

The 10th International Conference on Multi-functional Materials and Applications

(ICMMA 2016)

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Dr. Wijitra Jenwiriyakul (Applied Chemistry)

Agenda of ICMMA2016 - Opening Ceremony

(Host by Prof. Dr. **Saksit Chanthai**)

08:50~09:00	Report address by Prof. Dr. Vittaya Amornkitbamrung (Khon Kaen University, Thailand) – Conference Chairman	
09:00~09:30	09:00~09:10	Opening Address by Prof. Dr. Kittichai Triratanasirichai (Khon Kaen University, Thailand) –The President of KKU-
	09:10~09:20	Address by Prof. Dr. Won-Chun Oh (Hanseu University, Korea) – Conference Vice Chairman Introduction of Potential Scientists
	09:20~09:30	Address by Prof. Dr. Daosheng Sun (Vice President, Anhui Jianzhu University, China) Introduction of ICMMA2017
09:30~09:40	"Award of Appreciation Plaque" Plaque to Prof. Dr. Zhigang Chen (Suzhou University of Science and Technology, China)	
09:40	The conference chairman announces ICMMA 2016 begins	
09:50	Group photo	

Conference Program

December 1 (Thursday), 2016

12:00-18:00	Onsite Registration
18:00-20:00	Welcome Reception
20:00~	Conference Committee Board Meeting (for ICMMA2017)

December 2 (Friday), 2016

08:30~	Onsite Registration
08:50-10:00	Opening Ceremony (Khon Kaen University, Thailand)
Session A (10:10-10:50) (Chairman : Prof. Dr. Shin Mukai)	
10:00-10:25	Invited Lecture 1 Dr. Hiroaki Murase (Frontier Materials Laboratories, Osaka Gas, Chemicals Co., Ltd., Japan) <i>Synthesis of polysilanes using Mg with Lewis acid catalysts and its application for coating materials to polyethylene pipe interface</i>
10:25-10:50	Invited Lecture 2 Prof. Dr. Zhigang Chen (Suzhou University of Science and Technology, China) <i>Excellent SERS of SiO₂ fiber membrane embedded with Ag nanoparticles</i>
10:50-11:10 Coffee break	
Session B-1 (11:10-12:00) (Session Chairman : Prof. Dr. Zhigang Chen)	
11:10-11:35	Invited Lecture 3 Prof. Dr. Seung-Kyu Park (Department of Chemical Engineering, Hoseo University, Korea) <i>Upgrading of heavy oil or vacuum residual oil: Aquathermolysis and demetallization</i>
11:35-12:00	Invited Lecture 4 Dr. Jyothi Rajesh Kumar (Convergence Research Center for Development of Mineral Resources (DMR), Korea Institute of Geoscience & Mineral Resources (KIGAM), Korea) <i>Separation and recovery of rare earths for sustainable developments: By environmentally sound solutions</i>
Session B-2 (11:10-12:00) (Session Chairman : Prof. Dr. Won-Chun Oh)	
11:10-11:35	Invited Lecture 5 Prof. Dr. Makoto Ogawa (Vidyasirimedhi Institute of Science and Technology (VISTEC), Thailand) <i>Interactions of nanoparticles with layered solids</i>
11:35-12:00	Special Lecture 1 Prof. Dr. Gang He (School of Physics and Materials Science, Radiation Detection Materials & Devices Lab, Anhui University, China) <i>Modulation of interface quality and band offset and investigation of electrical properties of high-k/III-V gate stacks</i>
12:00-13:10 Lunch	

Session C-1 (13:10-14:50) (Session Chairman : Prof. Dr. Zaoqi Sun)	
13:10-13:30	Special Lecture 2 Prof. Benhong Yang (Analytical and Testing Center, Hefei University, China) <i>Tg improvement and thermal stability enhancement mechanism of polyolefins by incorporating POSS</i>
13:30-13:50	Special Lecture 3 Dr. Masaaki Yoshikawa (Energy Technology Laboratories Osaka Gas Co., Ltd., Japan) <i>Roadside air pollution reduction technology by activated carbon fibers</i>
13:50-14:10	Oral Lecture 1 Prof. Dr. Chan Kyung Kim (Department of Chemistry and Chemical Engineering, Center for Design and Applications of Molecular Catalysts, Inha University, Korea) <i>Computational studies on bimetallic clusters of platinum</i>
14:10-14:30	Oral Lecture 2 Prof. Dr. Ki-Choong Mah (Department of Optometry, Eulji University, Korea) <i>Changes in subjective fatigue and pupil diameter induced by watching LED TV</i>
14:30-14:50	Oral Lecture 3 Prof. Dr. Saksit Chanthai (Department of Chemistry, Faculty of Science, Khon Kaen University, Thailand) <i>Quenching effect of Hg(II)-GQDs as a sensitive fluorescent turn-on sensor for selective detection of cyanide and iodide in water sample using specific masking agents</i>
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13:10-13:30	Special Lecture 4 Prof. Dr. Chen-Hao Wang (Department of Materials Science and Engineering, National Taiwan University of Science and Technology, Taiwan) <i>Non-precious metal catalysts of Fe-based nanomaterials for low temperature fuel cell</i>
13:30-13:50	Special Lecture 5 Prof. Dr. Jae-Won Lee (Department of Energy Engineering, Dankook University, Korea) <i>Technologies to enhance the properties of commercial Ni-rich cathode materials for lithium-ion batteries</i>
13:50-14:10	Oral Lecture 4 Prof. Nan Xu (Jiangsu Key Laboratory of Environmental Functional Materials, School of Chemistry Biology and Material Engineering, Suzhou University of Science and Technology, China) <i>Transport behaviors of titanium dioxide nanoparticles in saturated sand column in the presence of ammonium and hydrochar</i>
14:10-14:30	Oral Lecture 5 Prof. Dr. Prawit Nuengmatcha (Department of Chemistry, Faculty of Science and Technology, Nakhon Si Thammarat Rajabhat University, Thailand) <i>Photocatalytic and sonocatalytic performance of ZnO-graphene-TiO₂ nanocomposite for degradation of dye pollutants</i>
14:30-14:50	Oral Lecture 6 Dr. Kasama Urkasame (Division of Applied Chemistry, Graduate School of Engineering, Hokkaido University)

	<i>A simplified model for simulation of photocatalytic systems with TiO₂-SiO₂ microhoney combs</i>
14:50-15:10 Coffee break	
Session D-1 (15:10-17:10) (Session Chairman : Prof. Dr. Saksit Chanthai)	
15:10-15:30	Special Lecture 6 Prof. Dr. Baolin Wang (Nanjing Normal University, China) <i>First-principles prediction and laboratory synthesis of new calcium silicate phases</i>
15:30-15:50	Oral Lecture 7 Dr. Kwang Youn Cho (Ceramic Fiber and Composite Materials Center, Korea Institute of Ceramic Engineering and Technology, Korea) <i>Low-oxygen curing on polycarbosilane precursor for synthesis of silicon carbide fiber</i>
15:50-16:10	Oral Lecture 8 Dr. Woo Sik Kim (Ceramic Fiber and Composite Center, Korea Institute of Ceramic Engineering and Technology, Korea) <i>Development of the high performance nano composites; the ultra-light weight nano fibers and flexible composites</i>
16:10-16:30	Oral Lecture 9 Prof. Dr. Jin Do Chung (Dept of environmental Engineering, Hoseo University, Korea) <i>Study on the high vacuum thin film deposition efficiency improvement under vapor deposition technology</i>
16:30-16:50	Oral Lecture 10 Prof. Dr. Xianbiao Wang (School of Materials and Chemical Engineering, Anhui Jianzhu University, China) <i>Structure induced selective adsorption performance of ZIF-8 nanocrystallines and their application in water purification</i>
16:50-17:10	Oral Lecture 11 Prof. Dr. Goutam Mukhopadhyay (BCDA College of Pharmacy & Technology, India) <i>RSM study in the foam fractionation of native whey (waste)</i>
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15:10-15:30	Special Lecture 7 Prof. Dr. Fung-Jun Zhang (Anhui Key Laboratory of Advanced Building Materials, Anhui Jianzhu University, China) <i>Preparation and photocatalytic performance of bismuth oxide modified by Ag</i>
15:30-15:50	Oral Lecture 12 Prof. Dr. Ashish A. Gawai (Anuradha College of Pharmacy, India) <i>Cleaning validation study for common equipment's used in manufacturing and preparation of pediatric suspension and simple Linctus</i>
15:50-16:10	Oral Lecture 13 Prof. Dr. Ram K. Agarwal (Editor-in-Chief, Asian Journal of Chemistry) <i>Analytical, biological and medicinal characteristics of semicarbazones derived from</i>

	<i>pyrazolone and their lanthanide(III) complexes</i>
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16:30-16:50	Oral Lecture 15 Prof. Dr. Shou-Qing Liu (Suzhou University of Science and Technology, China) <i>The effects of metal cations on the activity of the Prussian blue photocatalyst</i>
16:50-17:10	Oral Lecture 16 Ms. Pimpisa Kaewanan (Materials Chemistry Research Center, Department of Chemistry and Center of Excellence for Innovation in Chemistry, Faculty of Science, Khon Kaen University, Thailand) <i>A fluorescent turn-on/off method based on Hg²⁺ quenched graphene quantum dots as a fluorescent probe using thioacetamide for selective determination of Ag⁺ in water samples</i>
Poster Session (17:10-18:00) (Session Chairman : Prof. Dr. Chuyang Xu) with Coffee and Beverage	
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19:50-20:00	Closing Remark (Prof. Dr. Chankyung Kim)

December 3 (Saturday), 2016

8:30 ~	Conference Tour
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Invited Lecture

Synthesis of polysilanes using Mg with Lewis acid catalysts and its application for coating materials to polyethylene pipe interface

Hiroaki Muraseⁱ

*Frontier Materials Laboratories, Osaka Gas Chemicals Co., Ltd., 5-11-61 Torishima,
Konohana-ku, Osaka 554-0051, Japan*

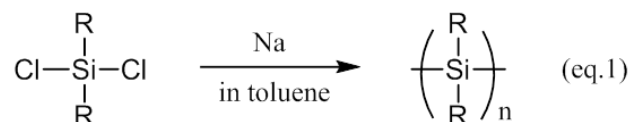
ABSTRACT

Polysilane (PSi) is a kind of silicon polymers composed of only silicon atoms (Si-Si bonds) as the main chain and organic substituents like methyl and phenyl groups as the side chain. The preparation method of PSi hitherto known was highly limited. In this paper, the highly practical method for the synthesis of PSi was introduced.

As an applied research of PSi, the effects of coating materials on polyethylene (PE) pipe interface were investigated. The fusion strength of PE pipes would be generally reduced when sand particles adhered on the pipe interface. However, it has been found that a kind of PSi was very effective for maintaining the fusion strength even when sand particles were adhered on the fusion interface.

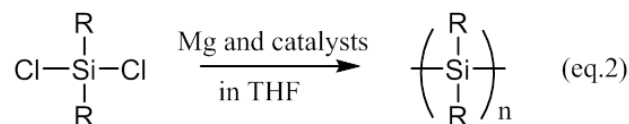
INTRODUCTION

PSi has attracted considerable attention due to their usefulness as the precursors for thermally stable ceramics, materials for microlithography, and materials for solar cell elements and so on. In contrast to the growing interest with PSi, the method of preparation hitherto known was highly limited. Almost the only practical method developed so far was the condensation of organo-dichlorosilane with alkali metal (Kipping Method [1]). This reaction, which is shown by eq. 1, proceeds at an elevated temperature (over 100°C) in an inert solvent using appropriate alkali metal in dispersion.



This reaction condition is very vigorous, so that it was necessary to find a new synthetic method for PSi under milder reaction conditions.

It has been found in this study that the reduction of organo-dichlorosilane with Mg metal particles as reducing agents and metal chlorides as catalysts at room temperature could be successfully attained, that is, Si-Si bond was formed and various types of PSi were obtained in good yield (eq.2) [2].



Since the Gas Utility Industry Law was revised to permit the use of PE pipes in 1982 in Japan, the PE pipes are steadily spreading as gas feed pipes. The most popular and generally applicable method for connecting the PE pipes is to use electrofusion joints.

However, the pipe surface may suffer from dirt such as fine sand particles due to wind blowing at the work sites irrespective of pre-cleaning. The fusion strength of electrofusion joints depends on the amount of sand particles adhered to

ⁱEmail: murase_hiroaki@ogc.co.jp, Tel: +81-6-6467-1571,

the interface (Figure 1) because flow rate of molten resins is poor at the fusion interface on electrofusion joints.

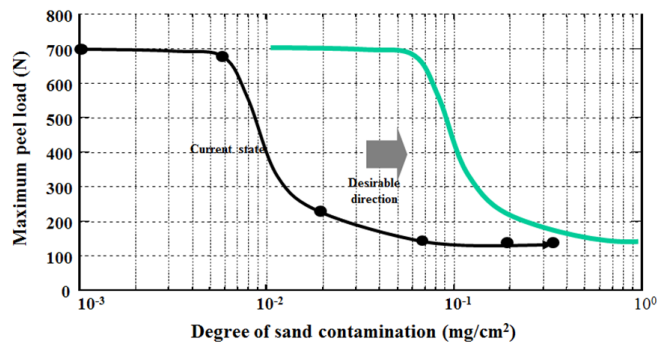


Figure1. Harmful effect of sand to fusion strength

It was found that decrease of fusion strength may be suppressed in the presence of PSi at the fusion interface of electrofusion joints, even when sand particles were adhered on the joint. A kind of PSi was very effective for maintaining the fusion strength at electrofusion joints when sand particles were adhered on the fusion interface.

Excellent SERS of SiO₂ fiber membrane embedded with Ag nanoparticles

Jun-Chao Qian, Cheng-Bao Liu, Zheng-Yin Wu, Feng Chen, and Zhi-Gang Chen

*School of Chemistry, Biology and Materials Engineering, Suzhou University of Science and Technology,
Suzhou, China, 215009*

ABSTRACT

Uniformly distributed Ag nanoparticles supported on SiO₂ fiber membrane materials were successfully synthesized by electrospinning and pyrolysis. In this study, the electrostatic spinning solution is composed mainly of PVP, TEOS and AgNO₃. The structural and morphological studies of the materials after calcination at 650°C were investigated by X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and thermogravimetry–differential scanning calorimetry (TG–DSC). The results indicated that the sample had a rough surface structure and the load on the nanofibers was the metal silver (Ag), and the number and grain size of Ag nanoparticles increased as the relative amounts of AgNO₃ increased. Furthermore, the surface enhanced Raman scattering (SERS) activity of the Ag/SiO₂ was investigated using the common antibiotic enrofloxacin (ENR) as a probe. It was found that the amorphous silica fiber with uniform loading of Ag nanoparticles exhibits a strong SERS enhancement effect. This good analytical performance predicts excellent potential for SERS detection of trace antibiotics.

Keywords: *Ag nanoparticles; membrane materials; electrospinning; SERS enrofloxacin*

Upgrading of heavy oil or vacuum residual oil: Aquathermolysis and demetallization

Seung-Kyu Parkⁱⁱ and Dong-Ho Park

Department of Chemical Engineering, Hoseo University, Asan 336-795, Korea

ABSTRACT

Even though the oil price seems not to be increased quickly in a few years, it is generally forecasted that the price will resume an upward trend in both the medium- and long-term [1-3]. The OPEC group estimates that the oil price rises by an average of about \$5 per year over the course of this decade, only reaching \$80 per barrel in 2020. The oil prices seem not jump to triple-digit territory within a decade, but it will quickly increase as the political issues for reduction of manufacturing appear [2-4]. This has led to consideration of alternative energy sources such as heavy crude oil and natural bitumen [5,6]. They are considered one of the most crucial sources to meet future energy demand. The total resources of heavy oil and bitumen in known accumulations are 3,396 and 5,505 billion barrels of original oil in place (OOIP) and among these, 30 and 993 billion barrels of oil are prospective additional oil, respectively [3,4,7].

Heavy oil contains heavy hydrocarbon compounds, resins and asphaltenes, containing carbon chains more than sixty carbon atoms [8]. High content of heavier fraction corresponds with high molecular weight, viscosity, and boiling point. The hydrocarbons in the oil sand and natural bitumen are forms of crude oil that are extremely dense and viscous, with a consistency ranging from that of molasses for some extra-heavy oil to as solid as wax at room temperature, making extraction difficult. They often contain high concentrations of sulfur and heavy metals, particularly nickel and vanadium, which interfere with refining processes. We have studied regarding on upgrading of heavy oil and vacuum residual oil by demetallization by combination of solvent distillation and adsorption by mesoporous adsorbents for several years [9-11]. Recently, our concern was expanded to upgrading of heavy oil by aquathermolysis reaction. In this talk, I will review the recent studies regarding on aquathermolysis and demetallization of heavy oil and vacuum residual oil that we have conducted.

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ⁱⁱEmail: skpark@hoseo.edu, Tel : +82 41 5409686, Fax : + 82 41 5405758

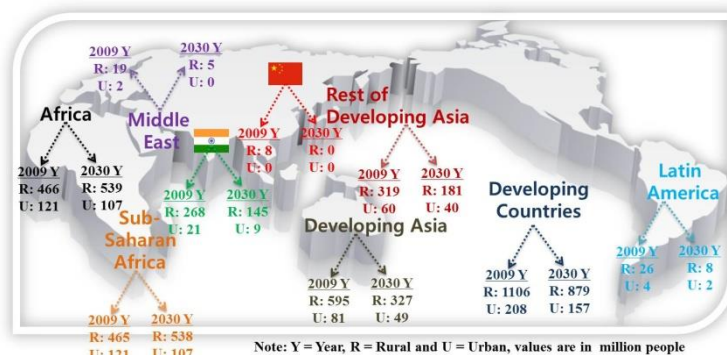
Separation and recovery of rare earths for sustainable developments: By environmentally sound solutions

Jyothi Rajesh Kumarⁱⁱⁱ and Jin-Young Lee

Convergence Research Center for Development of Mineral Resources (DMR), Korea Institute of Geoscience & Mineral Resources (KIGAM), Daejeon 34132, Korea

ABSTRACT

Rare earths are ruling the new millennium high world by their unique applications in the field of electronic materials manufacturing. Korean products exporting all over globe especially, mobile phones, computers, electrical goods such as air-conditioners, televisions etc. Country like South Korea having very limited rare earths based natural resources as well as land filling problem arise based on generating the manufacturing waste. Rare earths are having wide applications in various area's such as phosphors, permanent magnets, alloys, catalysts, nuclear reactor control rods, glass, dating materials, ceramics, catalysts and electronics. The major application was in magnets it occupies 26% worldwide, and then followed by metal alloys (19%), polishing (16.5%), catalysts (15%), glass/phosphors (6%) and ceramics/other (5.5%). For metal recovery the three primary routes were established: 1) pyro, 2) hydro 3) electro metallurgical routes. Hydrometallurgy deals the aqueous processing of the metals. It has many advantageous rather than one disadvantage much wastewater generation. And one more major objective for the rare earths processing is the energy crisis, as per world energy outlook survey by the year 2030 all over world number of people without access electricity was estimated and the figures and facts motivated the people work on rare earths processing.



Number of people without access to electricity by region in the new policies scenario

(http://www.iea.org/publications/freepublications/publication/weo2011_energy_for_all.pdf)

ⁱⁱⁱ Email: rkumarphd@kigam.re.kr, Tel: +82-42-868-3313, Fax: +82-42-868-3418.

Interactions of nanoparticles with layered solids

M. Ogawa*

*School of Energy Science and Engineering, Vidyasirimedhi Institute of Science and Technology (VISTEC),
555 Moo 1 Payupnai, Wangchan, Rayong 21210, Thailand.*

ABSTRACT

Nanoparticles have attracted increasing interests due to the wide range of applications in catalysts, imaging, optics, electronics and so on. In addition to the size and shape controlled synthesis, the immobilization of nanoparticles on or within solid supports has been a topic of interests for such applications as supported catalysts, sensing, and imaging. As to the nanoparticles supported solids, the size, shape and the distribution of the nanoparticles on or within solid supports are important parameters to determine the materials' performances. The available approaches for the preparation of hybrid materials containing nanoparticles can be roughly classified into two; one is based on the *in-situ* formation of nanoparticles on supports and the other is the immobilization of pre-synthesized nanoparticles on supports by such means as impregnation.

Here, we report the hybrid materials composed of nanoparticles with layered solids. Semiconductor and metallic nanoparticles have been synthesized in the interlayer spaces of layered silicates and titanates for possible catalysts applications.¹⁻³⁾ Pre-synthesized nanoparticles of iron oxides and titanium dioxides have been complexed (immobilized) with layered double hydroxide and silicate.³⁻⁸⁾ The amounts and the spatial distribution of the nanoparticles on layered solids are important parameter to determine the materials performances of the resulting hybrids.⁹⁾

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*E-mail: waseda.ogawa@gmail.com

Special Lecture

Modulation of interface quality and band offset and investigation of electrical properties of high-k/III-V gate stacks

Gang He,^{iv} Juan Gao, and Zhaoqi Sun

School of physics and Materials Science, Radiation Detection Materials & Devices Lab, Anhui University, Hefei 230601,

P.R. China

ABSTRACT

In this report, the reduction and removal of surface native oxides (GaO_x , AsO_x) from the as-received InGaAs surface by using dimethylaluminumhydride (DMAH)-derived AION and ALD-derived Al_2O_3 passivation layer with self-cleaning effect prior to HfTiO deposition is reported to solve Fermi level pinning challenge. XPS analysis has revealed that complete consumption of native oxides of AsO_x and GaO_x at the InGaAs surface, but no effect to InO_x , has been realized by MOCVD AION and ALD-derived Al_2O_3 at 300°C. Meanwhile, the regrowth of the native oxides at the interface of HfTiO/InGaAs gate stacks has been detected by inserting AION passivation layer. Valence band spectra of HfTiO/AION/InGaAs gate stacks show reduction in valence band offset and increase in conduction band offset compared to that of HfTiO/InGaAs. Electrical measurements of MOS capacitor with HfTiO/ Al_2O_3 /InGaAs gate stacks with dielectric thickness of ~4 nm indicate improved electrical performance. The improved interface control and suitable band offset relative to InGaAs make high-k/III-V as promising gate stacks in future InGaAs-based MOSFET devices.

Keywords: *High-k gate dielectrics; Interface chemistry; III-V-based CMOS devices*

Supported Program: National Natural Science Foundation of China (51572002, 11474284)

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G. He, J. Gao, H. S. Chen, J. B. Cui, X. S. Chen, and Z. Q. Sun, *ACS Appl. Mater. Interfaces* 6, 22013-22025 (2014)

^{iv}Email: hegang@ahu.edu.cn

T_g improvement and thermal stability enhancement mechanism of polyolefins by incorporating POSS

Benhong Yang*

Analytical and Testing Center, Hefei University, Hefei 230601, China

ABSTRACT

Three types of poly(olefin-*co*-octavinyl-polyhedral oligomeric silsesquioxane) organic-inorganic nanocomposites were synthesized via free radical polymerization and characterized by ¹H NMR, ²⁹Si NMR, DSC and TGA. The results indicate that POSS contents in nanocomposites can be tailored by varying the POSS feed ratios. DSC and TGA measurements show that the incorporation of POSS into polyolefin matrix can apparently improve their thermal properties. The drastic T_g and T_{dec} increases are mainly due to the formation of network structures of the nanocomposites, where POSS cubes behave as the joint points and block the motion and degradation of the polymeric chains.

Keywords: *nanocomposites; polyolefin; POSS; thermal properties*

*Email: yangbh@hfu.edu.cn

Roadside air pollution reduction technology by activated carbon fibers

Masaaki Yoshikawa^v

Energy Technology Laboratories, Osaka Gas Co., Ltd.

ABSTRACT

The technology against air pollution using Activated Carbon Fibers (ACF) does not use the electric power and utilizes only the natural wind. Our research group has developed the ACF unit for roadside that can remove air pollutants by parallel wind flow through slit shape structure. Ministry of Land, Infrastructure, Transport and Tourism of Japan has been proceeded the installation of ACF unit at the national highway where the air pollution from traffic was very severe since 2007. Observed NO₂ and NO removal at the roadside was 84% and 19% on average, respectively. The duration of ACF is enhanced by catalytic performance to oxidize NO_x into NO₃⁻ ion, which can be washed out by rain fall easily. Estimated duration of ACF at the roadside is assumed for over 7 years.

INTRODUCTION

Activated Carbon Fibers (ACF) has been developed and manufactured by commercial scale in Japan for over 30 years. It has been also manufactured in China and Korea since 2000. The structure of ACF is porous fibrous carbon which has fiber diameter of 10~20 micron and has excellent performance for the speed of both adsorption and desorption. So far, ACF has been utilized for water purifier and solvent recovery equipment. ACF can be easily made into various forms such as paper, felt, and mold by the advantage of fibrous structure (Fig.1). Recently, a demand on the countermeasure for the air pollution in the urban area has been increased. Accordingly, we have developed ACF optimized for the removal of low concentration of NO and NO₂ in the atmosphere.

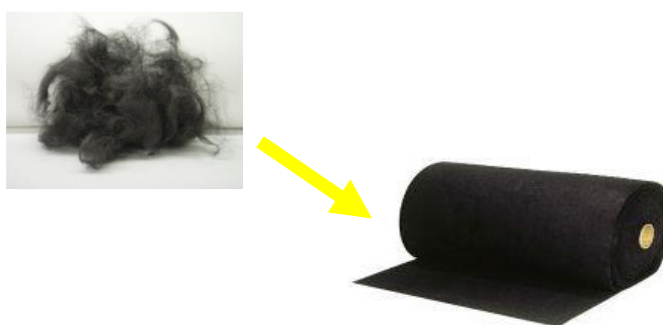


Fig.1. ACF Felt for NO_x removal

ACF PARALLEL WIND UNIT FOR NO_x REMOVAL AT THE ROADSIDE

Using this ACF Felt, a unit which can reduce the air pollution at the roadside was developed (Fig.2). Different from conventional filter unit, this ACF unit makes air pass in parallel flow. Pressure drop of ACF unit gives only 200 Pa at the wind velocity of 2 m/sec, which is one fourth of the conventional air filter. By this peculiar structure, ACF unit can purify polluted air at the wide area of roadside without using electric powered fan.

^vEmail: yoshikaw@osakagas.co.jp



Fig.2. ACF unit for NO_x removal and example of the installation at the roadside in Japan

NO_x removal performance of the ACF unit was measured at actual national road in Osaka, Japan. Fig.3 shows the NO₂ removal performance as a function of the natural wind velocity. NO₂ removal performance was stable against wind velocity, and average removal ratio was 84%. On the other hand, the NO removal ratio was relatively low, 19 % on average, and it tended to lower by the increase of the wind velocity. We are improving the NO removal of ACF at present.

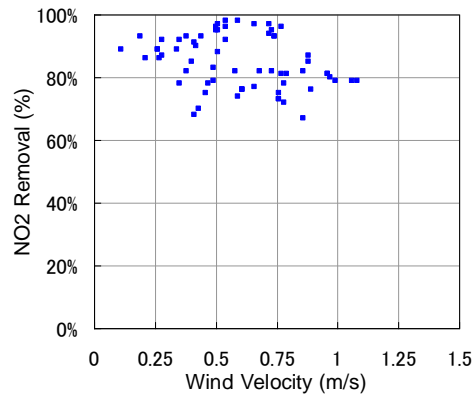


Fig.3. NO₂ removal performance of ACF unit at the roadside in Japan

Non-precious metal catalysts of Fe-based nanomaterials for low temperature fuel cell

Chen-Hao Wang^{vi}

Department of Materials Science and Engineering, National Taiwan University of Science and Technology,
Taipei 10607, Taiwan

ABSTRACT

Fuel cell is energy device converting chemical energy of hydrogen and oxygen via the electrochemical process into electricity energy. Since its product is only water, fuel cell is considered of eco-friendly and green energy. In order to speed up sluggish reaction rates of electrochemical reactions, platinum-based catalysts and other precious metal catalysts are employed in the electrodes. Compared to the hydrogen oxidation reaction rate occurs in the anode, the oxygen reduction reaction (ORR) is much slower, and thus more platinum-based catalysts are loaded in the cathode. We have synthesized Fe-based catalysts supported by metal organic framework (MOF) and modified CNT (Fe-based MOF/CNT catalyst). With carefully modifying the process parameters, Fe-based MOF/CNT catalyst demonstrates an excellent ORR ability with the electron-transfer number of 3.99, as shown in Figure 1, which is very close to the ideal four electron-transfer number. The excellent catalytic performance is probably attributed to two reasons. One is that the co-existence of unique structure and high amount of unoccupied graphitic-N π^* play the role of the active sites for the ORR. The other reason is attributable to the formation of porous structure and high conductivity of CNT.

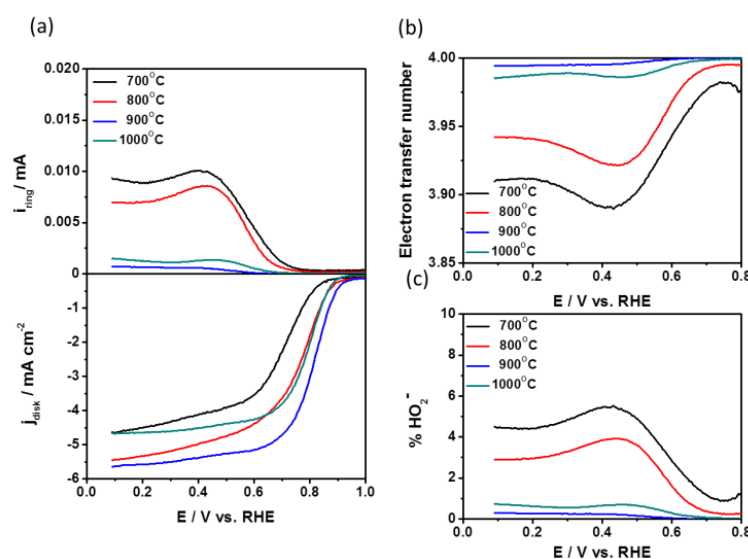


Fig. 1. The rotating ring-disk electrode technique showing electrochemical behaviors of Fe-based MOF/CNT catalysts by various temperatures: (a) the disk currents (lower part) and the ring currents (upper part); (b) the electron-transfer numbers; (c) the yields of hydrogen peroxide ion

^{vi}Email: chwang@mail.ntust.edu.tw

Technologies to enhance the properties of commercial Ni-rich cathode materials for lithium-ion batteries

Dong-jin Kim, Ji-won Choi, and Jae-won Lee

Department of Energy Engineering, Dankook University, Cheonan, Republic of Korea

ABSTRACT

Recently, there have been great demands for lithium-ion batteries (LIBs) that have high energy to meet the requirements for the power sources of electric vehicles or energy storage systems. Ni-rich cathode materials with a layered structure are being widely used to realize LIBs with high energy density as they have higher capacity than conventional cathode materials such as LiCoO_2 or LiMn_2O_4 . However, Ni-rich cathode materials suffer from poor cycling stability and rate capability. To overcome these problems, several technologies have been developed. In this study, some commercial technologies to enhance the properties of Ni-rich cathode materials including surface modification and doping are introduced. In addition, we also report a novel coating method to increase rate and cycling performance of Ni-rich cathode materials. Lithium aluminum titanium phosphate (LATP), one of the Li-ion conductors, was coated on $\text{LiNi}_{0.6}\text{Co}_{0.2}\text{Mn}_{0.2}\text{O}_2$ (NCM622) by simple dip-coating process. The LATP-coated NCM622 exhibited higher capacity and better cycling stability and rate capability than the pristine material. Electrochemical impedance spectroscopy (EIS) and galvanostatic intermittent titration technic (GITT) analysis demonstrated the improvement is due to the lowered interfacial resistance and higher Li-ion diffusion coefficient of the LATP-coated NCM622. Lithium silicate (Li_4SiO_4 , LSO) was also coated on the surface of $\text{LiNi}_{0.8}\text{Co}_{0.1}\text{Mn}_{0.1}\text{O}_2$ (NCM811) particles by a sol-gel process. Similarly, the LSO-coated NCM811 also showed better cycling stability and rate capability for the same reason with the LATP-coated NCM622. The coating technology with Li-ion conductor appears to be promising to overcome the problems in cell performances of Ni-rich cathode materials.

First-principles prediction and laboratory synthesis of new calcium silicate phases

Xiaoqiu Wang,¹ Baolin Wang,^{2,3} Guihua Hou,³ and Qinfang Zhang*,³

¹Department of Physics, Jinling Institute of Technology, Nanjing, Jiangsu, 211169, China

²School of Physical Science and Technology, Nanjing Normal University, Nanjing 210023, China

³Key Laboratory for Advanced Technology in Environmental Protection of Jiangsu Province, Yancheng Institute of Technology, Yancheng 224051, China

ABSTRACT

Calcium silicate is the main mineral of Portland cement clinker, in which low heat consumption and exhaust emissions require low calcium content. Therefore, exploring the presence of low calcium minerals will lay the foundation for the design and research of Portland cement clinker with energy-saving and low-emission. Using an efficient structure search method based on a particle swarm optimization algorithm and experimental technique, we study the compositional and structural evolution of calcium silicate phase, i.e., probable existing mineral phase from combining calcium oxide with silica oxide, preparing condition and hydration properties of $3\text{CaO}\cdot 2\text{SiO}_2$ (C_3S_2). Our results show that five calcium silicate phases including C_3S , C_2S , C_3S_2 , CS and CS_2 are stable. C_3S_2 , less concerned phase, forms under the temperature arranged from 1100°C to 1460°C and its hydraulic activity is low in the room temperature with the hydration productions containing C-S-H gel and $\text{Ca}(\text{OH})_2$. The possible hardening mechanism by carbonization of C_3S_2 is also discussed. This integrated process—first-principles prediction of new compounds followed by laboratory synthesis and characterization—could be a route to the discovery of novel functional materials.

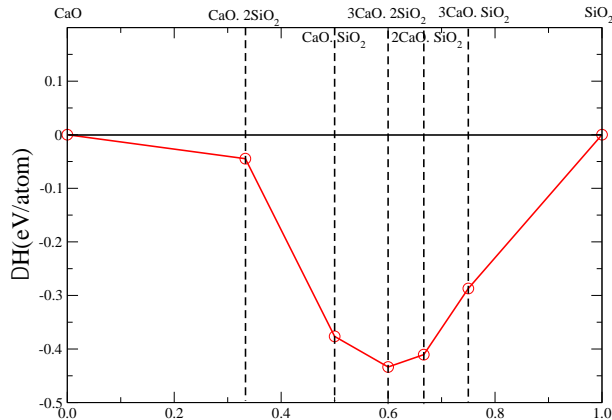


Fig. 1. Relative enthalpies of formation per atom for different C-S Phases

*Email: qfangzhang@ycit.edu.cn, Fax: +86-515-88298920

Preparation and photocatalytic performance of bismuth oxide modified by Ag

Xuan Li,¹ Feng-Jun Zhang,^{1,2,*} Tie-Nan Zhang², and Jie Ye¹

¹ Anhui Key Laboratory of Advanced Building Materials, Anhui Jianzhu University, Hefei Anhui, P. R. China, 230022

² Key Laboratory of Functional Molecule Design and Interface Process, Anhui Jianzhu University, Hefei Anhui, P. R. China, 230601

ABSTRACT

The liquid phase synthesis and photochemical deposition method are used to prepare a series of different Ag contents of the Ag/BiOBr composite photocatalyst. The catalysts were characterized by X-ray powder diffraction (XRD), scanning electron microscope (SEM) and Energy Dispersive spectroscopy (EDS), the photocatalytic degradation of Rhodamine B activity was evaluated by using the visible light of 550nm as the light source, The effects of different concentrations of Ag and different bromine sources (NaBr, CTAB) on the photocatalytic activity of BiOBr were investigated. Ag can significantly inhibit photoproduction electronic (e^-) and holes (h^+) composite. The existence of Ag increased significantly the BiOBr activity of photocatalytic degradation of dye. When the mass fraction of Ag (W) was about 2%, the photocatalytic activity of BiOBr was the most significant. Ag/BiOBr composite photocatalyst has a higher catalytic activity because of the strong absorption ability of the composite photocatalyst to visible light, Silver inhibits the recombination of the Ag/BiOX (X=Cl, Br, I) photo electron hole.

ACKNOWLEDGEMENTS

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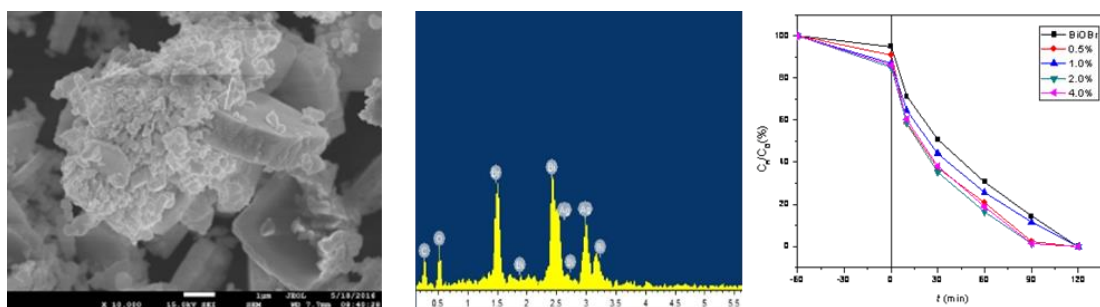


Fig. 1. SEM, EDS and photocatalytic performance of of Ag/BiOBr composite

*Email: zhang-fengjun@hotmail.com, Tel: +86-551-6382-8262 Fax: +86-551-6382-8106

Oral Lecture

Computational studies on bimetallic clusters of platinum

Nasir Shahzad, and Chan Kyung Kim

Department of Chemistry and Chemical Engineering, Center for Design and Applications of Molecular Catalysts, Inha University, 100Inharo, Nam-gu, Incheon 22212, Korea

ABSTRACT

Hydrogen is used as a fuel in proton exchange membrane (PEM) fuel cells. However, the PEMs have a strict prerequisite for the quality of the amount of impurities present. Currently, hydrogen is produced on large scale from the carbon-based materials and water gas shift (WGS) reaction is used for CO oxidation and hydrogen enrichment. The water gas shift reaction is an exothermic process requiring a high activation barrier and favors in the forward direction at low temperature. Hence, iron and other high-temperature non-precious metal catalysts are not advantageous. So, we need some noble metal catalysts that operate at low temperature. Among them, platinum is considered as the best catalyst. However, pure platinum has its own glitches: for instance, it is poisoned by H₂S that reduces its activity up to 40% after three cycles, coke formation is prevalent and the high cost of platinum raises the price of generated hydrogen. Coke formation is caused by strong adsorption of CO on platinum surface. Owing to this phenomenon, the dissociation reaction is dominated over oxidation. Designing a catalyst that can overcome these hurdles is pertinent to the green energy production.

To rationalize the low temperature platinum-based catalysts for the WGS reaction, we have selected some highly active sub-nanoclusters of platinum and then doped with the first row transition metals to examine their properties. In this work, more than sixty percent of platinum was replaced by the first row transition metals. This study shows that the platinum bimetallic sub-nano clusters doped with Ti and Mn not only prefer the CO oxidation over dissociation but also show enhanced tolerance towards H₂S and these clusters suppress the coke formation but enhance the hydrogen formation. Therefore, the bimetallic platinum sub-nanoclusters designed in this work are promising catalysts for the water gas shift reaction. All the calculations were done using the Gaussian 09 package.

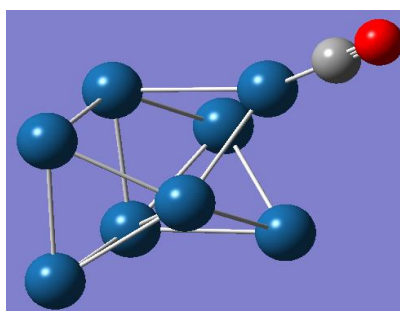


Fig. The most stable complex of Pt₈-CO

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Changes in subjective fatigue and pupil diameter induced by watching LED TV

Bon-Yeop Koo, and Ki-ChoongMah^{vii}

Department of optometry, Eulji University, Seongnam, South Korea, 553

Sangseong-daero Sujeonggu Seongnamsr Gyeonggi do 461-713 South korea

ABSTRACT

This study aimed to analyze changes in pupil diameter and subjective fatigue induced during watching viewing contents in different viewing conditions (Luminosity and physical form of the display surface).

All subjects were selected, applying the following criteria: Those who had not experience ophthalmic or psychiatry diagnosis, treatment and drug delivery; had monocular uncorrected vision or corrected vision of 0.8 or higher at distance; did not have dyschromatopsia; and had stereopsis of less than 100sec. of arc at near. With 108 persons (Under 20, 20 to 40 and Over 40, 36 persons each), the pupil diameter was measured, using an eye movement tracking device while they were watching two viewing contents in different viewing conditions. The data on the pupil diameter collected by the eye tracking device while they were watching the viewing contents were divided into 10 section with a unit of three minutes to analyze changes according to each condition. Their subjective fatigue was evaluated by conducting a survey before and after watching the viewing contents.

Key words: LED TV, Eye tracking device, Curved display, Pupil diameter

RESULTS

The more the viewing time, the less the pupil diameter tended to become, which showed a significant difference ($p < 0.05$). Also, it decreased, increased and decreased again, respectively, at the sections of the viewing time, nine, 24 and 27 minutes, and there were significant correlations in both linear and non-linear third-degree polynomial expressions.

The relative impact of viewing conditions on the pupil diameter showed significant correlations in luminosity and display ($p < 0.05$).

The subjective fatigue increased more after watching the viewing contents than before and significantly increased in younger subjects ($p < 0.05$).

CONCLUSIONS

Changes in subjective fatigue and the pupil diameter induced by watching viewing contents played on LED TV differed depending on the physical form of the display, luminosity of the background or the viewing contents, while the pupil diameter decreased with a pattern of regression in linear and third polynomial expressions as the viewing time increased.

A follow-up study to investigate and reveal the correlations of these changes more precisely is necessary.

^{vii}Email: kcмах@eulji.ac.kr

Quenching effect of Hg(II)-GQDs as a sensitive fluorescent turn-on sensor for selective detection of cyanide and iodide in water sample using specific masking agents

Prawit Nuengmatcha, Phitchan Sricharoen, Nunticha Limchoowong,

Ratana Mahachai and Saksit Chanthai*

Materials Chemistry Research Center, Department of Chemistry and Center of Excellence for Innovation in Chemistry,

Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand

ABSTRACT

A simple and rapid method of dual analysis for cyanide (CN⁻) and iodide (I⁻) ions was developed with the use of mercury quenched graphene quantum dots (Hg²⁺-GQDs) as a fluorescent probe. The Hg²⁺ ions would interact on their negatively charged surface of GQDs, resulted in drastically quenching of the fluorescent intensity (turn-off). When CN⁻ or I⁻ was added into the Hg²⁺-GQDs solution, their fluorescent enhancement was observed (turn-on). However, in the specific masking agent, persulfate ion S₂O₈²⁻ permitted to turn-on fluorescent probe of the Hg²⁺-GQDs for CN⁻ detection. Alternatively, in the presence of hydrogen peroxide its turn-on fluorescent probe could be selective for I⁻. Under the optimum conditions, the limits of detection for CN⁻ and I⁻ were 0.17 and 0.20 μM, respectively. While the limits of quantification for CN⁻ and I⁻ were 0.99 and 0.78 μM, respectively. No effect of interfering ions was found the selective determination of CN⁻ and I⁻ ions. The proposed method was successfully applied for dual detection of both CN⁻ and I⁻ in real water samples with satisfied recovery ranges of 72.97–112.41% and 78.61–117.09% for CN⁻ and I⁻, respectively.

Keywords: Graphene quantum dots; Cyanide; Iodide; Mercury; Masking agent; Fluorescent sensor

*E-mail: sakcha2@kku.ac.th

in the presence of ammonium and hydrochar

Cheng Liu, Kairong Zhou, Nan Xu,* Xiaoting Xu

Jiangsu Key Laboratory of Environmental Functional Materials, School of Chemistry Biology and Material Engineering, Suzhou University of Science and Technology, Suzhou 215009, China

ABSTRACT

Soil and water environments are inevitably contaminated by the excess of artificial nanoparticles (NPs) and ammonium (NH_4^+) fertilizers. There is a possibility of ammonium effect on the transport of nanoparticles titanium dioxides (nTiO_2). It is a great urgency and high priority to investigate the hydrochar-modified nTiO_2 retention mechanisms and accurately describe their transport in the presence of ammonium. Rutile nTiO_2 with hydrochar modified through the saturated porous sand columns were observed under the conditions (0-25 mM NaCl or NH_4Cl electrolyte, pH 6.0 and 8.0). The applicability of classic Derjaguin-Landau-Verwey-Overbeek (DLVO) theory and the two-site kinetic retention model was used to describe the transport of hydrochar-modified nTiO_2 in the sand columns in the presence of NH_4^+ . The experimental results showed that the hydrochar facilitate the transport of nTiO_2 by hydrochar carrying nTiO_2 attachment on the surface. It is attributed to the lower attachment efficiency, clean-bed filter coefficient and deposition rate coefficient of nTiO_2 in sand column. The transportability of hydrochar-modified nTiO_2 at different electrolytes obeys the order as follows: $\text{NH}_4^+ > \text{Na}^+ > \text{Na}^+ + \text{NH}_4^+$ at the same ion strength (IS). The two-site kinetic retention model provides the good simulation for their transport behavior. The lower critical coagulation concentration (CCC) of rutile nTiO_2 in NH_4^+ solution results in the more reversible deposition associated with greater K_2 on Site 2 (from model) in sand column compared by that in Na^+ solution. The more concern should be paid on the transport behavior of NPs in the simultaneous presence of complex impact factors.

Keywords: Nanoparticle titanium dioxide (nTiO_2); Transport; Phosphorus; Particle size; Ionic concentration; pH

Acknowledgements: This research was financially sponsored by the National Natural Science Foundation (NSF) of China (grant No. 21377090), NSF of Jiangsu Province (grant No. BK20131152), Qing Lan Project of Jiangsu Province, and Open Projects of the Jiangsu Key Laboratory for Environmental Functional Materials (No. SJHG1309).

* E-mail: nanxu@mail.usts.edu.cn; +86 512 68083175; Fax: +86 512 68083175.

Photocatalytic and sonocatalytic performance of ZnO-graphene- TiO_2 nanocomposite for degradation of dye pollutants

P. Nuengmatcha,^{1,viii} S. Chanthai,² and W.C. Oh,³

¹*Department of Chemistry, Faculty of Science and Technology, Nakhon Si ThammaratRajabhatUniversity, Nakhon Si Thammarat 80280, Thailand.*

²*Department of Chemistry, Faculty of Science, KhonKaen University, KhonKaen 40002, Thailand.*

³*Department of Advanced Materials Science & Engineering, Hanseo University, Chungnam 356-706, South Korea.*

ABSTRACT

ZnO-graphene-TiO₂(ZGT) was synthesized by a simple solvothermal method. The as-obtained samples were characterized by X-ray diffraction, transmission electron microscopy and energy dispersive X-ray spectroscopy. The band gap energy of the as-synthesized catalysts were performed by UV-vis diffuse reflectance spectroscopy. For sonocatalysis, the sonocatalytic activities of catalysts were tested by the oxidation of various dyes under ultrasonic irradiation, and compared with ZnO-graphene (ZG), graphene, ZnO and TiO₂, respectively. The results indicated ZGT displayed higher ultrasound activated sonocatalytic activity than other catalysts. The optimum conditions including irradiation time, pH, dye concentration, catalyst dosage and ultrasonic intensity were 120 min, 9, 20 mg/L, 1.00 g/L and 40%, respectively. In addition, the photocatalytic activities of as-obtained catalysts were assessed based on the degradation of both standard and industrial dyes under visible-light irradiation. ZGT exhibited higher visible-light-activated photocatalytic activity than did other samples. It is therefore evident that the ZGT can be applied not only as a highly effective sonocatalystbut also highly performance photocatalystfor dye pollutants. Moreover, a possible sonocatalyticand photocatalytic degradation mechanismsare discussed.

Keywords: *ZnO-graphene-TiO₂; Photocatalytic and sonocatalyticdegradation; Dye pollutants*

^{viii}*E-mail: pnuengmatcha@gmail.com; Tel. +66-7537-7443, Fax +66-7537-7443*

A Simplified model for simulation of photocatalytic systems with TiO₂-SiO₂ microhoneycombs

KasamaUrkasame, Seichiro Yoshida, ShinichiroIwamura, Isao Ogino, and Shin R. Mukai^{ix}

Division of Applied Chemistry, Graduate School of Engineering, Hokkaido University

1. INTRODUCTION

Photocatalyst particles are generally used as slurry or packed bed, or coated on a flat plate [1]. Our previous work has suggested the potential application of titania-silica microhoneycomb (MH) photocatalysts synthesized by ice-templating method [2]. These photocatalysts have high specific surface area, allow rapid mass transfer and cause only a low hydraulic resistance.

In this work, to examine the potential of MH photocatalysts, a simple theoretical model has been proposed to simulate the photocatalytic reaction system, in which some parameters are expected to be position dependent.

2. EXPERIMENTAL

Microhoneycomb TiO₂-SiO₂ photocatalysts (10 mol % TiO₂) were prepared by modifying the method reported in Ref. 2. In short, an acidic titania sol was added to a silica sol, followed by adding a neutral titania sol to adjust pH independently from titania content. This method was found to give more reproducible results than the old method. Calcination of samples was done in air at 873 K.

Decolorization of aqueous methylene blue (MB) solution was conducted using uncalcined and calcined photocatalysts in a continuous flow system schematically shown in Fig.1. A synthesized MH was held vertically and MB solution at a specified concentration was passed through it, and the effluent solution was analyzed by a UV-vis spectrophotometer to determine conversions. A simulation model was constructed by assuming plug flow with a superficial liquid velocity of v through a sample having bulk density of ρ and the first order reaction with respect to the adsorbed capacity of MB (q) where the rate constant k accounts for the dependency of light intensity and q on position z (Eq.(2)). At steady-state operation, the rate equals to the mass transfer of MB from the bulk liquid to the catalyst surface (Eq.(1)).

$$-v \frac{dc}{dz} = k(z)\rho q = K_f a \left(C - \left(\frac{q}{K} \right)^n \right) \quad (1)$$

$$\frac{d \ln k}{dz} = \varepsilon_1 + \varepsilon_2 q \quad (2)$$

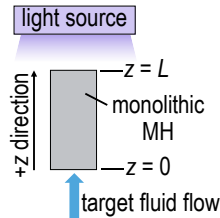


Fig. 1. Schematic drawing of photocatalytic system, showing the direction of z in the model

The rate constant k is a function of light absorption coefficients from blank monolith (ε_1) and adsorbed MB (ε_2), respectively. The equations were solved numerically by MATLAB by varying $k(z)$ at $z=L$. The mass transfer coefficient $K_f a$ and Freundlich adsorption isotherm parameters K and n were obtained from batch adsorption experiments.

^{ix}Email: smukai@eng.hokudai.ac.jp

3. RESULTS AND DISCUSSION

Synthesized MH photocatalysts have the channel size of 15-40 μm (Fig. 2). The proposed model could well predict the conversion in the low feed concentration region whereas some deviations were observed in higher concentration region probably because of greater influence of axial dispersion of MB. Calcination increased the adsorption capacity of MB. The modeling results indicate that the effective irradiation depth is longer for the uncalcined sample than the calcined one because of higher degree of light attenuation by adsorbed MB in the latter photocatalyst. However, the overall reaction rate is affected by q to a greater extent. Therefore, the overall conversion of calcined sample was higher. This simplified model has the potential to be used as a tool for morphology selection to maximize the overall performance of a photocatalyst.

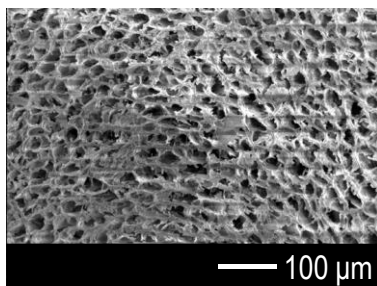


Fig. 2. SEM image of aTiO₂-SiO₂ microhoneycomb

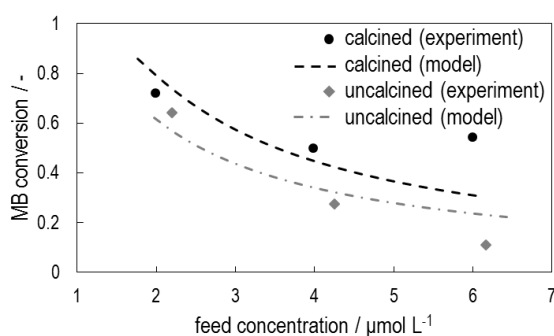


Fig.3. Photocatalytic activity of 10 mol% titania samples

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Low-oxygen curing on polycarbosilane precursor for synthesis of silicon carbide fiber

Khos-Erdene Khishigbayar, Kwang Youn Cho, and Jong Min Seo^x

Ceramic Fiber and Composite Materials Center, Korea Institute of Ceramic Engineering and Technology, 101, Soho-ro, Jinju-si, Gyeongsangnam-do, 660-031 Korea

ABSTRACT

The reduced pressure curing method having presence of iodine vapor is more effective on pyrolysis with early stage crystallization of β -SiC at 1300°C. Crystal size of β -SiC, cured at 0.008 kPa is around 3-4 nm larger than cured at 101 kPa.

INTRODUCTION

The presence of oxygen in the fiber causes high temperature instability, it is incorporated with thermal degradation and carbothermal reduction [1]. Many scientists reported non-oxidation curing methods on PCS precursor such as electron beam radiation [2], UV assisted radiation [3], cyclohexane vapor curing [4], unsaturated hydrocarbon vapor [1] and others.

METHOD

Polycarbosilane powder was melted at 150 °C for 1h with a vacuum and stabilized at 190°C for 2hs with the low vacuum condition in a single-hole spinneret spinning machine. Curing proceeded with various pressures in range of 0.008-101 kPa at 200 °C for 2 h.

RESULTS

Fig. 1 represents the detailed structural analysis of fabricated SiC fiber carried out by TEM. The microstructure of fabricated SiC fibers was changed remarkably by the iodine vapor curing at reduced pressure. According to TEM, crystal size of SiC fiber cured at 101 kPa and 0.008 kPa were 1-3 nm and 3-6 nm, respectively.

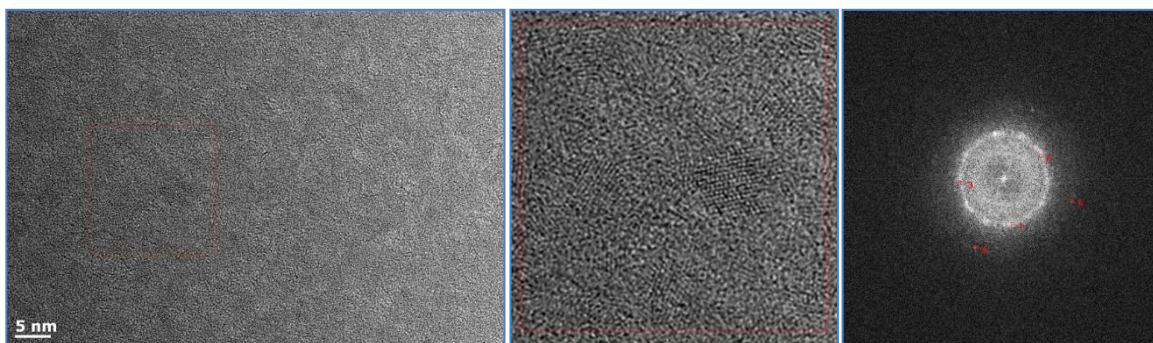


Fig.1. TEM analysis of fabricated SiC fibers cured at 0.008 kPa

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^xEmail: kycho@kicet.re.kr, Tel: +82-55-792-2710, Fax: +82-55-792-2530

Development of the high performance nano composites; The ultra-light weight nano fibers and flexible composites

Woo Sik Kim, Kwangyoung Cho and Dong-geun Shin^{xi}

Ceramic Fiber and Composite Center, Korea Institute of Ceramic Engineering and Technology, Jinju 52853, Korea.

ABSTRACT

In this research, graphene was prepared by unzipping of carbon nanotubes (CNTs), chemical exfoliation of graphite and electrochemical exfoliation of graphite rod. 3D foam like, 2D film like and 1D fiber like architectures of graphene composite were fabricated using various graphene-based nano materials.

INTRODUCTION

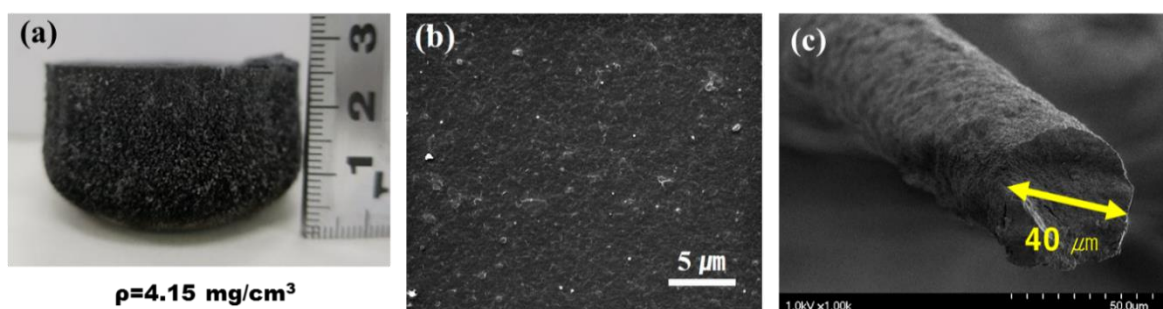
Graphene is comprised of a monolayer of hexagonally arranged sp²-hybridized C atoms. It has received much interest, because of its high electron mobility, thermal conductivity, elasticity, and stiffness. These properties make graphene attractive for application in nanoelectronic devices, sensors, functional composites, and energy storage.

METHOD

3D architecture of graphene foams were developed via the in situ self-assembly of graphene and CNTs hybrid prepared by mild chemical reduction. 2D architecture of graphene films were fabricated via the various methods such as electro-spray deposition, spin / spray coating and etc. 1D architecture of graphene fibers were prepared via continuously spun from graphene oxide suspensions followed by chemical reduction at room temperature.

RESULTS

The 3D architectures of graphene foam had low densities, high thermal stability, high electrical conductivity and high specific capacitance. The electrical conductivity and transmittance of 2D composite films were controlled. By varying wet-spinning conditions and complex with CNTs, a series of 1D graphene fibers were prepared. Their structural features, mechanical and electrical performances were investigated.



Figs. (a) optical image of 3D graphene foam, (b) surface morphology of 2D graphene film, (c) SEM image of 1D graphene fiber

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^{xi} Email: wskim@kicet.re.kr, Tel. +82-55-792-2431

Study on the high vacuum thin film deposition efficiency improvement under vapor deposition technology

Sang Hyun Park,^{1,2} Jin Do Chung,^{1,xii} Yeon BoK Cho,¹ and Do Won Hwang²

¹ Dept of environmental Engineering, Hoseo Univ., Asan, Chung, Korea, 32117

² Alpha -plus Co. Ltd, Asan, Chung, Korea, 32117

ABSTRACT

As the deposition technology has been developed in the modern society, the devices have also been developed small accordingly. Among those devices, as the use of the display has been increased, it has been being researched in a variety of fields from the related academic fields to the government oriented industrial aspect, and in the field of the Organic Light Emitting Diode (OLED), being used in the modern display fields, the research on the uniformity of the thin film that affects the quality of the products has been vividly performed for its significance. In order to solve these problems, the prediction of the final process is necessary, and for this reason, the purpose of this study is to understand the movement of the molecules in the environment of the high-degree vacuum which is necessary for the deposition of the OLED thin film, to predict the feature in the aspect of the evaporation sources through the simulation and to suggest the efficient deposition process to form the thin film uniformly. The condition of the simulation is to change the inside of the vapor deposition in the high-degree vacuum environment and to confirm the index value of the cosign function [N] expressing the distribution chart of the thickness of the thin film and to compare and analyze it with the experiment data. As a result, the fact that if the amount of the evaporation is smaller, the value [N] is lager has been confirmed.

Keywords : DSMC, OLED, Cap, Direct simulation Monte Carlo, Deposition

^{xii} Email: jindo7@naver.com

Structure induced selective adsorption performance of ZIF-8 nanocrystallines and their application in water purification

Yan Ding, Yongfei Xu, Bing Ding, Zhen Li, Fazhi Xie, Fengjun Zhang, Jin Liu, and Xianbiao Wang^{xiii}

School of Materials and Chemical Engineering, Anhui Jianzhu University, Hefei, 230601, P. R. China

ABSTRACT

Inspired by the surface charge and uniform pore size of Zeolitic Imidazolate Framework-8 (ZIF-8), we prepared ZIF-8 nanocrystallines and investigated their selective adsorption performance and potential application in water purification by adsorption of phenol, methyl orange (MO) and Cr(VI) in aqueous solution. The obtained ZIF-8 nanocrystallines have uniform size (~50 nm in diameter), high BET surface area (1291 m²/g) and tunable surface charge. The adsorption experiments indicate that the ZIF-8 adsorption capacity follows the order of Cr(VI)>MO>phenol. Meanwhile, the adsorption behaviors were investigated to fit well with a pseudo-second-order model. The adsorption selectivity towards Cr(VI) and MO was due to the electrostatic interaction between the positively charged surface of ZIF-8 and Cr(VI) or MO anions. Further, the adsorption capacity for Cr(VI) is much more than that of MO, exhibiting size selectivity. This work not only gives an insight into the adsorption behavior and adsorption mechanism of ZIF-8, but also provides an excellent adsorbent with selective adsorption performance for the process of water treatment and purification.

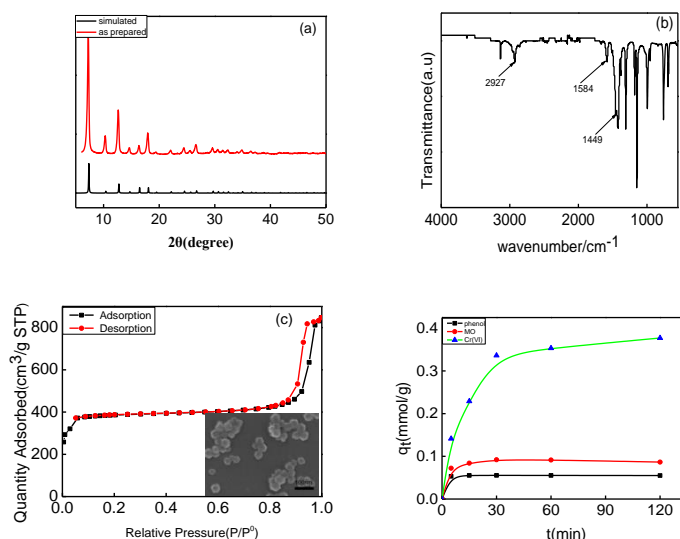


Fig. 1. (a) XRD patterns, (b) FTIR spectrum, (c) nitrogen adsorption-desorption curves of ZIF-8 nanocrystallines (inset: SEM image) and (d) kinetic adsorption curves for phenol, MO and Cr(VI)

^{xiii} Email: xianbiao.wang@hotmail.com, liujin@ahjzu.edu.cn

RSM study in the foam fractionation of native whey (waste)

(Subtitle: Statistical Analysis in Enrichment of Total Whey)

Dr. Goutam Mukhopadhyay^{xiv}

BCDA College of Pharmacy & Technology Kolkata, India

ABSTRACT

The objective of the present study was to optimize the operating conditions in the separation of the total whey proteins from whey by continuous foam fractionation method using response surface methodology (RSM). The effects of the different process variables such as pH (X1) of proteins in feed, Gas flow rate, GFR (X2) of initial feed solution, protein:surfactant ratio, PSR (X3) and volumetric flow rate, VFR (X4) were investigated on the performance criteria of fractionation of raw processed whey. Four factors, three levels Box-Behnken design was used for the optimization procedure. Quadratic model regression equations and response surface plots correlate independent variables (X₁, X₂, X₃ and X₄) and dependent variables (response) such as concentration of Foamate (C_f), Enrichment ratio (E_r), and percentage Recovery (%R_p) of total whey proteins can be achieved easily. All the four factors had significant effects on the response variables. The model predicted that the optimized values of the factors (X₁, X₂, X₃, X₄) were 5, 290, 1.5, 14 respectively. The predicted responses were (concentration of Foamate, Enrichment ratio, and percentage Recovery) such as 6647.32, 13.27, and 78.02 respectively. Experiments were performed with the predicted values of factors.

Keywords: *Box-Behnken design, Optimization, Foam separation, Whey.*

^{xiv} Email: goutam_bst@yahoo.com

Cleaning validation study for common equipment's used in manufacturing and preparation of Pediatric Suspension and Simple Linctus

Ashish A. Gawai, and S. Lokhande. Biyani K. R.^{xv}

Anuradha College of Pharmacy, Anuradha Nagar, Chikhli, Dist-Buldana, M.S, India

ABSTRACT

The drug tragedy of sulfanilamide elixir which killed over 100 people is a classical example of pharmaceutical contamination. The contamination of pharmaceutical products with other pharmaceutically active ingredients and microorganisms are the real concerned which questions the integrity and safety of the pharmaceutical product. In most cases contamination of pharmaceutical products occurs when a common facility is utilized to manufacture many products.

Regulatory agencies like United State of Food and Drug Administration (USFDA), European Medicinal Evaluation Agency (EMA), Australia's Therapeutic Goods Administration (TGA) established requirements for cleaning of such established requirements for cleaning of such common instruments/ facility and validation of such process which is documented evidence with a high degree of assurance that one can consistently clean a system to predetermined and acceptable limits. Production of Paracetamol Suspension Pediatric 120mg/5ml and Simple Linctus BP in a common facility, where Paracetamol and Simple Linctus could be a possible cross contaminant.

Hence the present study was carried out to validate the cleaning validation of Paracetamol Suspension Pediatric 120mg/5ml and Simple Linctus BP were observed by visual inspection, swab sampling for chemical residue and swab sampling for microbiological analysis. Upon the compiled data, it was concluded that the results were found to be satisfactory and there is no chance of cross contamination with Paracetamol Suspension Pediatric 120mg/5ml and Simple Linctus BP to next product.

Keywords: *Paracetamol, Simple Linctus, Cross Contamination, Cleaning Validation*

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^{xv}Email: drashishgawai@gmail.com

Analytical, biological and medicinal characteristics of semicarbazones derived from pyrazolone and their lanthanide(III) complexes

Ram K. Agarwal^{xvi}

Former Head, Department of Chemistry, Lajpat Rai Postgraduate College (C.C.S. University)

SAHIBABAD-201005 (Ghaziabad) INDIA

Editor-in-Chief, ASIAN JOURNAL OF CHEMISTRY

ABSTRACT

Medicinal inorganic chemistry is an emerging topic of growing significance in both therapeutic as well as diagnostic tools. The discovery and development of the antitumour compound cis-platin (*cis* [Pt(NH₃)₂Cl₂] played a potent role in field of medicinal inorganic chemistry. The history of the development and basic concepts of biological/medicinal inorganic chemistry have been available in literature. The field now covers active metal complexes, metal ions and even metal-binding compounds as potential agents. Metal ions can be removed from a biological system by judicious use of metal-binding molecules (termed ligands from the Latin word *ligare*, meaning that which binds). From early days, the physiological properties of heterocyclic piperazines have generated interest since they are found to exert various physiological effects. Pyrazolone (n-heterocyclic compound) is an active moiety as a pharmaceutical ingredient, especially in non-steroidal anti-inflammatory agents used in the treatment of arthritis and other musculoskeletal and joint disorders. Semicarbazones, a class of Schiff bases are reported to possess versatile structural features and good antifungal and antibacterial properties. A good number of semicarbazones derived from 4-aminoantipyrine are reported from our laboratory and studied their biological/medicinal characteristics. Lanthanide (III) compounds frequently have magnetic, catalytic and optic properties and therefore they are widely used in industries. In recent years, new experimental methods have been developed due to which new role of lanthanides in the biochemical processes operating in cellular membranes, organelles and cytoplasm have been obtained. In present lecture, the author will summarize the work on lanthanides(III) complexes of semicarbazones especially derived from 4-aminoantipyrine and their analytical, biological and medicinal characteristics.

Keywords: *Lanthanides(III), Complexes, Semicarbazones, 4-Aminoantipyrine, Analytical, Biological, Medicinal characteristics.*

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^{xvi} Email: ramagarwallrpg@gmail.com, ram_agarwal54@yahoo.com

Demonstration of improved the photocatalytic effect with PtSe₂ and TiO₂ decorated large area graphene obtained by CVD method

Shu Ye and Won-Chun Oh*

Department of Advanced Materials Science & Engineering, Hanseo University, Chungnam 356-706, Korea

ABSTRACT

Here, we report our method on enhancing the photocatalytic effect with PtSe₂ and TiO₂ treated large area graphene (LAG). The LAG was growth on copper foil at a low temperature (500 °C) under atmospheric pressure by chemical vapor deposition (CVD) method [1-2]. A facile, fast ultrasonic method was then used to successfully synthesize PtSe₂-LAG/TiO₂ nanocomposites. The composites that were obtained were characterized using X-ray diffraction (XRD) spectroscopy, scanning electron microscopy (SEM) with energy dispersive X-ray (EDX) spectroscopy, transmission electron microscopy (TEM), Raman spectroscopic analysis, and X-ray photoelectron spectroscopy (XPS). UV-vis diffuse reflectance spectra (DRS) analyses were also performed, and the catalytic behavior was investigated by the decomposition of methylene blue (MB). The as-prepared LAG with a Raman D band was obtained, and graphene layers can be clearly seen in High-Resolution Transmission Electron Microscopy (HRTEM) images. The degradation performance of the MB solution was determined via UV-Vis spectrophotometry. This improved photocatalytic activity is a result of the positive synergetic effect between PtSe₂ and LAG in the heterogeneous photocatalyst. In this study, the LAG behaves as an electron transfer agent, contributor, collector, and source of active adsorption sites. The optical properties were also observed to be affected by the different weight ratios of the LAG in the composites by observing their respective band gaps from diffuse reflectance spectra.

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*Email: wc_oh@hanseo.ac.kr, Tel: +82-41-660-1337, Fax: +82-41-688-3352

The effects of metal cations on the activity of the Prussian blue photocatalyst

Shou-Qing Liu, Ze-Da Meng, Feng Chen, and Zhi-Gang Chen

Provincial Key Laboratory of Environmental Science and Engineering, College of Chemistry, Bioengineering and Material Engineering, Suzhou University of Science and Technology, Suzhou 215009, China

ABSTRACT

The formula of Prussian blue could be denoted as $\text{KFe(III)Fe(II)(CN)}_6$. So, Prussian blue is capable of use as a heterogeneous photo-Fenton reagent for the degradation of organic species. Some anions such as Cl^- , Br^- , SO_4^{2-} and NO_3^- have been investigated on the effects of the activity of photocatalysts, however, the effects of alkali cations on the photocatalytic activity have not been studied. The emphasis of this work is laid on the effects of alkali metal cations on the photo-Fenton process. The facts show that alkali cations strongly affect the degradation rate of organic species. The degradation rates of Rhodamine B, Malachite Green, and Methyl Orange in the presence of KCl , KNO_3 , and K_2SO_4 , respectively, are faster than their degradation rates in the presence of the corresponding sodium salts. The average degradation rates of Rhodamine B in 0.2 M KCl , NaCl , RbCl , and CsCl solution, are 0.0960, 0.0343, 0.0247, and 0.0179 $\text{mg}\cdot\text{L}^{-1}\cdot\text{min}^{-1}$, respectively, while the rate without salts is 0.0543 $\text{mg}\cdot\text{L}^{-1}\cdot\text{min}^{-1}$. Thus, potassium ions accelerate the degradation rate, but sodium, rubidium, and cesium ions decrease the rate. The order of the rates is $R_{\text{K}} > R > R_{\text{Na}} > R_{\text{Rb}} > R_{\text{Cs}}$, which is consistent with that of the oxidation currents in electrochemistry. This phenomenon is attributed to the molecular recognition of the microstructure in Prussian blue nanoparticles by the alkali cations. The reaction mechanism of the photo-Fenton process has also been explored.

A fluorescent turn-on/off method based on Hg²⁺ quenched graphene quantum dots as a fluorescent probe using thioacetamide for selective determination of Ag⁺ in water samples

Pimpisa Kaewanan, Prawit Nuengmatcha, Saksit Chanthai^{xvii}

*Materials Chemistry Research Center, Department of Chemistry and Center of Excellence for Innovation in Chemistry,
Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand*

ABSTRACT

A selective fluorescence sensor for the determination of silver ion (Ag⁺) was developed based on graphene quantum dots (GQDs). GQDs were prepared by the citric acid pyrolysis method. In the presence of mercury ion (Hg²⁺), the fluorescence intensity of GQDs decreased linearly and it was fully recovered by thioacetamide (TAA). This is aimed to use as fluorescent sensor for determination of Ag⁺. Upon the addition of Ag⁺, the fluorescence intensity of the TAA-(Hg²⁺ quenched GQDs) decreased as a linear function of the Ag⁺ concentration. The GQDs acquired showed steady, selective, and highly sensitive detection of Ag⁺. The experimental parameters affecting the fluorescence sensor were investigated and optimized. The optimum conditions included 4 μM Hg²⁺ concentration, 70 μM TAA concentration, solution pH 7 and 5 min reaction time. Under the optimized conditions, the working linear concentration range and the limit of detection for Ag⁺ were 0-12 μM and 0.2 μM, respectively. The proposed method was successfully implied to determine Ag⁺ in water samples.

Keywords: *Graphene quantum dots, turn-on/turn-off, fluorescence probe, thioacetamide, mercury ion, silver ion*

^{xvii} Email: sakcha2@kku.ac.th

Poster Presentation

Catalytic reduction potential of silver nanoparticles for selenium analysis in water sample by flow injection-hydride generation atomic absorption spectrometry

Ruttiya Poonyaka and Saksit Chanthai^{xviii}

*Materials Chemistry Research Center, Department of Chemistry and Center of Excellence for Innovation in Chemistry,
Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand*

ABSTRACT

Few analytical methods have been developed for an ultra-trace determination of selenium in complex matrices. In this study, selenium speciation, both Se(IV) and Se(VI), under catalytic reduction using silver nanoparticles (AgNPs) associated with flow injection-hydride generation atomic absorption spectrometry (FI-HGAAS) was developed. The AgNPs were freshly prepared in an excess of sodium borohydride solution, and the pale yellow solution of AgNPs exhibits a characteristic absorption peak at 355 nm. By using AgNPs either in the presence or in the absence of borohydride for Se analysis, the results demonstrated that they did not affect any selective catalyst for Se(IV) analysis, but they acted as a catalytic pre-reducing agent for Se(VI). Thus, the dispersed AgNPs could indeed enhance in sensitivity for selenium analysis. The Se(VI)-to-Se(IV) conversion and its recovery study for Se speciation in drinking water samples were also validated using AgNPs in comparison with the common pre-reducing agent used. Both LOD and LOQ of the method were $0.5 \mu\text{g L}^{-1}$ and $1.0 \mu\text{g L}^{-1}$, respectively. The precision of the calibration curve using Se(VI) standard solution between $5 \mu\text{g L}^{-1}$ and $25 \mu\text{g L}^{-1}$ ($n = 10$) was shown within the acceptable ranges of RSD between 3.23% and 5.69% for an inter-day and an intra-day analysis, respectively. For real sample analysis, the determination of Se in the presence of AgNPs was successfully achieved ranging from $0.03\text{-}0.10 \mu\text{g mL}^{-1}$, $0.12\text{-}1.0 \mu\text{g mL}^{-1}$ and $0.22\text{-}0.97 \mu\text{g mL}^{-1}$ for Se(IV), Se(VI), and total Se, respectively.

Keywords: *Selenium, Silver nanoparticles, Hydride generation, Catalytic reduction, Pre-reducing agent*

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^{xviii} Email: sakcha2@kku.ac.th

Mild acid ultrasonic assisted extraction of arsenic residues in different parts of hot chilli prior to ultra-trace determination by flow injection-hydride generation atomic absorption spectrometry

Sugunya Phongsirirux,^a Phitchan Sricharoen,^a Nunticha Limchoowong,^a Suchila Techawongstien,^b and Saksit Chanthai^{a,xix}

^a*Materials Chemistry Research Center, Department of Chemistry and Center of Excellence for Innovation in Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand*

^b*Department of Plant Science and Agricultural Resources, Faculty of Agriculture, Khon Kaen University, Khon Kaen 40002, Thailand*

ABSTRACT

Mild acid ultrasonic assisted extraction (UAE) of arsenic residues in hot chilli peppers was introduced as a green approach due to simple, efficient and rapid method in association with flow injection-hydride generation atomic absorption spectrometry (FI-HGAAS). The optimized conditions of UAE are certainly investigated in details, in particular several variables that could affect the performance of the extraction method. In this study, arsenic species, As(III) and As(V), were determined in different parts of chilli fruits including seed, pericarb and placenta. This procedure leads to improve mild extraction conditions using 0.1 g of ground sample in 10 mL of 1 M acid mixture of HCl : HNO₃ (3:1, v/v) and 1.5 mL H₂O₂ for 15 min sonication (35 kHz) and 25 °C. Analytical features of merit for both FI-HGAAS and FAAS measurements were obtained and compared. Actually, trace amounts of total As in these samples were found very lower than LOQ of FAAS. Therefore, the ultra-trace amounts of As(III), As(V) and total As in the chilli samples determined by FI-HGAAS were found in the ranges of 1.9-6.4 ng g⁻¹, 1.2-19.1 ng g⁻¹, 3.3-22.4 ng g⁻¹, respectively. Among three varieties of these chilli samples, higher contents of As were mostly found in seed of the fruits. The proposed method is, therefore, a novel one and can be implied for a routine work for arsenic in fruits and vegetables with its emerging applications.

Keywords: *Ultrasonic assisted extraction, Hydride generation, Atomic absorption spectrometry, Chilli, Arsenic.*

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^{xix} Emai: sakcha2@kku.ac.th

Colorimetric detection of dichlorvos using polydiacetylene incorporated with fatty acid on paper

R. Pimsen,^{xx} J. Janruang, and S. Sangsampan

*Department of Chemistry, Faculty of Science and Technology, Nakhon Si Thammarat Rajabhat University,
Nakhon Si Thammarat 80280, Thailand.*

ABSTRACT

A new colorimetric method for the detection of dichlorvos based on polydiacetylene incorporated with fatty acid on paper is developed. Dichlorvos is a widely used organophosphate pesticide which possesses both acute and chronic toxicity instigating hazardous risks to humans and environment. The toxicity of dichlorvos is closely related to its strong acetylcholinesterase inhibition activity. Based on this enzyme inhibition activity, a sensitive and selective colorimetric detection of dichlorvos is developed with a polydiacetylene (PDA) on paper. Using a threshold concentration of myristoylcholine, poly(10,12-pentacosadynoic acid) on paper was induced to exhibit a blue-to-red color transition. When incubating with acetylcholinesterase, myristoylcholine is enzymatically hydrolyzed to myristic acid and choline that preclude the color transition of the PDA on paper. When acetylcholinesterase is mixed with dichlorvos prior to the incubation with myristoylcholine, the color transition is resumed upon the addition of the PDA on paper. From the results, the optimum conditions for dichlorvos detection were MC 200 μM , AChE 3 U/mL and pH 6.5. Moreover, the color transition is also observable by naked eye in which 500 ppb dichlorvos. The addition of fatty acids such as lauric acid, myristic acid, palmitic acid and stearic acid, polydiacetylene/30% stearic acid can be visually detected. The limit of detection is lowered to 150 ppb. It is therefore evident that the developed method can be successfully applied to the determination of dichlorvos for on-site environmental monitoring.

Keywords: *Dichlorvos, acetylcholinesterase, polydiacetylene, organophosphate*

^{xx}Email: rung_cha@yahoo.com; Tel. +66-7537-7443, Fax +66-7537-7443

Analysis of optical performance in blue light blocking spectacle lenses

Hang-seok Lee, and Ki-choong Mah^{xxi}

Department of Optometry, Graduated School of Eulji University, Seong-Nam

ABSTRACT

To analyze the performance of the blue light blocking lens, the blue light transmittance of 16 blue light blocking lenses having luminous transmittance more than 80 % were measured by spectrophotometer, and the influence of the blue light blocking lens on the color accuracy and the clarity in LED display at different luminance levels(20 nit, 110 nit and 400 nit) were measured by the camera image quality evaluation equipment.

The blue light blocking lens showed the difference in the optical performance depending on the manufacturing method. The coated lens showed higher luminous transmittance and blue light transmittance than the tinted lens, and it showed the significant difference in the luminous transmittance($p < 0.05$). The luminous transmittance and blue light transmittance of coated lens showed significant positive correlation($r = 0.714$), but the tinted lens did not show the significant correlation between the luminous transmittance and the blue light transmittance.

The luminous transmittance and the blue light transmittance of the blue light blocking lens was showed significant positive correlation($r = 0.433$), and both the luminous transmittance and the blue light transmittance did not show the significant correlation with the changes in the color accuracy and the clarity.

The color accuracy and the clarity by the blue light blocking lens was increased at high luminance(400 nit), but it was decreased at low luminance(20 nit and 110 nit).

Conclusively, the difference in the optical characteristics based on manufacturing method was verified, and that the influence on the color accuracy and the clarity was verified according to the luminance level of LED display. Therefore, the results of this study were considered to suggest the basic data for the performance of blue light blocking lens.

Keywords: *Blue light blocking lens, Luminous transmittance, Blue light transmittance, Color accuracy, Clarity*

^{xxi}E-mail: kcmah@eulji.ac.kr, Tel: 031-740-7262, Fax: 031-740-7365,

Green synthesis, characterization and application of silver nanoparticles for antibacterial

P. Porrawatkul^{xxii} M. Thongsom, P. Khaosuk and T. Dolohmi

Department of Chemistry, Faculty of Science and Technology, Nakhon Si Thammarat Rajabhat University, Nakhon Si Thammarat 80280, Thailand.

ABSTRACT

Silver nanoparticles (AgNPs) were successfully synthesized via a simple solvothermal process using rind extract of *Garcinia mangostana* Linn. (Mangosteen) as reducing agent. The intrinsic characteristics of as-obtained samples were performed using a variety of techniques including ultraviolet-visible spectroscopy (UV-Vis), fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDX). For optimization study, the effects of pH, reaction temperature and reaction time were investigated in details. From the results, the optimum conditions for AgNPs preparation were achieved at pH 7 with a reaction temperature 80 °C and 5 hours for complete reaction time. The synthesized AgNPs showed the UV-Vis spectra at 420 nm which is the main peak of silver nanoparticles. The obtained characteristic peaks from FTIR and EDX spectra confirmed the presence of elemental signature of silver indicating the AgNPs were successfully synthesized. SEM image exhibited that the particle size of the synthesized AgNPs is in the range of 100 to 200 nm. In addition, the synthesized AgNPs showed a moderate antibacterial activity against *Staphylococcus aureus* and *Escherichia coli*.

Keywords: Silver nanoparticles, *Garcinia mangostana* Linn. Antibacterial activity

^{xxii}E-mail: paweena.n@gmail.com; Tel. +66-7537-7443, Fax +66-7537-7443

Decomposition of N_2H_4 in the HYBRID decontamination process

Huijun Won, Seonbyung Kim, Sangyoon Park, Wangkyu Choi, and Jeikwon Moon

NPP D & D Technology Development Division, Korea Atomic Energy Research Institute, Daejeon 305-353, Korea

ABSTRACT

As the increase of an operation age of a nuclear power plant, a radioactivity is accumulated on the internal loop of a primary coolant system. Radiation exposure of workers can be reduced by the application of the chemical decontamination process. Ordinary chemical decontamination processes generate a secondary waste as an ion exchange resin. A new chemical decontamination process was developed by KAERI. HYBRID represents a name of the process (HYdrazine Base Reductive metal Ion Decontamination, $N_2H_4-Cu^+-H^+$). It was found that the three kinds of decomposition reaction of N_2H_4 occur during the application of HYBRID process. Firstly, N_2H_4 is decomposed into nitrogen, hydrogen and ammonia by radiolysis. Secondly, N_2H_4 is decomposed into ammonia, nitrogen, hydrazoic acid and ammonium nitrate in the presence of ferrous ion above 120 °C. Thirdly, N_2H_4 is decomposed into nitrogen and water by H_2O_2 during the secondary waste volume reduction.

Key words: *decontamination; hydrazine; decomposition; radiolysis; H_2O_2 ; Cu^+*

Microstructure and permanentmagnetic properties of W-type hexagonal ferrites $\text{Ba}_{1-x}\text{Sr}_x\text{Fe}_2^{2+}\text{Fe}_{16}^{3+}\text{O}_{27}$

Xiansong Liu,^{xxiii} Farui Lv, Xiaofei Niu, and Shuangjiu Feng

Engineering Technology Research Center of Magnetic Materials, School of Physics & Materials Science, Anhui University, Hefei 230601, PR China

ABSTRACT

A series of W-type hexagonal ferrites with the composition $\text{Ba}_{1-x}\text{Sr}_x\text{Fe}_2^{2+}\text{Fe}_{16}^{3+}\text{O}_{27}$ ($0 \leq x \leq 1$) were prepared by the ceramic process in a nitrogen atmosphere during the whole process of pre-sintering and sintering. The phase composition, micromorphology, and magnetic properties of the particles were investigated by XRD, SEM and VSM. The results of XRD show that the single phase was observed in the W-type ferrites with different Sr content. The micro-morphology of the particles exhibits the uniform plane hexagonal structures of W-type ferrites with different Sr content. The coercivity (H_c) of the particles increases with the increase of Sr content (x), while the saturation magnetization (M_s) of the particles first decreases with x from 0 to 0.2, and then begins to increase when x continues to increase.

The permanent magnetic properties of the $\text{Ba}_{1-x}\text{Sr}_x\text{Fe}_2^{2+}\text{Fe}_{16}^{3+}\text{O}_{27}$ ($0 \leq x \leq 1$) magnets were obtained by using a B - H hysteresis curve measurement. The intrinsic coercivity (H_{cj}), magnetic induction coercivity (H_{cb}) and maximum energy product ($(BH)_{\max}$) of magnets decrease with the Sr content (x) increases. However, the remanence (B_r) of the magnets increases at first, reaches to the maximum value (402.4 mT) at $x=0.3$ and then decreases. Meanwhile, at $x=0.6$, other magnetic properties of the magnets were obtained, including intrinsic coercivity ($H_{cj}=146.7$ kA/m), coercivity magnetic induction ($H_{cb}=136.6$ kA/m) and maximum energy product ($(BH)_{\max}=27.1$ kJ/m³).

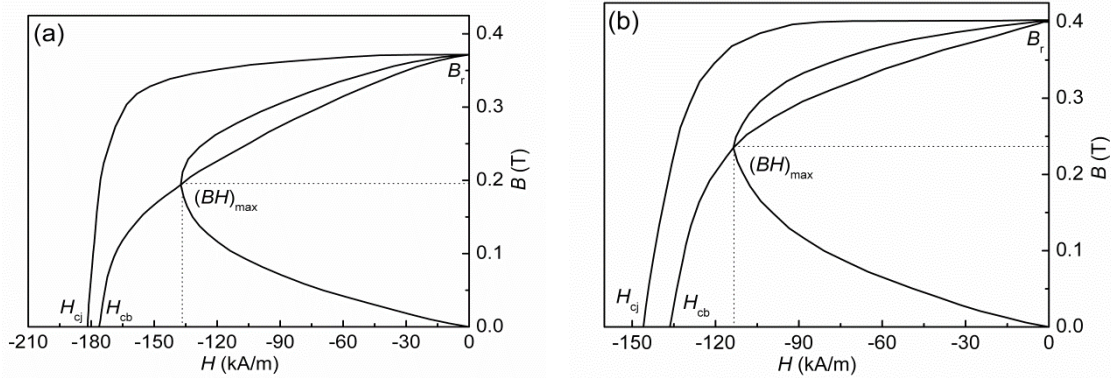


Fig. 1 Demagnetization curve of the $\text{Ba}_{1-x}\text{Sr}_x\text{Fe}_2^{2+}\text{Fe}_{16}^{3+}\text{O}_{27}$ ($0 \leq x \leq 1$) magnets with an Sr content of (a) $x=0.3$ and (b) $x=0.6$.

^{xxiii} Email : xiansongliu@ahu.edu.cn

Introduction of additional micropores and tunable macropores into carbon gels

Kazuki Sakai, Takeshi Mori, Takanori Tsuchiya, Shinichiro Iwamura, Isao Ogino and Shin R. Mukai

Division of Chemical Process Engineering, Graduate School of Engineering, Hokkaido University, N13W8, Kita-ku, Sapporo, 060-8628, JAPAN

ABSTRACT

Porous carbon materials are widely used for electrical devices and catalyst supports due to their electrical conductivity, chemical stability and high surface area. While micropores in carbon materials provide most of the functional surfaces of the material, mesopores and macropores are also necessary to enhance the accessibility of substances to such surfaces. Thus, the structural controlling of each category of pores of the material is inevitable to maximize its performance, but such controlling is difficult for typical carbon materials such as conventional activated carbons. It has been reported that the size of mesopores of carbon gels can be easily controlled by adjusting synthesis conditions of its precursor [1]. However, the structural controlling of its micropores and macropores still remain as a challenge. In this work, we report simple methods which allow the introduction of additional micropores, through CO₂ activation, and tunable macropores, through templating, into carbon gels. Fig.1 shows N₂ adsorption isotherms of CO₂-activated carbon gels. It can be confirmed that a significant amount of additional micropores can be introduced into carbon gels through CO₂ activation. It was also confirmed that surface areas comparable to chemically activated carbons can be easily obtained even when a conventional oxidizing agent, CO₂, is used for activation. Fig.2 shows SEM images of carbon gels into which macropores were introduced using polymethyl methacrylate nanoparticles as the template. It can be confirmed that macropores with controllable sizes can also be introduced into carbon gels through a simple method. By combining these methods, a porous carbon with a hierarchical and tunable pore system of micro-, meso- and macropores can be obtained.

Keywords: Carbon gel; Porous material; CO₂ activation; Polymer template

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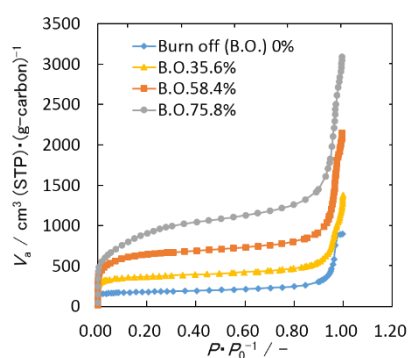


Fig. 1 N₂ adsorption isotherms of CO₂-activated carbon gels

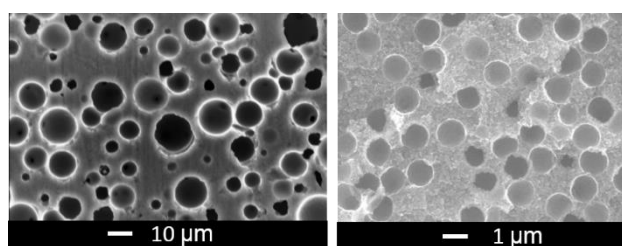


Fig. 2 SEM images of macroporous carbon gels prepared by polymer templates with different sizes

Heat irradiation properties of silicon carbide fibers under microwave

Khos-Erdene Khishigbayar, Kwang Youn Cho,^{xxiv} and Jong Min Seo

Ceramic Fiber and Composite Materials Center, Korea Institute of Ceramic Engineering and Technology, Korea

ABSTRACT

SiC fibers have been reacted different ways with microwave irradiation depending on their fabrication conditions. The influence of these properties on microwave heating effect has been analyzed with electric field distribution in the microwave oven. It reveals that SiC fibers can be heated in microwave oven at the 2.45GHz of frequency.

INTRODUCTION

SiC fibers with an excellent mechanical properties have been used in a wide range of industrial application and its utilization area is extending, continuously [1]. SiC fibers are a kind of anisotropic microwave absorbing materials due to their fiber shaped semi-conductive properties [2].

METHOD

In this study, SiC short fibers were prepared and their microwave absorbing properties have been analyzed with infrared thermal imaging camera.

RESULTS

The maximum irradiation temperature of SiC fiber with microwave is strongly depended on halogen concentration, which was used during PCS curing process to obtain SiC fiber. The optimal amount of halogen to PCS fiber was found 1:1 at our experimental condition.

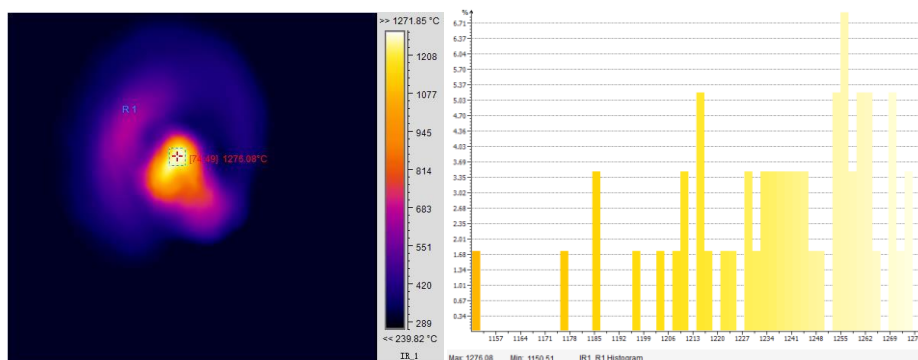


Fig.1. Temperature profile of IR-camera measurement analysis of fabricated SiC fiber

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^{xxiv} Email: kycho@kicet.re.kr, Tel: +82-55-792-2710, Fax: +82-55-792-2530

Oxy-stabilization on iodine-dopped PCS fiber

Kwang Youn Cho,^{xxv} Khos-Erdene Khishigbayar, and Jong Min Seo

Ceramic Fiber and Composite Materials Center, Korea Institute of Ceramic Engineering and Technology, Korea

ABSTRACT

Iodine-converged polycarbosilane(PCS) has used as a starting material to obtain PCS fiber for fabrication of SiC fiber. FT-IR, GPC, TGA and SEM analysis were used to determine the optimal reaction temperature and the iodine doping ratio to PCS. Tensile strength of the obtained SiC fiber was 1.5 GPa.

INTRODUCTION

Fiber shaped polycarbosilane prepared by melt spinning method and then, stabilized with the presence of iodine[1]. The iodine should be volatilized to lead the iodine diffusion into PCS. Generally, this stabilization method is considered a harmful for human body due to gaseous state of iodine. In this study, we tried to minimize the amount of iodine, which is used for stabilization process of SiC fiber fabrication.

METHOD

PCS and iodine were dissolved respectively into toluene and mixed together for convergence of PCS and iodine. The converged-PCS was melt spun and stabilized at various temperatures for 24 hours.

RESULTS

A softening and melting point of originally used PCS were increased significantly after the convergence reaction. The average tensile strength of obtained SiC fiber was 1.5 GPa, which was stabilized at 180 °C for 24 hours.

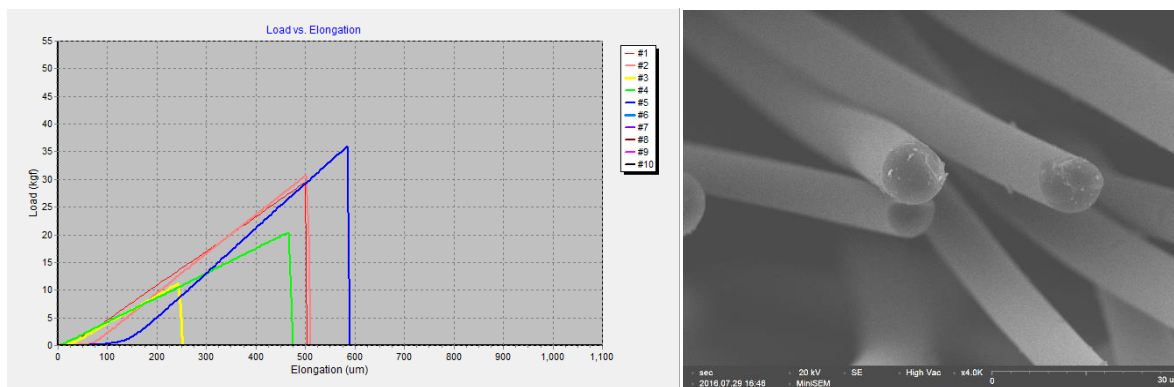


Fig.1. Tensile strength curve of SiC fiber and its cross section image

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^{xxv}Email: kycho@kicet.re.kr, Tel: +82-55-792-2710, Fax: +82-55-792-2530

Reduced pressure curing on iodine-converged PCS fiber

KwangYoun Cho,^{xxvi} Khos-Erdene Khishigbayar, and Jong Min Seo

Ceramic Fiber and Composite Materials Center, Korea Institute of Ceramic Engineering and Technology, 101, Soho-ro, Jinju-si, Gyeongsangnam-do, 660-031 Korea

ABSTRACT

The convergence of PCS and iodine could be minimized the amount of iodine, which is used for the curing stage of SiC fiber fabrication. Ceramic yield of PCS was increased from 75% to 83% after the 1% iodine convergence.

INTRODUCTION

SiC fiber can be obtained from preceramic polymer such as polycarbosilane (PCS) by melt spinning, stabilization and heat treatment process [1]. In this study, iodine doped PCS fiber was stabilized at reduced pressure [2], it can be potentially lead to avoid the oxygen diffusion into the fiber body.

METHOD

PCS and iodine were dissolved into toluene and converged in vacuum oven. The converged-PCS was melt spun and stabilized at 180 °C for 24 hours under 1.6 torr of pressure. And then, the stabilized PCS fiber was heat treated at 1300 °C.

RESULTS

The optimal amount of iodine ratio and stabilization pressure was found at 1% and 1.6 torr, respectively. The ceramic yield was increased from 75% to 83% at this condition.

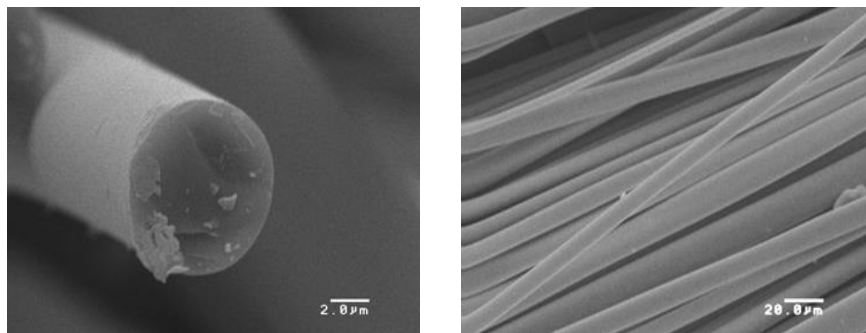


Fig.1. Surface and cross sectional images of the converged fiber

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^{xxvi} Email: kycho@kicet.re.kr, Tel: +82-55-792-2710, Fax: +82-55-792-2530

Heat conversion behavior of SiC fiber sheet under microwave

KwangYoun Cho,^{xxvii} Khos-ErdeneKhishigbayar, and Jong Min Seo

Ceramic Fiber and Composite Materials Center, Korea Institute of Ceramic Engineering and Technology, 101, Soho-ro, Jinju-si, Gyeongsangnam-do, 660-031 Korea

ABSTRACT

Irradiation behavior of SiC fiber and microwave is depending on SiC fiber sintering and the frequency of microwave. Heat conversion efficiency of SiC fiber sheet under microwave irradiation was measured and oxidation degree of fiber was monitored after the microwave irradiation.

INTRODUCTION

High temperature resistant behavior of SiC fiber can provide a wide range of application and it is continuously extending its utilization area [1]. Microwave heating is induced by internal molecular vibration of heated body. Therefore, the heating rate value is much higher than conventional heating technology [2].

METHOD

PCS fiber sheet was prepared by the cured fiber and heat treated at high temperature to obtain SiC fiber sheet. The prepared SiC fiber sheet was irradiated under microwave and the heat conversion temperature was measured by IR thermal camera.

RESULTS

Heat conversion temperature of SiC fiber sheet under microwave is strongly depended on the iodine concentration, which was used during the curing stage. The maximum heat conversion temperature was measured at 1107 °C.

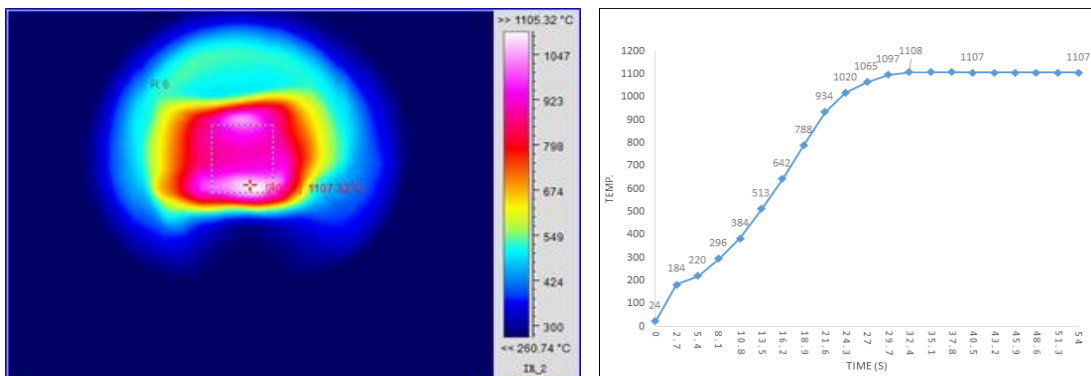


Fig.1. The heat conversion temperature profile and heating rate

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^{xxvii}Email: kycho@kicet.re.kr, Tel: +82-55-792-2710, Fax: +82-55-792-2530

Measurement of Ce(IV) concentration and oxidation of Ce(III) in foam decontaminant

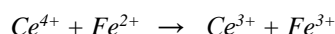
Chong-Hun Jung,^{xxviii} Wang-Kyu Choi, and Jei-Kwon Moon

Decontamination & Decommissioning Research Division, Korea Atomic Energy Research Institute, P.O. Box 105, Yuseong, Daejeon, Korea, 305-600

ABSTRACT

A nanoparticle-based foam decontaminant is composed of a surfactant and nanoparticles for the generation and maintenance of foam, and a chemical decontamination agent made of Ce(IV) dissolved in nitric acid. Ce(IV) will be reduced to Ce(III) through the decontamination process. Oxidizing cerium (III) can be reused as a decontamination agent, Ce(IV). Oxidation treatment technology by ozone uses its strong oxidizing power. It can be regarded as an environmentally friendly process, because ozone cannot be stored and transported like other industrial gases (because it quickly decays into diatomic oxygen) and must therefore be produced on site, and used ozone can immediately begin to decompose.

In order to regenerate Ce(III) into Ce(IV) in nanoparticle-based foam decontaminant containing a TBS surfactant, it is necessary to determine the optimal conditions for ozonation treatment. Previous to this study, research was carried out to determine whether the potentiometric titration method can be used for an analysis of the Ce(IV) concentration in nanoparticle-based foam decontaminant. In the potentiometric titration method, the reaction of Ce(IV) and Fe(II) is as follows:



Potentiometric titration with Fe(II) is able to effectively analyze the concentration of Ce(IV) in nanoparticle-based foam decontaminant containing a surfactant regenerated through ozonation treatment.

The oxidation conversion rate of Ce(III) was increased with an increase in the flow rate of the gas mixture and ozone injection amount. The oxidation time for 100% oxidation conversion of Ce(III) at an ozone injection amount of 9.0 g/h and 7.5 g/h was 6.0 h and 7.0 h, respectively. The time required for 100% oxidation conversion of Ce(III) to Ce(IV) at a specific ozone injection amount can be predicted from these experimental data.

Keywords: Foam, Decontamination, Cerium, Ozone, Oxidation, TBS Surfactant

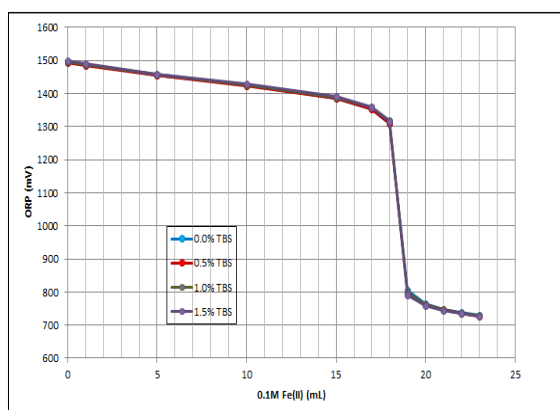


Fig. 1. Potentiometric titration curves using Fe(II) according to TBS concentration of 0-1.5% in 1M sulfuric acid solution.

^{xxviii} Email: nchjung@kaeri.re.kr

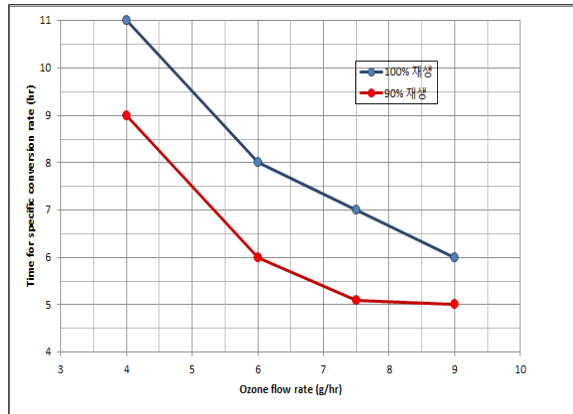


Fig. 2. Oxidation time for specific Ce(III) conversion rate on the variation of ozone flow rate.

The adsorption and desorption study of the carotenoid extract from plant pigments using graphene oxide associated with different functionalized surfactants as a specific modified adsorbent

Chinawooth Sakaew, Saksit Chanthai^{xxix}

Materials Chemistry Research Center, Department of Chemistry and Center of Excellence for Innovation in Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand

ABSTRACT

Graphene, the two-dimensional carbon based materials was mostly used in physical and chemical features of an adsorption study. Based on their advantages including photoluminescence, rigid structure, and electrochemical behaviors with various applications, the numerous benefits have been worldwide demonstrated. In this study, the adsorption-desorption application of graphene oxide (GO) for carotenoids was carried out in the presence of different functionalized surfactants. The carotenoids extracts, the common phytochemicals which are found in the variety of colorful fruits and vegetables, were adsorbed on and then desorbed from the GO surface. The GO was prepared following the optimized conditions of the Hummer's method and its characterization was done by FT-IR. The adsorption and desorption conditions of β -carotene using GO as an adsorbent were investigated in detail, since previously, the study of β -carotene was mostly concerned on bleaching, pre-concentration and determination. The insight theme of interaction/mechanism has not been clarified yet. To overcome this approach, this study proceeds to enhance their robustness and/or uses. The functionalized surface improvement of the GO with sodium dodecyl sulfate (SDS) was a choice to carry out. SDS is the anion surfactant (as reducing agent) which helps β -carotene contacting to the GO surface by its functional polar group. Testing of β -carotene adsorption using these materials was then carried out. Desorption study of the plant pigments was also investigated. Determination of β -carotene was spectrophotometrically validated with 0.1-20 ppm linearity range. This work is, therefore, applicable in a color bleaching, purification, pre-concentration and determination of the carotenoids in plant extracts by using of GO associated with specific functionalized surfactant as an adsorbent.

Keywords: *Graphene oxide, carotenoids, adsorption, desorption, plant pigments, surfactants, adsorbent*

^{xxix} Email: sakcha2@kku.ac.th

Preconcentration and trace determination of copper(II) in Thai food recipes using Fe₃O₄@Chi–GQDs nanocomposite as a new magnetic adsorbent

Nunticha Limchoowong, Saksit Chanthai^{xxx}

Materials Chemistry Research Center, Department of Chemistry and Center of Excellence for Innovation in Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand

ABSTRACT

This study describes preparation, characterization and application of magnetic chitosan-graphene quantum dots nanocomposite (Fe₃O₄@Chi–GQDs) as a new adsorbent for preconcentration and trace determination of Cu(II) in Thai food recipes or the so-called “Som Tam” (green papaya salad). Physicochemical characterization of the Fe₃O₄@Chi–GQDs was investigated in detail. Spectroscopic and magnetic properties including morphology and thermal property were also analyzed using FTIR, EDX, XRD, TGA, VSM and TEM, respectively. Sample preparation of Cu(II) was done by ultrasound-assisted extraction under the optimized conditions (i.e. extraction acid and its concentration, and extraction time) prior to determination by inductively coupled plasma-optical emission spectrometry (ICP-OES). For preconcentration study, the optimization conditions including pH, dosage of adsorbent, sample volume, adsorption-desorption time, concentration and volume of the elution acid, and reusing time, were investigated. Good linearity was obtained ranging from 0.05 to 2500 µg L⁻¹ with correlation coefficient (R²) of 0.999. Limit of detection was 0.015 µg L⁻¹. Their relative recoveries of 85.4 to 107.5 were satisfactorily achieved from real samples. It is, therefore, evident that the nanocomposite can be applied as a magnetic adsorbent for trace determination of Cu(II) in various food samples.

Keywords: *Chitosan-graphene quantum dots; magnetic nanocomposite; copper; food recipes*

^{xxx}Email: sakcha2@kku.ac.th

Fe₃O₄/hydroxyapatite/graphene quantum dots nanocomposite for pre-concentration and determination of copper in Thai food ingredients based ultrasound application

Phitchan Sricharoen, Saksit Chanthai^{xxxi}

Materials Chemistry Research Center, Department of Chemistry and Center of Excellence for Innovation in Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand

ABSTRACT

A new Fe₃O₄/hydroxyapatite/graphene quantum dots (Fe₃O₄/HAP/GQDs) nanocomposite was synthesized and characterized by scanning electron microscopy, transmission electron microscopy, Fourier transform infrared spectroscopy, X-ray diffraction, energy dispersive X-ray spectroscopy and magnetization measurement. The Fe₃O₄/HAP/GQDs was applied to preconcentrate copper residues in Thai food ingredients prior to determination by inductively coupled plasma-optical emission spectrometry. Experimental parameters affecting the magnetic solid-phase extraction based on ultrasound-assisted optimization were conducted, such as solution pH, amount of the magnetic nanoparticles, adsorption and desorption time, and type of an elution acid and its concentration. Under the optimal extraction conditions, a linear range of 0.05–2500 ng mL⁻¹ ($R^2 > 0.999$), limit of detection of 0.58 ng mL⁻¹ and limit of quantification of 1.94 ng mL⁻¹ were obtained. The precision, expressed as the relative standard deviation of the calibration curve slope ($n = 5$), for intra-day and inter-day analysis was 0.87 and 4.47%, respectively. For real samples analysis, the method recovery of copper was ranged between 83.5% and 104.8%. This approach offers the enrichment factors of 39.2, which guarantees the trace determination of copper. Findings of the present work suggest that this nanocomposite has high potential and is suitable candidate for both preconcentration and separation of Cu(II) from food samples and can be used repeatedly by retreatment with deionized water.

Keywords: *Magnetic solid-phase extraction, copper, hydroxyapatite, graphene quantum dots, nanoadsorbent, ultrasound-assisted extraction*

^{xxxi} Email: sakcha2@kku.ac.th

Adsorption of Malachite green from aqueous solution using Tilapia bone powder

M. Sriuttha,^{1,xxxii} K. Pongpratea,¹ B. Hemung¹ and W. Tongpoothorn²

¹Faculty of Applied Science and Engineering, KhonKaen University, NongKhai Campus, Nongkhai 43000, Thailand

²Department of Chemistry, Faculty of Engineering Rajamangala University of Technology Isan, KhonKaen Campus, KhonKaen 40000, Thailand

ABSTRACT

The Tilapia bone powder was used as an adsorbent for adsorption of malachite green from aqueous solution. The surface structure and the functional groups of Tilapia bone powder were characterized using Scanning Electron Microscopy (SEM) and Fourier Transform Infrared Spectrophotometer (FTIR), respectively. The effect of contact time was studied and reached to equilibrium of 180 minutes. At equilibrium time, the adsorption of Langmuir and Freundlich isotherms were evaluated. The adsorption isotherm of Langmuir isotherm ($R^2 = 0.9716$) showed better fit than Freundlich isotherm ($R^2 = 0.9267$), showing a monolayer adsorption. For kinetic analysis, the kinetic analysis of malachite green by Tilapia bone powder described well by the pseudo second order kinetic sorption.

Keywords: *Tilapia bone powder; malachite green; adsorption*

^{xxxii} Email: manosr@kku.ac.th, Tel. +66-4241-5600, Fax +66-4241-5699

A fluorescent turn-on/off method based on Hg²⁺ quenched graphene quantum dots as a fluorescent probe using thioacetamide for selective determination of Ag⁺ in water samples

Pimpisa Kaewanan, Prawit Nuengmatcha, Saksit Chanthai^{xxxiii}

*Materials Chemistry Research Center, Department of Chemistry and Center of Excellence for Innovation in Chemistry,
Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand*

ABSTRACT

A selective fluorescence sensor for the determination of silver ion (Ag⁺) was developed based on graphene quantum dots (GQDs). GQDs were prepared by the citric acid pyrolysis method. In the presence of mercury ion (Hg²⁺), the fluorescence intensity of GQDs decreased linearly and it was fully recovered by thioacetamide (TAA). This is aimed to use as fluorescent sensor for determination of Ag⁺. Upon the addition of Ag⁺, the fluorescence intensity of the TAA-(Hg²⁺ quenched GQDs) decreased as a linear function of the Ag⁺ concentration. The GQDs acquired showed steady, selective, and highly sensitive detection of Ag⁺. The experimental parameters affecting the fluorescence sensor were investigated and optimized. The optimum conditions included 4 μM Hg²⁺ concentration, 70 μM TAA concentration, solution pH 7 and 5 min reaction time. Under the optimized conditions, the working linear concentration range and the limit of detection for Ag⁺ were 0-12 μM and 0.2 μM, respectively. The proposed method was successfully implied to determine Ag⁺ in water samples.

Keywords: *Graphene quantum dots, turn-on/turn-off, fluorescence probe, thioacetamide, mercury ion, silver ion*

^{xxxiii} Email: sakcha2@kku.ac.th

Composites of graphene oxide and silica gel from rice husk ash adsorbents for removal of methylene blue

Kongsak Pattarith^{xxxiv}

Department of Science, Faculty of Science and Technology, Phranakhon Si Ayutthaya Rajabhat University, Phranakhon Si Ayutthaya 13000, Thailand

ABSTRACT

Methylene blue (MB) is the most common among all other dyes of its category, is generally used in textile industries for dyeing cotton and silk. Adsorption techniques are widely used to remove certain classes of pollutants from waters. The purpose of this work investigates the adsorption of MB onto composites of graphene oxide and silica gel from rice husk ash. The effects of different initial MB concentration and contact time were studied. Adsorption equilibrium was attained within 240 min. Equilibrium data were fitted to the Langmuir isotherm model and the optimum MB removal was found to be 100.45 ± 0.35 mg/g.

Keywords: *methylene adsorption; equilibrium; graphene oxide; silica gel composites*

^{xxxiv} Email: pkongsak@hotmail.com; Tel. +66 3527 6555 - 9, Fax +66 3532 2076

Napier grass stem as a low cost adsorbent for the removal of acid red dye from aqueous solution

W. Tongpoothorn,^{1,xxxv} M. Saenggo¹ and M. Sriuttha²

¹*Department of Chemistry, Faculty of Engineering Rajamangala University of Technology Isan, KhonKaen Campus, KhonKaen 40000, Thailand*

²*Faculty of Applied Science and Engineering, KhonKaen University, NongKhai Campus, Nongkhai 43000, Thailand*

ABSTRACT

Adsorption of acid red dye from aqueous solution onto Napier grass stem, a low cost agricultural material in a batch process was investigated. The adsorption behavior of acid red dye at different contact time, initial dye concentration, solution pH and adsorbent dose were performed. Under optimum conditions as 12 h of contact time, 80 mg/L of initial dye concentration and 0.5 g of adsorbent, it gave the highest percentage of adsorption (88.75%) and adsorption capacity (1.40 mg/g). However, pH of dye solution has not effect on adsorption in this study. The Freundlich isotherm model showed well fitted to the equilibrium adsorption data, indicating multilayer adsorption. The kinetic data were well described by the pseudo-second order. The adsorption process was endothermic with a mean of enthalpy (ΔH) +8.62 kJ/mol and non-spontaneous with a mean free energy of (ΔG) +11.90 kJ/mol. Therefore, it can be used napier grass stem as an alternative adsorbent for removal of acid red dye solution. Additionally, it was added value of this plant as well.

Keywords: *Napier grass; acid red dye; adsorption*

^{xxxv} *Email: aammytt@hotmail.com; Tel. +66-817177347*

Molecular dynamics simulation study of binary mixture solution

Byung Ho Park,¹ Hui Zhang,² Daming Gao,² and Chan Kyung Kim¹

¹Department of Chemistry and Chemical Engineering, Center for Design and Applications of Molecular Catalysts, Inha University, 100 Inharo, Nam-gu, Incheon 22212, Korea

²The Chemical and Material Engineering Department, Hefei University, 373 Huangshan Road, Hefei, China

ABSTRACT

Molecular dynamics (MD) simulation has been studied for describing various natural phenomenon by using classical mechanics. Binary mixture solution is an adequate system for molecular dynamics simulation because it has only two simple solvent molecules. The purpose of this study is to provide theoretical insights into binary mixture solution. First, initial coordinates were generated by using the Amorphous Cell, a module for creating initial point for MD simulations by packing molecules in a defined region. Initial coordinates were generated according to the solution mole fraction.

In the case of ethanol - water mixture, the number of water molecules was fixed to 500 and the number of ethanol molecules were varied according to the mole fraction. Each initial volume was also defined by computing the liquid density and compared with the experimental densities of binary mixtures.[1,2] After minimizing the initial coordinates with the Forcite MD module, the next simulations were carried by using the previous output as new input coordinates files. Two properties, Radial Distribution Functions (RDFs) and Self-diffusion Coefficients, were obtained by analysis of MD simulation trajectories. All molecular dynamics simulation were carried by using the Material Studio 7.0 package.[3] The COMPASS force field was used throughout the simulations. All MD simulations were performed under the periodic boundary condition (PBC) in constant pressure. Temperature was set to 298K by using Berendsen thermostat. For the 2.0 ns trajectories, the snapshot of the coordinates was taken every 1.0 ps. The structures obtained from the MD simulations were compared with those from quantum chemical calculations.

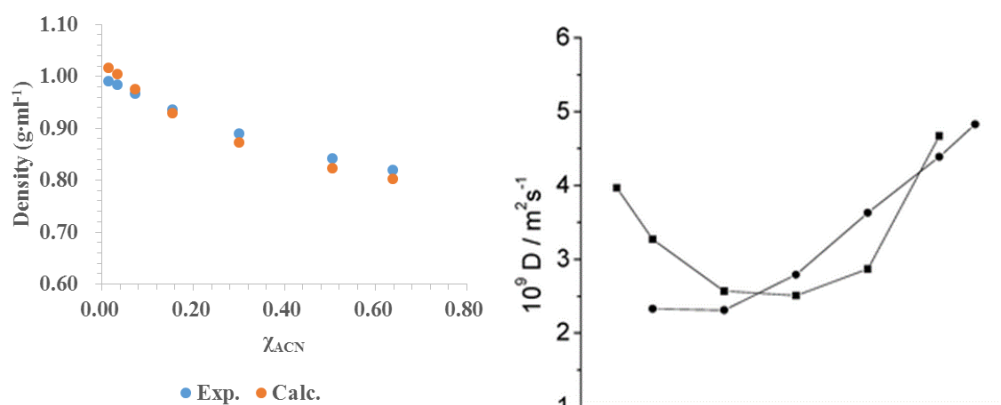


Fig. MD results for H₂O-MeCN binary system

ACKNOWLEDGEMENTS: This work was supported by Inha University and the BK21 Plus Program.

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Structural studies on the binary solvent mixture: Propionic acid-water system

Young-Min Kwon,¹ Hui Zhang,² Daming Gao,² and Chan Kyung Kim¹

¹Department of Chemistry and Chemical Engineering, Center for Design and Applications of Molecular Catalysts, Inha University, 100 Inharo, Nam-gu, Incheon 22212, Korea

²The Chemical and Material Engineering Department, Hefei University, 373 Huangshan Road, Hefei, China

ABSTRACT

Propionic acid, one of the smallest carboxylic acids, is widely used in industry. It is a very useful reactant for production of various chemicals such as amide, ester, and halide derivatives. It has a good solubility with water. In pure solvent, a number of small clusters exist in the liquid phase including a stable dimer. When propionic acid is mixed with water to form a binary solvent system, the number of homo- and hetero-clusters increases rapidly. The structures of these clusters are quite diverse. In particular, the clusters of solvent molecules can influence various physical and chemical properties of the solvent. Therefore, it is necessary to understand the cluster structures in order to study chemical reaction and physical phenomena in a binary mixture.

In this work, several clusters in the propionic acid-water binary system were studied using the B3LYP/6-31+G(d) level of theory. Especially, we calculated all the possible isomers of homo-dimers and -trimers of propionic acid and water, respectively, and hetero dimers and trimers of propionic acid-water mixture. All calculations were performed by using the Gaussian 09 package.

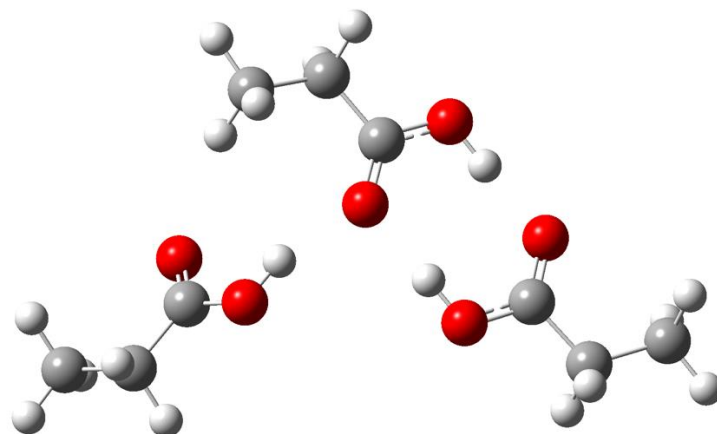


Fig. 1. Propionic acid trimer

ACKNOWLEDGEMENTS: This work was supported by Inha University and BK21 plus project.

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The structure feature of ZnO@e-HNbWO₆ nanocomposite and its photocatalytic performance

Lifang Hu,^{1,2} Rui Li,² Jie He^{2,xxxvi}

¹ School of Earth and Environment, Anhui University of Science and Technology, Huainan, 232001, China;

² School of Chemical Engineering, Anhui University of Science and Technology, Huainan, 232001, China;

ABSTRACT

ZnO@e-HNbWO₆ nanocomposite was prepared by exfoliation-restacking method through HNbWO₆ nanosheet and ZnO nanoparticle sol. The as-prepared materials were characterized by means of X-ray powder diffraction (XRD), scanning electron microscopy (SEM), Fourier transform infrared (FT-IR) spectroscopy, and UV-visible diffuse reflectance spectroscopy (UV-vis DRS). The photocatalytic activity of the as-prepared materials was evaluated by degradation for methylene blue under visible light irradiation. The results show that there is an obvious interaction and synergistic effect between host HNbWO₆ nanosheets and guest oxide ZnO nanoparticles. Due to this synergistic effect, the host-guest crosslinking had an effect on electronic coupling and the transfer of photo-generated electron in the photocatalytic process, and result to the catalysts had good photocatalytic activity for degradation of methylene blue visible light irradiation

Keywords: HNbWO₆ nanosheet; ZnO nanoparticle; Structural features; synergistic effect; Photocatalytic activity

^{xxxvi} Email: jhe@aust.edu.cn, Tel.: +86 554 6668520, Fax: +86 554 6668520

Dislocation structure and work hardening of $L1_2$ -Ni₃Al intermetallic compound

Chang-Suk Han^{xxxvii}

*Dept. of ICT Automotive Engineering, Hoseo University
Hoseo-ro 79beon-gil, Baebang-Myun, Asan City, Chungnam 31499, KOREA*

ABSTRACT

Temperature dependence of stress-strain curves and dislocation structures were studied in a temperature range between 77 and 500 K. Increase in dislocation density in the early stage of deformation is noted and is correlated with rapid work hardening observed at high temperatures. The origin of the anomalous strengthening of the structure-sensitive character is discussed on the basis of these observations. The strengthening at 77 K is explained by dislocation interactions that produce long and straight dipole loops of screw and mixed characters on primary (111) slip planes. The observed rapid increase in dislocation density at 500 K is correlated with the rapid work hardening by taking account of the shortening of the edge segments linked to immobile screw dislocations. An extremely fine slip was noted after deformation at 500 K, indicating that the usual Frank-Read source is not operative at high temperatures due to the strong Kear-Wiltsdorf (KW) locking.

Keywords: *Temperature dependence, Stress-strain curve, Dislocation structure, Work hardening*

^{xxxvii} *Email: hancs@hoseo.edu, Tel: +82 41 5409542;*

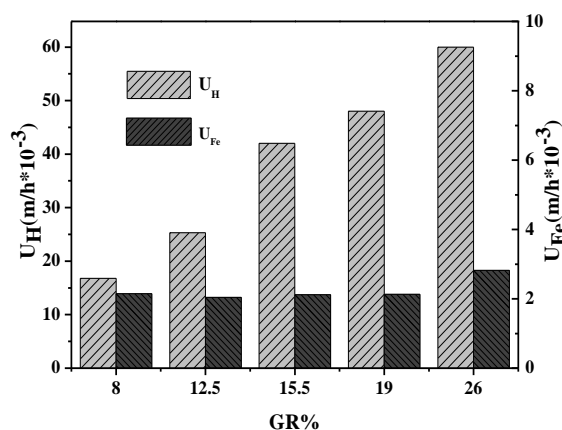
Branched polymer based on PVA for acid recovery via diffusion dialysis

Congliang Cheng, Xianhai Hu, Wengzong Xu, Jin Liu^{xxxviii}

School of Material and Chemical Engineering, Anhui Jianzhu University, Hefei 230022, PR China

ABSTRACT

Branched polymer named as allyltrimethylammonium chloride (TMA) was grafted on Polyvinyl alcohol (PVA) chain by free radical polymerization in water. A series of branched polymer hybrid membranes are prepared with branched polymer and Tetraethoxy-silicone (TEOS) acted as a cross-linking by sol-gel reaction. The obtained membranes were characterized with ion exchange capacity (IEC), water uptake (W_R), linear expansion ratio (LER), tensile strength (TS), elongation at break (Eb), thermal decomposition temperature (Td) and initial decomposition temperature (IDT), acid resistance etc. Their diffusion dialysis (DD) performances are tested with a simulated feed containing 0.81M HCl + 0.18M FeCl₂. Research shows that diffusion dialysis coefficient (U_H) is between 0.0168-0.060 m/h and the separation factor (S) is in 7.8-22.5, which are better than commercial membrane DF-120 (0.009 m/h for U_H , 18.5 for S). As long as the grafting rate is appropriate, anion exchange membrane with excellent performance for diffusion dialysis can be obtained and the preparation process is basically green and simple.



Dialysis coefficient of hydrochloric acid (HCl) and ferrous chloride (FeCl₂) for different graft ratio of hybrid membranes

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^{xxxviii} Email: ccl8888858@163.com. Tel.: +86 (551) 63513136

Positive effects of Al³⁺ partially substituted by Co²⁺ cations on the catalytic performance of Co_{1+x}Al_{2-x}O₄ (x=0-0.2) for methane combustion

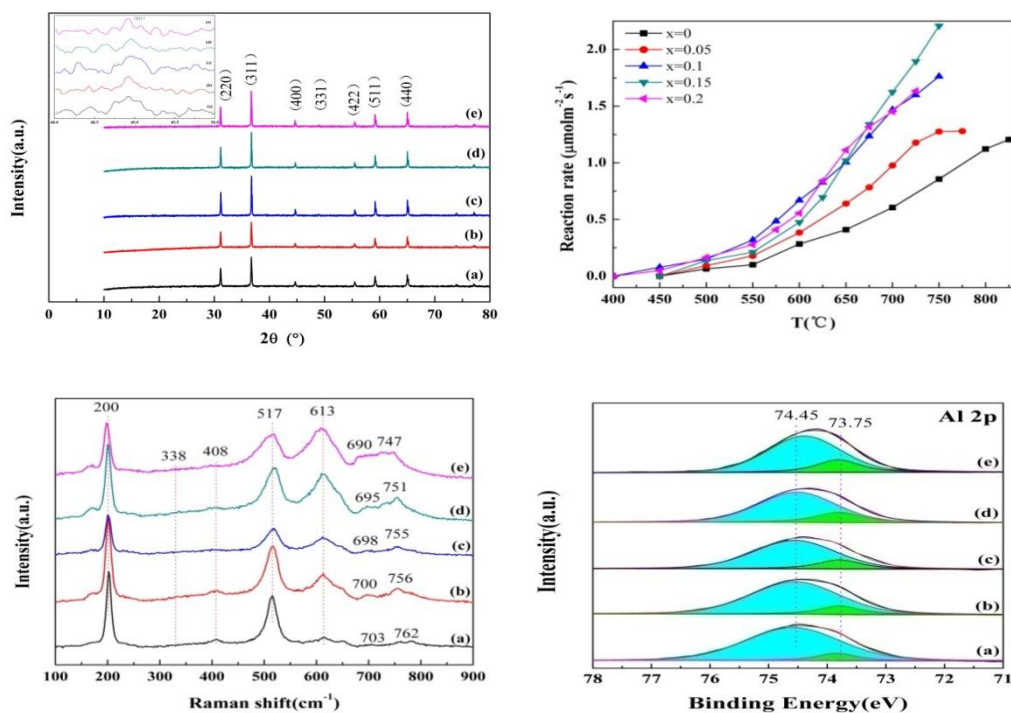
Weiwei Zha, Zhenghui Zhou, Donglin Zhao and ShaojieFeng*

School of Materials Science and Chemical Engineering, Anhui Jianzhu University, Hefei, Anhui, 230601, China

ABSTRACT

Co_{1+x}Al_{2-x}O₄ (x=0-0.2) catalysts were prepared by sol-gel method using citric acid as a chelating agent calcined at 1100°C and then investigated for methane combustion. The catalytic activity of CoAl₂O₄ was significantly enhanced after Al³⁺ partially substituted by Co²⁺ cations in methane combustion. X-ray diffraction showed that all the Co_{1+x}Al_{2-x}O₄ (x=0-0.2) samples displayed a spinel-type single phase. Raman spectroscopy deduced that Al³⁺ partially substituted by Co²⁺ cations created structural defects and lattice distortion, which was indicated to be favorable for the formation of oxygen vacancy and weakening the bond strength of Al-O. X-ray photoelectron spectroscopy revealed that the excellent catalytic activity for methane combustion may be attributed to the active octahedral coordinated Co³⁺ cations and surface oxygen vacancies.

Keywords: spinel-type oxides; Co_{1+x}Al_{2-x}O₄; oxygen vacancy; methane combustion



ACKNOWLEDGMENTS

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Enriched nitrogen porous organic polymers synthesis and hydrogen storage properties

Wen-Ya Zhou,¹ Jin Liu,^{1,2,xxxix} Rong-Liang Jiang,¹ Zhen Li,² Tai Wang,¹ and Sai-Sai Chen¹

¹Anhui Key Laboratory of Advanced Building Materials, Anhui Jianzhu University, Hefei 230601, P. R. China

²School of Materials Science and Chemical Engineering, Anhui Jianzhu University, Hefei 230601, P. R. China

ABSTRACT

The porous organic polymers (POPs) mainly composed of light elements such as C, N, O and have light skeleton density, which can be synthesized with different monomers and many methods. POPs have extensive application in the gas storage and separation etc. with its high specific surface area and special pore structure becoming the research focus of porous materials. In our works, enriched nitrogen porous organic polymers (ENP) were derived from melamine (MA) and terephthalic-aldehyde (TA) by solvothermal reaction via Schiff reaction (Fig.1a). The effects of reaction conditions (time, feed ratio and temperature) and reaction medium on the polymerization of microporous polymers were studied. And the structure and hydrogen storage properties were characterized by infrared spectroscopy (IR), scanning electron microscope (SEM), and the N₂ adsorption and hydrogen storage analyzer. The results show that the melamine and terephthalic-aldehyde without catalyst, formed by solvothermal method is aldehyde amine structure (-N-CR₁R₂-N-) and not to the imine (>C=N-). The hydrogen storage properties of different ENP were determined to hydrogen storage analyzer (FineSorb-3110). Among all the samples of ENP, when the monomer molar ratio was 2:3 (amine: terephthalic-aldehyde), the BET specific surface area was 389m²/g, and the structure of ENP exhibit "microporous-mesoporous-macroporous". Hydrogen uptake capacity of ENP23 was 9.02wt.% at 298K, 5MPa. (Fig.1b)

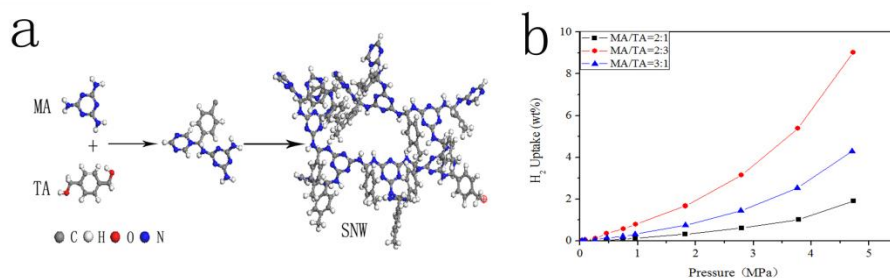


Fig.1 a: synthesis of highly ENP scheme; b: ENP H₂ adsorption at 298K, 5MPa

ACKNOWLEDGMENTS

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^{xxxix} Email: liujin@ahjzu.edu.cn

Zirconium metal-organic frameworks UIO-66(H₂ADC) with 9, 10-dicarboxylic acids anthracene as ligand synthesis and hydrogen storage properties

Sai-Sai Chen,¹ Sheng-Bao Xiao,¹ Jin Liu,^{1,2,xl} Zhen Li,² Jiong Xu,¹ and Xin-Cui Wang¹

¹Anhui Key Laboratory of Advanced Building Materials, Anhui Jianzhu University, Hefei 230601, P. R. China

²School of Materials Science and Chemical Engineering, Anhui Jianzhu University, Hefei 230601, P. R. China

ABSTRACT

Metal-organic frameworks(MOFs) because of its structure can be designed, light density and high specific surface area, has shown its important application in gas storage and separation. But available of MOFs had not major breakthrough in hydrogen storage. So many researchers try to improve the polar organic ligands, in order to improve the MOFs for hydrogen adsorption. In our works, the new nano-size zirconium metal-organic frameworks (Zr-MOF) UIO-66(H₂ADC) were synthesized with 9, 10-dicarboxylic acids anthracene (H₂ADC) and zirconium chloride by the simple solution method and solvothermal reaction. Its structural was studied by powder X-ray diffraction (PXRD) and infrared (IR) spectroscopy. The results showed that UIO-66(H₂ADC) and UIO-66 have the same face-centered cubic (**fcu**) topology from PXRD pattern and structural model and its structure is octahedral (Fig. 1A). What's more, the influence of different feed ratio on the structure of UIO-66(H₂ADC) was studied and when the feed ratio was 1:1.2 (metal: organic linker) named UIO-66(H₂ADC)-1.2, the crystallinity and BET specific surface area of the obtained MOFs were the best among all feed ratio. Specific surface area of UIO-66(H₂ADC)-1.2 was 432m²/g and that average pore diameter was 4.38nm belonged to mesoporous. The storage hydrogen properties of UIO-66(H₂ADC) were determined to high-pressure hydrogen storage analyzer (FineSorb-3110). Hydrogen uptake capacity of UIO-66(H₂ADC)-1.2 was 13.86wt%, 5.45wt%, respectively, at 77K and 298K, 5MPa according to the hydrogen adsorption isotherm (Fig. 1B). When considering of unit the specific surface area adsorption (USSAA) at 77K and pressure up to 1.8MPa¹, UIO-66(H₂ADC)-1.2 was 0.118 mg/m², but UIO-66 was 0.025 mg/m², which shown UIO-66(H₂ADC) have good hydrogen uptake capacity.

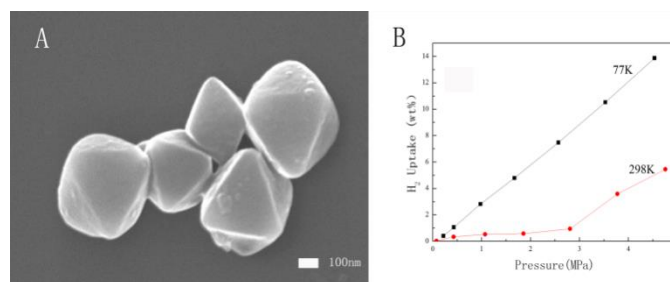


Fig. 1. A: SEM image of UIO-66(H₂ADC); B: UIO-66 (H₂ADC) -1.2 hydrogen adsorption curves.

ACKNOWLEDGMENTS

This work was financially supported by the Natural Science Foundation of China (NO.21171004), and the Science and Technology Project of Anhui Province (1604a0802113), and Anhui Province Academic Technology Leader Training Funded Projects.

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^{xl}Email: liujin@ahjzu.edu.cn

Hydrogen storage properties of new highly cross-linked polymers derived from chlorinated polypropylene and polyethylenimine

Sai-Sai Chen,¹ Jin Liu,^{1,2,xli} Sheng-Bao Xiao,¹ Zhen Li,² Wen-Ya Zhou,¹ Jiong Xu,¹ and Xin-Cui Wang¹

¹Anhui Key Laboratory of Advanced Building Materials, Anhui Jianzhu University, Hefei 230601, P. R. China

²School of Materials Science and Chemical Engineering, Anhui Jianzhu University, Hefei 230601, P. R. China

ABSTRACT

Compared to traditional metal-based hydrogen storage materials, the porous cross-linked polymer materials have a low density, high specific surface area, structure design and other characteristics. What's more, non-aromatic hydrocarbon polymers in contrast to the aromatic cross-linked polymers have good structural stability and higher polar. In our works, the new highly cross-linked polymer derived from chlorinated polypropylene (CPP) grafting polyethylenimine (PEI) was synthesized by hydrothermal amination reaction (Fig. 1). The influence of different reaction conditions on the structure and properties of high cross-linked polymer and effects of different conditions on the synthesis were studied. Structure of the polymers named CPP-g-PEI were characterized by Fourier transform infrared (FT-IR) spectroscopy, elemental analysis (EA), ¹³C solid-state NMR (¹³C-NMR), thermogravimetric analysis (TG), scanning electron microscope (SEM) and specific surface area ultrafine pore size analyzer. CPP-g-PEI had honeycomb-like pores (Fig. 2a) that belongs to the mesoporous at the pore average size 5.37nm in range from 2 to 50nm and thermally stable up to 250 °C. N content of CPP-g-PEI had increased after hydrothermal amination reaction. The hydrogen storage properties of different CPP-g-PEI were determined to hydrogen storage analyzer (FineSorb-3110), and among all the samples, CPP-g-PEI-2 could be achieved the highest 11.26wt% and 22.68wt% at 77K, 5MPa and 7MPa (Fig. 2b), while at 300K, 7MPa, was up to 4.77wt%. But CPP-g-PEI_{OH} obtained higher hydrogen uptake was 2.47wt% at 300K, 5MPa. BET specific surface area was not associated with hydrogen storage capacity, which shown the results of BET specific surface areas and hydrogen uptake. In summary CPP-g-PEI have good structural stability and hydrogen storage properties.

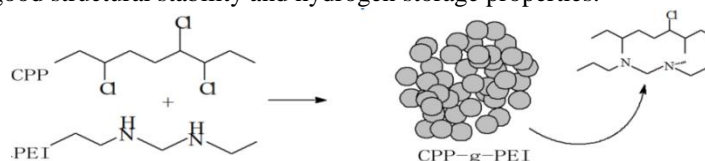


Fig. 1 Synthesis of highly cross-linked polymer CPP-g-PEI scheme

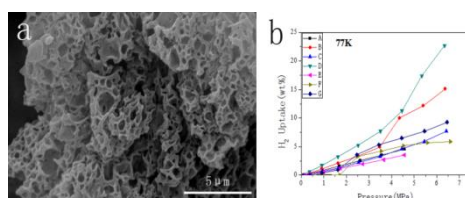


Fig. 2a: SEM image of CPP-g-PEI-1; b: H₂ adsorption properties at 5 and 7MPa: A- CPP-g-PEI_{Cl}; B- CPP-g-PEI_{OH}; C- CPP-g-PEI-1 ; D- CPP-g-PEI-2 ; E- CPP-g-PEI-3 ; F- CPP-g-PEI-4 ; G- CPP-g-PEI-5.

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^{xli}Email: liujin@ahjzu.edu.cn

Synthesis and stability of liquefied MDI with low viscosity

Tai Wang,¹ Zhen Li,^{1,2,xlii}; Jin Liu,^{1,2} and Sai-Sai Chen¹

¹Anhui Key Laboratory of Advanced Building Materials, Anhui Jianzhu University, Hefei 230601, P. R. China

²School of Materials Science and Chemical Engineering, Anhui Jianzhu University, Hefei 230601, P. R. China

ABSTRACT

Polyurethane elastomer (PUE) is an important applied polymer of containing urethane groups, which is synthesized through step-growth addition polymerization of polyol, the diisocyanate and the chain extender as reaction monomers. The superior performance of PUE is given by the unique microphase separation structure and design of structure, so it is widely used in national defense and national economy in all areas. The diphenyl methane diisocyanate (MDI) is the important hard segment monomer of PUE. However, MDI is solid at room temperature, and this will result in poor operability of the room temperature polymerization. Meanwhile, the synthesis of prepolymer have large viscosity and unstable. Therefore, it is significant to study the MDI liquefaction and keep its reaction property without change. In this paper, the low of viscosity liquefied MDI monomer prepared by polypropylene glycol and MDI, which can be replaced high toxicity isocyanate monomer, harm the environment, such as toluene diisocyanate (TDI). The effects of temperature, feed ratio and other factors on the viscosity and NCO content of liquefied MDI were studied (Fig.1), in addition, the change of the micro rheology over time of liquefied MDI was also studied (Fig. 2). Through the optimization of experimental conditions, the viscosity of liquefied MDI reached 310mPa s and NCO content reached 18%, and with the time increase the viscosity and NCO content changed little, from the perspective of rheology can be seen liquefaction MDI is relatively stable. All in all, at room temperature liquefied MDI can be applied synthetic casting polyurethane elastomers.

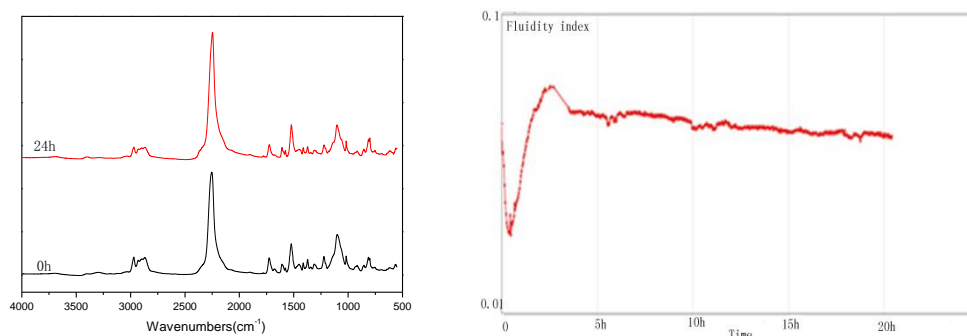


Fig. 1 FTIR spectra of liquefied MDI **Fig. 2** Rheolaser MASTER of liquefied MDI

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^{xlii} Email: zhen-li@yeah.net

A facile route to synthesis ternary type Cu₂O quantum dots/graphene-TiO₂ nanocomposites to the improved photocatalytic effect

Dinh Cung Tien Nguyen,[†] Kwang Yeon Cho[‡] and Won-Chun Oh^{†,xliii}

[†] *Department of Advanced Materials Science & Engineering, Hanseo University,*

Seosan, Chungnam, Korea, 356-706

[‡] *Korea Institutes of Ceramic Engineering and Technology, Soho-ro, Jinju-Si, Gyeongsangnam-do, Korea*

ABSTRACT

The novel material Cu₂O quantum dots/graphene-TiO₂ composite was successfully synthesized by using a facile hydrothermal method. During the hydrothermal reaction, loading of Cu₂O and TiO₂ particles onto graphene sheets were achieved. The obtained Cu₂O quantum dots/TiO₂ composite photocatalysts are characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray (EDX) analysis, transmission electron microscopy (TEM), Raman spectroscopy, and ultraviolet-visible (UV-vis) diffuse reflectance spectroscopy (DRS). The degradation of rhodamine B (RhB) was observed by measuring the decrease in the concentration by UV spectrophotometer. Furthermore, the quantum dot size of Cu₂O is promising to enhance the photocatalytic activity of Cu₂O quantum dots/graphene-TiO₂ composite in the visible light region.

Keywords: *Cu₂O quantum dots/graphene-TiO₂ composites, hydrothermal, UV-vis DRS, photodegradation, RhB*

^{xliii} *Email: wc_oh@hanseo.ac.kr; Tel: +82-41-660-1337, Fax: +82-41-688-3352,*

Study on the pyrolysis kinetic of larch bark and the characteristics of the produced gas components

Qun Shao,^{xliv} Haosheng Xin, Yuhao Wang

School of Materials and Chemical Engineering, Anhui Jianzhu University, Hefei 230601, China

ABSTRACT

Biomass is the only one renewable source of energy that can provide solid, liquid and gas fuels simultaneously. Pine bark is an important forestry processing waste and a crucial component of the biomass energy. The transform of pine bark into a new renewable energy by a reasonable and clean and efficient processing is of great significance. In this work, the pyrolysis characteristics and pyrolysis products were studied by taking larch bark as an object. In addition, the influence of pyrolysis process on produced composition, the mass loss characteristics and the evolution of gas components in the pyrolysis and combustion process were studied. The kinetic parameters were optimized against data for 30, 40 and 50 K/min heating rates. The pyrolysis mechanism of larch bark was revealed and the pyrolysis kinetics model was established. The optimized parameters were applicable to heating rates beyond those used to generate them.

Key Words: *larch bark, TGA, pyrolysis kinetic, kinetic model, Gas evolution*

^{xliv} Email: qunshao1234567@163.com

Effect of mix proportion and sintering temperature on the characteristics of lightweight aggregate from coal gangue and fly ash

Daosheng Sun,¹ Peng Sun,² Aiguo Wang,¹ Kaiwei Liu^{1,xlv}

¹ Anhui Key Laboratory of Advanced Building Materials, Anhui Jianzhu University, Hefei 230022, China

² Anhui Testing Center For Highway Engineering, Hefei 230051, China

ABSTRACT

Coal gangue and fly ash were used as main raw material to fabricate artificial lightweight aggregate, as well as dolomite powder was selected as a foaming agent. In the paper, effects of coal gangue/fly ash ratio by weight and sintering temperature on mineralogical compositions, porosity, apparent density, compressive strength and internal pore structure of LWA were investigated. The results show that the mineralogical compositions of LWA are cordierite, mullite, anorthite and quartz. The porosity and pore size of LWA slightly decreased whereas the apparent density and compressive strength of its increased, the diffraction peak of mullite increased, accompanied with the diffraction peak of quartz decreased with coal gangue/fly ash ratio from 9:1 to 5:5 at 1250 °C. The porosity of LWA gradually increased and the apparent density of LWA decreased, and then the diffraction peaks of cordierite increased with the increasing sintering temperature. The LWA with porosity of 54.86%, apparent density of 1169kg/m³, pore size of 0.1-1.5mm, compressive strength of 4.78 MPa was prepared with coal gangue/fly ash ratio = 5:5 at 1250 °C for 30 min.

Keywords: *Lightweight aggregate; coal gangue; fly ash; mineralogical composition; physical property*

ACKNOWLEDGMENTS

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^{xlv} Email: sundaosheng@163.com, Fax: +86 551 63828078.

Stable amino siloxane oligomer-linked graphene oxide for the efficient removal of U(VI) and Eu(III)

Dong-Lin zhao^{xlvi}

*Key Laboratory of Functional Molecule Design and Interface Process,
Anhui Jianzhu University, Hefei Anhui, P. R. China, 230601*

ABSTRACT

Stable amino siloxane oligomer-linked graphene oxide composite (PAS-GO) was fabricated by facile cross-linking reactions between graphene oxide (GO) and poly 3-aminopropyltriethoxysilane (PAS) oligomers. The morphology, structure and property of the synthesized PAS-GO composite were characterized. Sorption performance for U(VI) and Eu(III) was studied by a battery of sorption tests in an aqueous system under different experimental conditions. The sorption process was pH and temperature dependent. The maximum sorption capacity of U(VI) and Eu(III) on the PAS-GO at 298 K was 267.11 and 220.41 mg/g, respectively. The PAS-GO could be repeatedly used for more than five cycles with slight degradation of sorption. The modification by -NH₂ increased the sorption sites and improved the sorption capacities because of the synergistic effect of chelation with U(VI) and Eu(III). High sorption efficiency and excellent reusability make PAS-GO composites ideal candidates for the removal of U(VI) and Eu(III) from aqueous solution.

^{xlvi} Email: zhaodlin@126.com

Synthesis of graphene oxide-Cu₂Se nanocomposites with enhanced photocatalytic activity

Asghar Ali, Chang Sung Lim, Yonrapach Areerob and Won-Chun Oh^{xlvi}

*Department of Advanced Materials Science & Engineering, Hanseo University,
Seosan-si, Chungnam, Korea, 356-706*

ABSTRACT

In present time, we examined the photo-degradation efficiency of Cu₂Se-graphene nanocomposites synthesized by a facile and fast microwave-assisted technique. The prepared composites were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Raman spectroscopic analysis, XPS and UV-Vis absorbance spectra analysis. The photocatalytic performance was studied through decomposition of Rh B as a standard dye under visible light radiation. Our results indicate that Cu₂Se-graphene composite exhibited significant photodegradation efficiency, which is approximately 95% of Rhodamine (RhB) degradation after visible light irradiation for 180min. It is concluded that the synthesized Cu₂Se-graphene use as a suitable catalyst for dye pollutants.

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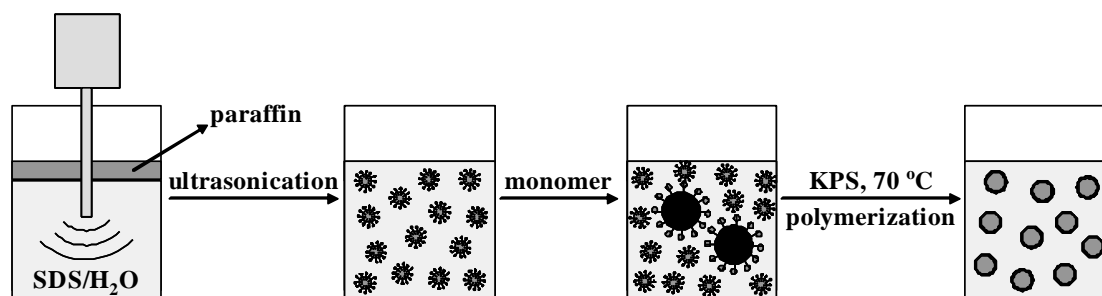
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^{xlvi} Email: wc_oh@hanseo.ac.kr, Tel: +82-41-660-1337, Fax: +82-41-688-3352

Preparation of paraffin/polystyrene nanocapsules via combined miniemulsion/emulsion polymerization

Feng Zhang*, En-tian Cui, Gui-hua Hou, and Qin-fang Zhang^{xlvi}

Key Laboratory for Advanced Technology in Environmental Protection of Jiangsu Province, Yancheng Institute of Technology, Yancheng, Jiangsu 224051, China



ABSTRACT

Paraffin/polystyrene (PSt) nanocapsules were prepared via a novel combined miniemulsion/emulsion polymerization. At first, miniemulsion with paraffin minidroplets dispersed in aqueous solution of sodium dodecylsulfate (SDS) was prepared. Then, styrene was added to the miniemulsion and the monomer droplets served as monomer reservoirs for the polymerization taking place in the minidroplets. Phase separation occurred during the polymerization and polymer shell was gradually formed around the paraffin minidroplets. The prepared paraffin/PSt nanocapsules were characterized by TEM, FTIR and DSC. The TEM and FTIR results demonstrate successful preparation of nanocapsules. The DSC curve of the prepared paraffin/PSt nanocapsules is similar to that of pure paraffin, indicating the microencapsulation does not influence the phase change behavior of paraffin.

^{xlvi} Email: zhangfeng.yc@gmail.com, Fax: +86-515-882827

Chemiluminescence and dual-switchable fluorescence sensing research of metal-organic frameworks

Ming-Hua Xie,¹ and Xiu-Li Yang

¹Key Laboratory for Advanced Technology in Environmental Protection of Jiangsu Province, Yancheng Institute of Technology, Yancheng, 224051

ABSTRACT

A 3D Metal-Organic Framework with remarkable chemiluminescence and dual-switchable fluorescence sensing properties was presented. An anthracene derivative with polyaromatic structure was employed as the linker to construct the 3D framework with direct POCL property, which represent the first example of direct chemiluminescent MOFs, while indirect CL can be achieved by the Lewis acidity of coordination unsaturated metal ions. Additionally, under the instruction of DFT calculations, the energy transfer between the linker and guest can be systematically modulated by varying the excitation wavelength, which resulted the observed dual switchable fluorescence sensing. The research has shown an alternative way in exploring optical MOFs, which will push forward the development of multifunctional MOFs.

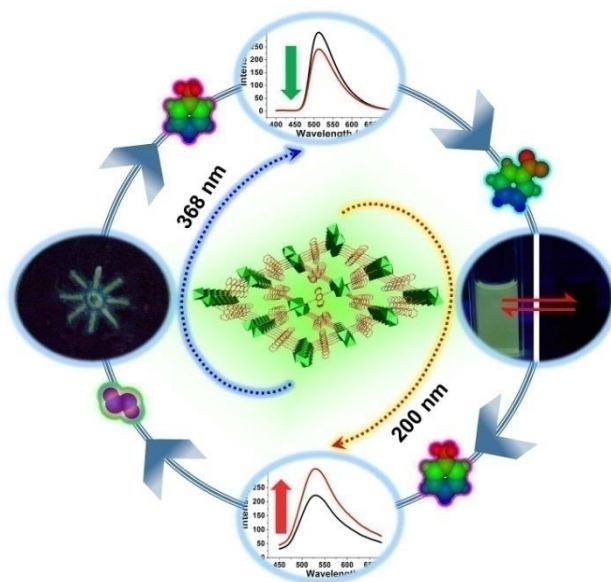


Fig. 1 Schematic illustration of the direct chemiluminescence and dual-switchable fluorescence sensing

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Porous metalloporphyrinic frameworks: Heterogeneous catalysis for CDC reaction and styrene epoxidation

Xiu-Li Yang,^{1,*} and Ming-Hua Xie

¹Collaborative Innovation Center for Ecological Building Materials and Environmental Protection Equipments, Yancheng Institute of Technology, Yancheng, 224051

ABSTRACT

Three metalloporphyrin octacarboxylates with different central metal ions were synthesized, which were used to construct porous metalloporphyrinic frameworks containing 3D nanopore cage or nanotubular channels by reacting with Cu^{II} or Zn^{II} under solvothermal conditions, respectively. The topologies and catalytic activities of the frameworks are highly dependent on the species of the central metal ions and the. The metalloporphyrinic frameworks were used as efficient heterogeneous catalysis for the CDC reaction and styrene epoxidation, the excellent catalytic activity originates from the immobilization of free accessible metal ions onto the pore surfaces. By forming frameworks, the porphyrin moieties showed enhanced catalytic activities and can be protected from suicidal self-oxidation. This research implies that incorporation of metalloporphyrin molecules is an effective and promising way in preparing biomimetic catalyst.

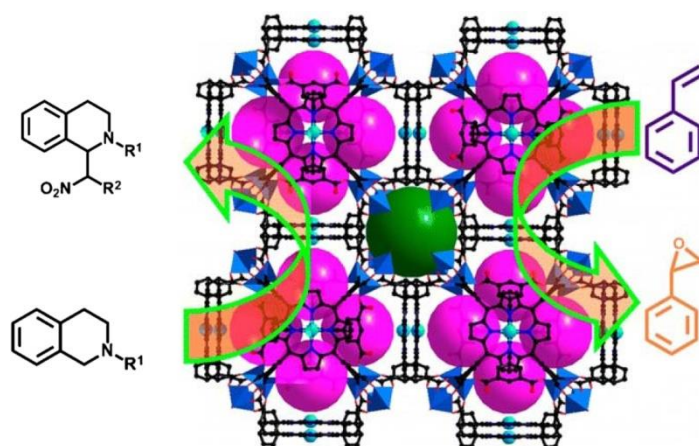


Fig. 1 Schematic illustration of the catalytic activities of the metalloporphyrinic frameworks

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Research on synthesis and hardening mechanism of C3S2 cement for new low - carbon Portland cement

Gui-Hua Hou, Hai-Lin Chen, Bi-Ming Dai, Bao Lu, Xiao-Jiao Gao, Qin-Fang Zhang

*Key Laboratory for Advanced Technology in Environmental Protection of Jiangsu Province,
Yancheng Institute of Technology, Yancheng, 224051*

ABSTRACT

High-energy consumption and exhaust emissions are two bottleneck items for the Portland Cements as the high content of CaO occurs in cement clinker. Therefore, it has important significance to study low-calcium cement clinker mineral and its hardening methods. Based on the preliminary works on different mineral phase types and corresponding structures of pure calcium silicate, this project mainly focuses on the research of $3\text{CaO}\cdot 2\text{SiO}_2$ (C3S2) synthesis conditions and its carbonation- hardening mechanism. Firstly, the synthesis conditions of C3S2 will be studied. Then carbonization process of C3S2 under the effect of CO_2 , hydration reaction induced by carbonization and their collaborative relationships are investigated. Consequently, the carbonization reaction kinetic equation of C3S2 is established. Furthermore, we will study the species, morphology, and crystal structure characterizations of carbonization products and observe the change regularity between porosity of hardening cement and carbonization time. The hardening processes and model by carbonization of C3S2 is concluded and established. The specific theoretic mechanism of this process is tried to find through the study above, and the durability of hardening test block is studied in typical use environmental conditions. On this basis, we preliminary study the differences on burnability, macro-properties and cement clinkers with different compositions which are mainly C3S2 and partially $2\text{CaO}\cdot \text{SiO}_2$ (C2S) . Thereby the novel cement clinker composition with features of low heat consumptions, low carbon dioxide emission and autogenously pulverization under calcination could be obtained. The novel cement can also absorb large amounts of carbon dioxides when it is hardening through carbonization. This may carve out a new way for low-carbon energy saving cement.

Keywords: *Low-carbon Portland cement; Saving energy cement; Cement carbonation- hardening*

Fabrication of hollow C@Co₃O₄@graphene composite anode for long-life lithium-ion batteries

Lu Yue,^a Ning Xu,^a Yang Wang,^a and Wen-Hui Zhang^{a,xlix}

^a Key Laboratory for Advanced Technology in Environmental Protection of Jiangsu Province, Yancheng Institute of Technology, Jiangsu 224051, China

ABSTRACT

Hollow C@Co₃O₄@graphene composite with hollow carbon core and graphene outer layer is fabricated. The nanocomposite exhibits high reversible capacity, good rate capability at high current densities and long-life performance, and retains a high capacity of 861 mAh g⁻¹ at 500 mA g⁻¹ after 700 cycles, making it a promising anode material for lithium-ion batteries.

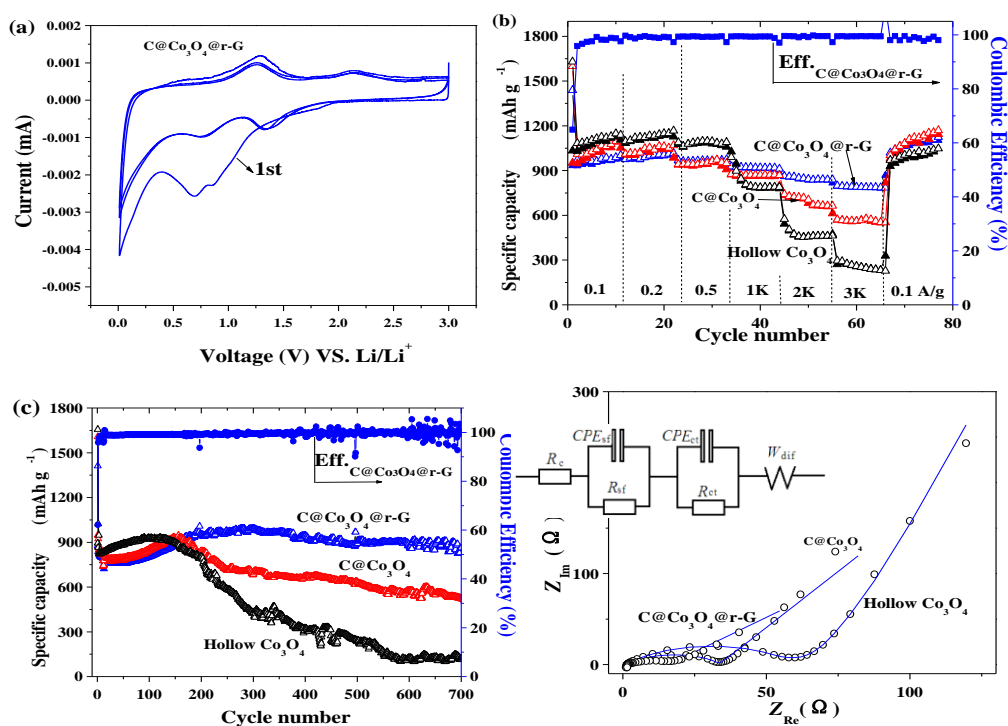


Fig. 1 (a) CV curves of C@Co₃O₄@r-G electrode in 0.01–3.0 V at a scan rate of 0.2 mV s⁻¹; (b) Rate performance of the electrodes; (c) Long-term cycling performance of the electrodes at 0.5 A g⁻¹; (d) EIS of the electrodes after 200 cycles; the spots correspond to the experimental data, the solid lines stand for the calculated data from the equivalent circuits in Figure 1d inset.

^{xlix} Email: zwhuizi000@sina.com, Tel./fax: + 86 051588298925

Controllable preparation and performance of WO₃ films

Pengyu Dong, Hao Tian, Xinguo Xi, and Guihua Hou

Key Laboratory for Advanced Technology in Environmental Protection of Jiangsu Province, Yancheng Institute of Technology, Yancheng 224051, China

ABSTRACT

In this paper, precursor was prepared by a sol-gel method using ammonium metatungstate, polyvinyl alcohol, and secondary deionized water as raw materials, then WO₃ porous films were prepared by spin coating process. The as-prepared samples were characterized by Thermo gravimetric-differential thermal analysis (TG-DTA), X-ray powder diffraction (XRD), scanning electron microscopy (SEM), Specific surface area analysis (BET). TG-DTA data showed that monoclinic phase was formed at 440 °C from amorphous phase for the pure WO₃ dry gel, while the monoclinic phase was formed at 480 °C for the WO₃ dry gel with polyvinyl alcohol as pore forming agent. Therefore, the WO₃ dry gel was calcined at 500 °C in this work. XRD data indicated that the monoclinic WO₃ films using the reagents as raw materials were successfully obtained by sol-gel, spin and calcining process. SEM images showed that the as-prepared samples had a pore structure, and the particle size was around 2-4 μm, and the pore size was about 2-4 μm. BET analysis showed that the specific surface area of WO₃ synthesized using polyvinyl alcohol as pore forming agent was larger than that of pure WO₃, because it had more pore structure. Finally, the photocatalytic activity of the samples was measured by degradation of methylene blue under the visible light irradiation. The results of photocatalytic degradation showed that the photocatalytic activity of WO₃ synthesized using polyvinyl alcohol as pore forming agent was higher than that of pure WO₃ sample.

Excellent visible light photocatalytic properties of novel graphene based CdLa₂S₄/TiO₂ heterojunction nanocomposite

Lei Zhu and Rong Shao

Key Laboratory for Advanced Technology in Environmental Protection of Jiangsu Province, Yancheng Institute of Technology, Yancheng, 224051

ABSTRACT

This paper introduced one pot method for the synthesis of hybrid CdLa₂S₄-graphene/TiO₂ nanocomposite. The generation of reactive oxygen species were detected through the oxidation reaction from 1,5-diphenyl carbazide (DPCI) to 1,5-diphenyl carbazone (DPCO). It is found that the photocurrent density and the photocatalytic effect increase in the case with the modified CdLa₂S₄. From the photocatalytic results, the excellent activity of CdLa₂S₄-graphene/TiO₂ nanocomposite for degradation of methylene blue (MB) and Texbrite BA-L (TBA) under visible irradiation could be attributed to both the effects between photocatalysis of the supported TiO₂ and charge transfer of the graphene nanosheet, and the introduction of CdLa₂S₄ to enhance the photogenerated electrons.

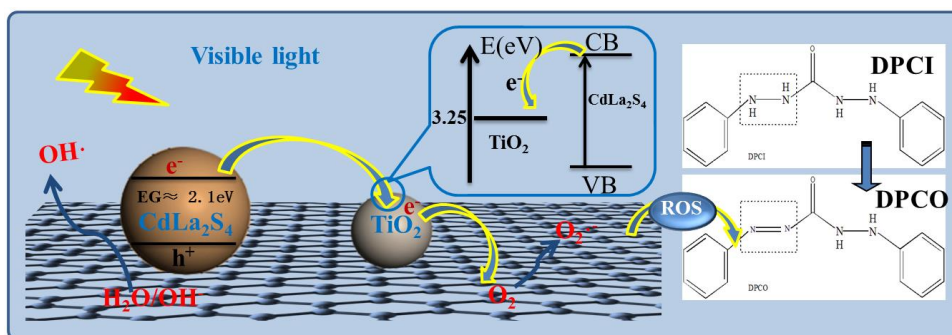


Fig. 1. Schematic drawing of photocatalytic degradation MB, TBA dyes and ROS generation on the interface of CGT sample under visible light irradiation.

Microwave sol-gel derived MMoO₄ (M=Ba, Ca, Sr) nanoparticles doped with Er/Yb, Ho/Yb, Ho/Yb/Tm and their upconversion photoluminescence properties for biomedical applications

Victor Atuchin,^{1,2,3,4} Maxim Molokeyev,^{5,6} Hee Kook Park,⁷ Beom Hyun Lee,⁷ Dong Min Won,⁷ Won-Chun Oh,⁷ and Chang Sung Lim^{7,1}

¹Laboratory of Optical Materials and Structures, Institute of Semiconductor Physics, SB RAS, Novosibirsk 630090, Russia

²Functional Electronics Laboratory, Tomsk State University, Tomsk 634050, Russia

³Laboratory of Semiconductor and Dielectric Materials, Novosibirsk State University, Novosibirsk 630090, Russia

⁴Institute of Chemistry, Tyumen State University, Tyumen 525003, Russia

⁵Laboratory of Crystal Physics, Kirensky Institute of Physics, SB RAS, Krasnoyarsk 660036, Russia

⁶Department of Physics, Far Eastern State Transport University, Khabarovsk 680021, Russia

⁷Department of Advanced Materials Science & Engineering, Hanseo University, Seosan 356-706, Republic of Korea

ABSTRACT

Rare earth-doped upconversion (UC) particles have attracted great interest in recent years due to the luminescent properties and potential applications in products such as lasers, three-dimensional displays, light-emitting devices, and biological detectors¹. The double molybdate compounds with general composition of MR₂(MoO₄)₄ (M: bivalent alkaline earth metal ion, R: trivalent rare earth ion) belong to a group of double alkaline earth lanthanide molybdates. It is possible that the trivalent rare earth ions in the disordered tetragonal phase could be partially substituted by Er³⁺/Yb³⁺, Ho³⁺/Yb³⁺ and Ho³⁺/Yb³⁺/Tm³⁺ ions, and the ions are effectively doped into the crystal lattice of the tetragonal phase due to the similar radii of trivalent rare earth ions of R³⁺, resulted in the excellent UC photoluminescence properties²⁻⁴. In this study, microwave sol-gel derived MR_{2-x}(MoO₄)₄ (M = Ca²⁺, Sr²⁺, Ba²⁺; R = La³⁺, Gd³⁺, Y³⁺) phosphors with suitable doping concentrations of Er³⁺/Yb³⁺, Ho³⁺/Yb³⁺ and Ho³⁺/Yb³⁺/Tm³⁺ ions were successfully synthesized, and the crystal structure refinement and upconversion photoluminescence properties were investigated in detail. The synthesized particles were characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM). Pump power dependence and Commission International de L'Eclairage (CIE) chromaticity of the UC emission intensity were evaluated in detail. The optical properties were examined comparatively using photoluminescence (PL) emission and Raman spectroscopy. These results led to high emitting efficiency and the involved materials can be considered potentially active components in new optoelectronic devices and in the field of luminescent imaging for biomedical applications.

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¹Email: cslim@hanseo.ac.kr

The status of refractive error and general binocular dysfunctions among elementary school children

Jung Un Jang^{li}

Department of optometry, Eulji University, Seongnam, South Korea, 553 Sangseong –daero Sujeong gu Seongnam sr Gyeonggi do 461-713 South korea

ABSTRACT

To assess the prevalence of non-strabismic accommodative and binocular dysfunctions among elementary school children in South Korea, 335 elementary school children (all 8-13 years of age) were given a thorough eye examination including binocular vision testing to determine of objective and subjective refraction, accommodative or binocular dysfunctions.

RESULTS

Table 1 presented the exam results. Of 335 subjects, 64.8% presented some kind of refractive errors, and 16.4% presented emmetropia. 15.8% of the subjects (53 subjects) presented binocular dysfunctions and met the criteria for this study. Of 15.8% subjects, various symptoms were presented (Table 2). The principal symptoms among the subjects were asthenopia, including asthenopia toward the end of the day (11.6%), followed by headache, including headache toward the end of day (3.9%). In addition, 1.8% of the subjects presented blurred vision at distance, 1.5% of the subjects presented intermittent diplopia, and 0.9% of the subjects presented intermittent blurred vision at near.

In this study, only subjects with abnormal symptoms were considered as prevalence of binocular dysfunctions. A breakdown of these results is given in Table 3. Of 53 subjects with general binocular dysfunctions, 30.2% (16 subjects) presented accommodative dysfunctions and 58.5% (31 subjects) presented vergence disorders. 11.3% (6 subjects) had binocular dysfunctions which were combined accommodative and vergence dysfunctions. As can be seen in Table 4, a greater prevalence of accommodative insufficiency (18.9%) was revealed, followed by accommodative infacility (7.1%). Also, convergence insufficiency was the most prevalent, followed by basic exophoria (5.7%), and convergence excess (3.8%).

CONCLUSION

Accommodative and non-strabismic binocular dysfunctions are prevalent in Korean elementary school children, especially convergence insufficiency was the most prevalent. Thus, it is important to diagnose and treat general binocular dysfunctions properly through an accurate and precise eye tests.

Keyword: *Binocular dysfunctions, Binocular dysfunctions symptoms, Refractive error*

^{li}Email: jjju@eulji.ac.kr

Table 1. Characters of subjects

	<i>n</i>	%
Emmetropia	55	16.4
Refractive error	217	64.8
Strabismus	3	0.9
amblyopia	5	1.5
None examinable	2	0.6
Binocular dysfunctions	53	15.8
Total	335	100

Table 2. Prevalence of students' symptoms

Symptoms	No. Subjects	Frequency of occurrence (%)
Asthenopia after 1 or 2 h	24	7.2
Asthenopia toward end of day	15	4.5
Headache	9	2.7
Headache toward end of day	4	1.2
Blurred vision at distance	6	1.8
Intermittent blurred near vision	3	0.9
Intermittent diplopia	5	1.5

Table 3. Prevalence of general binocular dysfunctions

Classification	<i>n</i>	%
Accommodative Dysfunctions	16	30.2
Accommodative insufficiency	10	18.9
Accommodative infacility	5	7.1
Accommodative excess	1	1.9
Vergence dysfunctions	31	58.5
Convergence insufficiency	26	49.1
Basic exophoria	3	5.7
Convergence excess	2	3.8
Combined accommodation and vergence dysfunctions	6	11.3
Combined accommodation and convergence insufficiency	4	7.5
Combined accommodation excess and convergence insufficiency	2	3.8
Total	53	100

A theoretical analysis of corneal transparency

Myung-Hee Lee, Su-Kyung Moon, Young Chul Kimⁱⁱⁱ

Department of optometry, Eulji University, Seongnam, South Korea

ABSTRACT

We investigated the effects of the corneal nano structures, collagen fibril diameters on light transmittance theoretically by using a 3d FDTD (Finite Difference Time Domain) method.

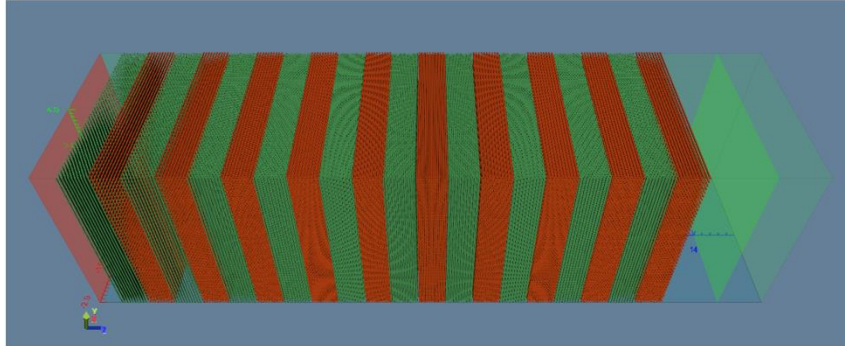


Fig. 1. Simulation Model

We performed comparative analysis of light transmittance with various collagen fibril diameters and structure in this study. We also tried to explain the extraordinary phenomena of high light penetration ratio of the cornea. According to our analysis, an optimized diameter was about 22.5 nm. The results are well corresponding to the real collagen fibril diameter dimension for humans.

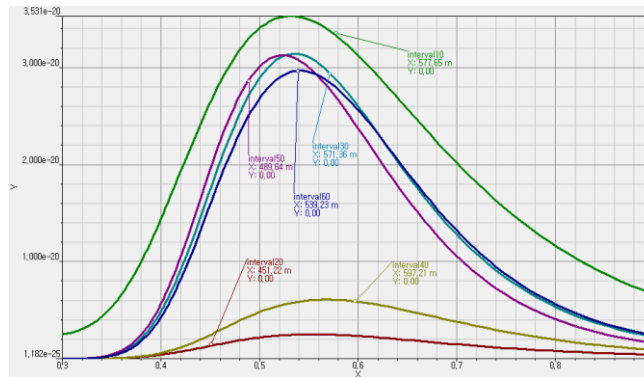


Fig. 2. Output light distribution versus wavelength

ⁱⁱⁱEmail: yckim@eulji.ac.kr

Comparison of thermal property of various ultrathin thermal sheets in the x-y plane direction

Ju Yong Cho,¹ Justin Solomon Manong'a,¹ and Won Kweon Jang^{1,*}

¹Department of Electronic Engineering, Hanseo University, Seosan, 356-706, Korea

ABSTRACT

With the development in the mobile devices, the demand for higher performance is getting intense. Minimizing heat generation and rapid spreading of generated heat are the main technical factors for the higher performance. One of the reasons reducing the reliability of the portable devices depends on how to reduce the spot heat up at the specific components such as microprocessor or battery. The solutions of heatsink and cooling fan cannot be used to avoid degradation of the device due to its volume. Alternative solution is ultrathin thermal sheet having the higher thermal dispersion property in the x-y plane direction. However, this solution has a problem that it is difficult to get the reliable thermal property values of ultrathin sheet with conventional measuring instruments. In this study, we have compared the simulation results of three types of copper, aluminum and graphite ultrathin sheets. The samples have the same dimension of 18 mm × 180 mm and 90 mm × 90 mm and the thickness of 100 μm, 70 μm, 25 μm.

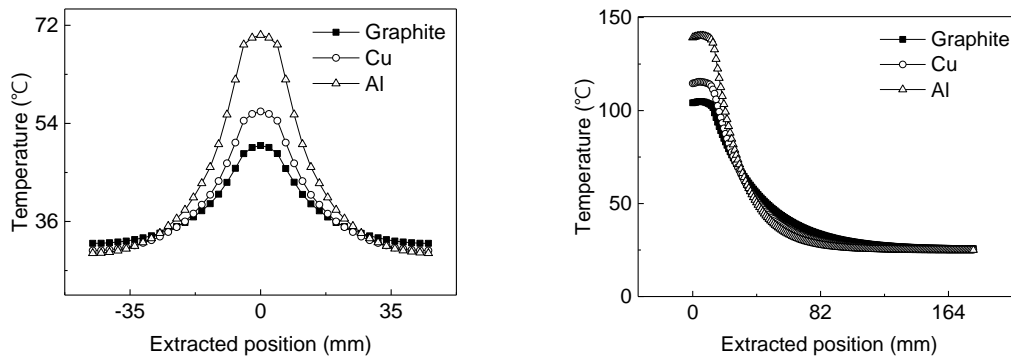


Fig. The temperature distribution on the sheets, (1) 18mm×180mm×100um, (2) 90mm×90mm×100um

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*Email: jwk@hanseo.ac.kr, Fax: +82-41-688-3448

Preparation of Ag-YAG:Ce³⁺-PMMA composite luminescent thin films and fluorescence enhancement

Rongfeng Guan,^{liii} XiaYe, Xianhu Chi, Jialiang Wang, Jinpeng Zhang

Laboratory for Advanced Technology in Environmental Protection of Jiangsu Province, Yancheng Institute of Technology, Yancheng, Jiangsu Province, 224051, China

ABSTRACT

The fluorescent substance, which is distributed on the surface of metal nanoparticles such as gold and silver or its sol, can produce plasma resonance coupling effect in the visible light waveband. The fluorescence emission intensity of the phosphor substance is greatly increased than that of the free state fluorescence emission intensity. In this paper, the yellow rare earth luminescent transparent composite films were prepared by the uniform glue coating method, this composite films is composed of Ag nanoparticles which was prepared used chemical reduction, YAG:Ce³⁺ and PMMA three kinds of mixed materials. The structure, morphology and fluorescence properties of the samples were analyzed by X-ray diffraction (XRD), scanning electron microscope (SEM), ultraviolet visible spectrum (UV-Vis) and fluorescence spectrophotometer; The results showed that the UV-Vis absorption peak of Ag nanoparticle was about 450 nm, the average particle size was 50-100nm, and the resonance absorption peak was located at the position of the fluorescence absorption peak of yellow phosphor YAG:Ce³⁺. The fluorescence emission intensity of the **Ag-YAG:Ce³⁺-PMMA** composite films firstly increases and then decreases with the increase of the doping concentration of nano Ag. When the amount of PMMA was fixed to 2g, the amounts of phosphor were YAG:Ce³⁺=0.2g, 0.3g, 0.4g and 0.5g, respectively, the optimal amount of doping silver was 0.5mg, and the maximum fluorescence enhancement factor was 1.3 times. But when YAG:Ce³⁺=1g, the optimal amount of doping silver was 1mg, the fluorescence enhancement factor was remained at about 1.3 times. The testing results of fluorescence quenching showed that film luminous intensity was lower than composite films of no doping Ag, fluorescence quenching phenomenon occurred, when the amount of silver doped was higher than 4mg in fluorescence power YAG:Ce³⁺=0.2-1g condition.

Keywords: PMMA composite film, YAG:Ce³⁺, Nano Ag, Fluorescence enhancement

^{liii}Email: rongfengg@163.com

Comparison of the electron emission characteristics of W and CNT field emitter for a microcolumn

Anjali Sharma,¹ Ho Seob Kim,^{1,liv} Dae-Wook Kim,¹ Seung Joon Ahn,¹ Tae Sik Oh,¹ and Young Chul Kim²

¹Dept. of information Display, Sun Moon University, Asan-si, Chungnam 336-708, Korea

²Department of Optometry, Eulji University, Seongnam, South Korea

1. INTRODUCTION

A microcolumn has been investigated to apply it as an electron beam inspection or lithography equipment. The processes using electron beam equipment take a long time because of its small field of view and the multi-beam system using multiple microcolumns has been developed to overcome this kind of limitation. In a microcolumn, a tungsten field emitter has usually been adopted as an electron emitter. However, the assembly and the fabrication of a microcolumn with long-term stability is not easy because of either the emission current stability or the difficulties in the alignment procedure of a W tip and the source lens aperture. In this study, we investigated three types of electron emitters and compared their emission characteristics for the application to a microcolumn system.

2. EXPERIMENTS

We have fabricated three types of electron emitters; (i) conventional W field emitter, (ii) a multi-wall carbon nanotube (CNT) emitter, and (iii) two-dimensionally distributed carbon nanotube (2D-CNT) emitter. And three sets of microcolumns have been assembled by adopting these three types of field emitters. The SEM images of the fabricated three types of emitters are presented in Fig. 1.

We have assembled three microcolumns with different field emitters and obtained emission current from each. Fig. 2 presents the I-V curves obtained from each microcolumn; (a) tip current obtained from the microcolumn with W field emitter, (b) with multi-wall CNT emitter, and (c) with 2D-CNT emitter. As expected, the emission current from a multi-wall CNT is much higher than that from a W emitter. Also, the emission current from a 2D-CNT emitter shows the highest value since lots of emitters are activated simultaneously.

The advantage of this 2D-CNT emitter is that it can reduce the difficulty in the column assembly procedure. That is, the alignment of field emitter and the source lens aperture is very easy when we adopt 2D-CNT emitter since the area which 2D-CNT covers is much larger than the area of the source lens aperture. We tried to obtain SEM images using standard Cu grid sample with the microcolumn adopting 2D-CNT emitter and one result is shown in Figure. 3.

3. RESULTS

We have fabricated three types of electron emitters including two dimensionally distributed CNT field emitter and studied their electron emission characteristics in microcolumns. Especially, the alignment procedure is much simple when adopting 2D-CNT emitter, and the preliminary performance result of the microcolumn with this emitter is presented.

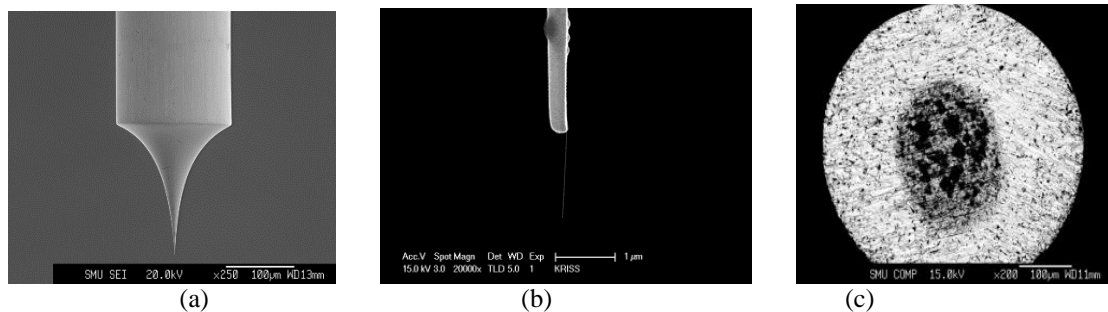


Fig. 1. The SEM images of the three types of field emitters. (a) tungsten (W) field emitter, (b) multi-wall CNT field emitter, and (c) two-dimensionally distributed CNT (2D-CNT) field emitter.

^{liv}Email: hskim3@sunmoon.ac.kr, Phone: +82-41-530-2264, Fax: +82-41-530-2260,

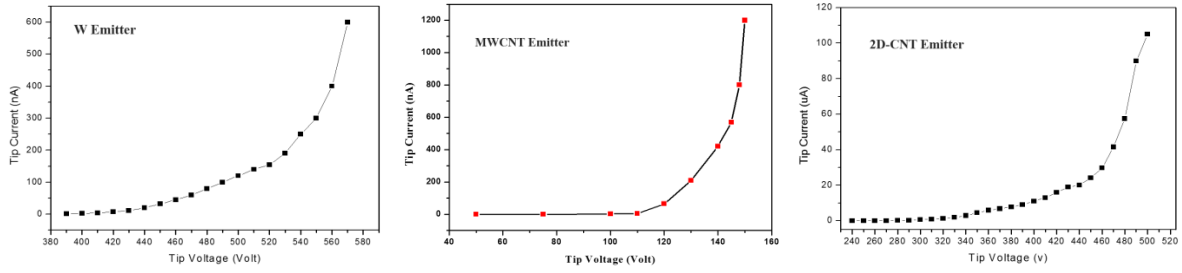


Fig. 2. Comparison of electron current emitted from the three types of field emitters. (a) tungsten (W) field emitter, (b) multi-wall CNT field emitter, and (c) two-dimensionally distributed CNT (2D-CNT) field emitter.

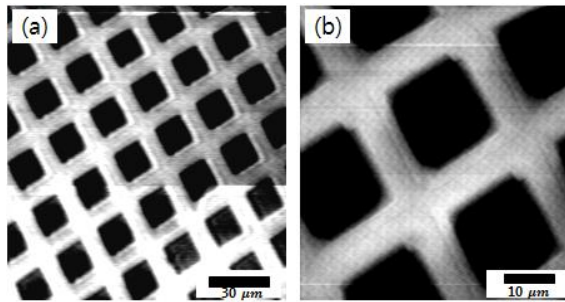


Fig. 3. Typical results of sample current images obtained with obtained with 2D-CNT microcolumn using a standard Cu grid

Physical and strength properties of matrix using red mud and water eluted from red mud

Yong Lee,^a Seungho Lee,^a Heontae Kim,^a Sangsoo Lee^{lv}

^a *Department of Architectural Engineering, Hanbat National University, Daejeon, 305-719, Korea*

ABSTRACT

As the use of fossil fuels as a source of energy has rapidly increased throughout the world since the industrial revolution in the 18th century, the amount of greenhouse gas which is generated artificially has increased greatly, causing the rise of the greenhouse level of the earth. Especially, among the greenhouse gas release, the ratio of carbon dioxide is 80%. Meanwhile, the construction industry in South Korea is an environmental hindrance which causes 42% of the entire carbon dioxide emission, 30% of the entire industrial waste, and 60% of the illegal waste, and it necessitates technical development for reducing carbon dioxide and environmental load. Accordingly, securing economic feasibility and reducing environmental load through the development of cement replacement material are being required. Therefore, in this study, an experiment was performed to draw the adequate ratio through a research on ternary hardening body using industrial byproducts of blast furnace slag, red mud, and fly ash of combined heat and power plant. An experiment replacing blast furnace slag and red mud was done as an advanced test, and fly ash of combined heat and power plant was added to adequate replacement ratio drawn. The experiment hardened blast furnace slag using high CaO contents of said fly ash without using alkali accelerator in order to reduce dosage of activator. Addition ratio of said fly ash was selected as 20, 30, 40, 50, and 60 (%); it revealed lower strength than Plain before addition ratio of the fly ash became 40% but it revealed higher strength in 40% hardening body than Plain; and then, it showed strength of gradually lowering. Liquidity showed a tendency to be lowered pursuant to addition ratio because absorption ratio of fly ash of combined heat and power plant was high. Absorption ratio showed a tendency to be lowered pursuant to increase in addition ratio of the fly ash but density showed a tendency to be heightened.

^{lv} *Email: sslee111@hanbat.ac.kr*

Synthesis of macromolecular modifiers PEPPTMS by ring-opening polymerization of EPPTMS

Jian Zhang, Xinglong Zhang, Chen Chen, Guojun Cheng^{lvi}

School of Materials Science and Engineering, Anhui University of Science and Technology, Xueyuan Road, Huainan 232001, Anhui, China

ABSTRACT

Coupling agent is a kind of materials possessing two different properties of functional groups, one is a group that adapts to inorganic and easily react with surface of inorganic; the other is a pro-organic group, which can react with others polymer or result in hydrogen bond dissolved in them. Unfortunately, there are some shortcomings when coupling agent is applied into between organic materials. In this case, the macromolecular modifier or the macromolecular coupling agent is advantageously produced. Macromolecule modifier can form chemical bond with inorganic system. In addition, the flexible structure of macromolecule chain can be combined well with organic material through physical entanglement or chemical bond, thus showing the advantages that small molecule coupling agent can not match. In the present work, a macromolecular modifiers of poly- γ -(2,3-epoxypropoxy) propyl trimethoxy silane (PEPPTMS) was prepared. This modification is an important method for obtaining new polymers with improved properties and therefore increases the scope of its applications. For successful synthesis of PEPPTMS, we take a novel method (Two-Step Feeding, TSF) with anionic ring-opening polymerization system. Fourier transform infrared spectroscopy (FTIR) shows that EPPTMS occurred to ring-opening polymerization, and nuclear magnetic resonance (NMR) confirmed EPPTMS occurred to ring-opening polymerization. Also Thermogravimetric analysis and differential scanning calorimetry were studied thermostability of PEPPTMS. In this work, DMSO acted as a significant role during the reaction and it can accelerate rate of the reaction. KH560 was dissolved in xylene into 250-mL round-bottomed flask-3-neck equipped with a magnetic stirrer for all 5 h at 80 °C under nitrogen. The optimal ratio between monomer and accelerant was 2:0.4. After reaction, the solution was added drop wise into a large excess of methanol, The isolated copolymer was washed with methanol, and the residual solvent of the final product was removed under vacuum at 80 °C for 8 h to yield pure white. The product is a single macromolecular analysed by DSC and TG analysis showed that the system decomposition temperature above 389 °C, which meet the stability of the composite material system machining process. And the polymer molecular weight above 20000 by GPC measurement. Also there is further work to solve the issue of broad molecular weight distribution, it became the focus of our next study. And consider shortcomings of the experiment and the future work needs to be done.

Keywords: EPPTMS, Anionic ring-opening, Second feeding, Macromolecular modifiers

^{lvi} Email: chengguojun0436@126.com

Effect of cationic monomer on flocculation performance of CPAM for slime water

Chuyang Xu,^{1,*} Yanfen Wang,¹ Rongchun Nie,² and Mengting Li

¹College of Materials Science and Engineering, Anhui University of Science & Technology, Huainan 232001, Anhui Province, P.R. China

²College of Chemical Engineering, Anhui University of Science & Technology, Huainan 232001, Anhui Province, P.R. China

ABSTRACT

As a linear high-molecular polymer, cationic polyacrylamide (CPAM) has a range of applications in chemical, power, agricultural and environmental engineering fields. Here, CPAM flocculants were successfully prepared with different cationic monomer by optical initiated polymerization method. The intrinsic viscosity, solid content and FT-IR were evaluated for the synthesized CPAM flocculants. In addition, the flocculation performance of CPAM was also examined for slime water.

Keywords: Flocculation performance, Slime water, Optical initiation, CPAM

*E-mail: rchnie@aust.edu.cn, Fax: +86-554-6668540

Fabrication and characterization of polypropylene and waste rubber powder blends with interfacial compatibilizers

Ji-nian Yang, Jin-bo Zhu, and Guo-xin Ding

School of Materials and Engineering, Anhui University of Science and Technology, Huainan 232001 P.R. China

ABSTRACT

To improve the performances of waste rubber powder filled polypropylene (PP/WRP) blends, two grafted polymers including maleic anhydride (MAH) grafted PP (mPP) and MAH grafted ethylene- α -octene copolymer (mEOC) were added and performed as interfacial compatibilizers. The influences of compatibilizers on the morphological structures, tensile properties and thermal behaviors of PP/WRP blends were carried out carefully. Results showed that interfacial compatibility between PP and WRP was enhanced. After adding compatibilizers, tensile properties of PP/WRP blends were improved. Thermal analysis revealed that, compared to pure PP, the blends were possessed of relative lower peak temperature of melting and degree of crystallinity. Despite of that, the values of activation of energy for blends were higher than that of pristine PP, and there were little variations on their reaction order, still exhibiting the first order reaction during the whole thermal decomposition of samples.

Key words: *Tensile property, Thermal stability, Reaction order, Activation energy*

Influence of Ni²⁺ content on the property of 0.5Ni_xZn_{1-x}Fe₂O₄-0.5CaTiO₃ composite ceramics

Yin Liu,* Chuan-chuang Wang, Yan-yan Zhu, Chen Chen, Qian Cheng, Chang-jue He

*School of Materials Science and Engineering, Anhui University of Science and Technology,
Huainan 232001, China*

ABSTRACT

0.5Ni_xZn_{1-x}Fe₂O₄-0.5CaTiO₃ (0.5 ≤ x ≤ 0.7) composite ceramics are prepared by conventional solid state route. The phase formation, microstructure, dielectric and magnetic properties were investigated by X-ray diffraction, SEM, precision impedance analyzer, and vibrating sample magnetometer, respectively. The results indicated that the composite ceramics are composed of both perovskite phase CaTiO₃ and spinel phase Ni_xZn_{1-x}Fe₂O₄. Dielectric constant and loss tangent of 0.5Ni_xZn_{1-x}Fe₂O₄-0.5CaTiO₃ composite ceramics show dispersion in the low frequency range. The Curie temperature of the dielectric constant shifts to lower temperatures with the increase x content. The saturation magnetization of 0.5Ni_xZn_{1-x}Fe₂O₄-0.5CaTiO₃ composite ceramics increases with the decreasing of x value. It can be seen that in 0.5Ni_xZn_{1-x}Fe₂O₄-0.5CaTiO₃ composites ceramics, 0.5Ni_{0.7}Zn_{0.3}Fe₂O₄-0.5CaTiO₃ composite ceramics has the optimum dielectric property and the saturation magnetization of the composites ceramics increases with the x value decreasing.

Keywords: Ni_xZn_{1-x}Fe₂O₄, CaTiO₃, Dielectric properties

*E-mail: yinliu@aust.edu.cn, Tel: +86-554-6668643

Interfacial performance of SBR/TiN nanocomposites modified by KH-570

Guojun Cheng,^{lvii} Jian Zhang, Chen Chen, and Jinbo Zhu

School of Materials Science and Engineering, Anhui University of Science and Technology, Xueyuan Road, Huainan 232001, Anhui, China

ABSTRACT

Γ -methacryloxypropyl trimethoxy silane (KH-570) was used for surface modification of nano titanium nitride (TiN) particles (nano-TiN). This modification strategy was designed for preparing styrene-butadiene-rubber (SBR)/TiN nanocomposites. The SBR/TiN nanocomposites were characterized by mechanical characteristics, Rubber processing analyzer (RPA), Differential scanning calorimetry (DSC) and HRTEM observations. The substantiated TiN/KH-570 coordination improved the dispersion of nano-TiN in the rubber matrix. It is illustrated that an organic coating layer was formed between modifiers and particles, together with the underwent interact of modified TiN nano-particles by KH-570 and SBR chains during the processing, KH-570 acted as an effective interfacial modifier to improve the dispersion of TiN nano-particles in rubber matrix and strengthen the rubber-TiN interfacial bonding for the vulcanizates. The mechanical properties and thermostability of nanocomposites was largely enhanced by strong interaction between modified TiN and SBR.

Key words: *TiN nano-particles, Silane coupling agent, Surface modification, Interfacial performance*

^{lvii} Email: chengguojun0436@126.com

Preparation and magnetic properties of (1-x) SrFe₁₂O₁₉ / x CoFe₂O₄ composites

Li Zhao, Yin Liu,* Linyi Zheng, Chuanchuang Wang, Yanyan Hu, Qian Cheng, and Chen Chen

*School of Materials Science and Engineering, Anhui University of Science and Technology,
Huainan 232001, China*

ABSTRACT

(1-x) SrFe₁₂O₁₉ / x CoFe₂O₄; 0 ≤ x ≤ 1.0, composites were compared by a conventional solid state route. The results exhibit that no reaction between hexagonal SrFe₁₂O₁₉ and spinel CoFe₂O₄ took place. Relative density of the composite sintered at 1230 °C for 2 h is 97.36%. All of the composites show typical single-phase magnetic behavior, suggesting the existence of exchange coupling. With the increase of CoFe₂O₄ content, the saturation magnetization of specimen sintered at 1230 °C is enhanced from 45.25 emu/g to 64.84 emu/g, which is ascribed to the high saturation magnetization of CoFe₂O₄ and the exchange coupling between SrFe₁₂O₁₉ and CoFe₂O₄. Compared with single-phase CoFe₂O₄, the coercivity is enhanced markedly from 9.71 kA/m to 116.66kA/m. With the increase of temperature, the saturation magnetization and coercivity of specimens are reduced.

Keywords: *SrFe₁₂O₁₉, CoFe₂O₄, Solid state route, Exchange coupling, Magnetic property*

Fabrication and properties of natural rubber/ modified lignocellulose composites

Guoxin Ding,^{lviii} Jinian Yang, Meixiu Guo, and Mingxu Zhang

*College of Materials Science and Engineering, Anhui University of Science and Technology,
Huainan, 232001, P. R. China*

ABSTRACT

Carbon black (CB) has been widely utilized as reinforcing filler in the rubber industry. However, CB is characterized by non-sustainable, of which the source is petroleum. And, it is hazardous and consuming lots of energy during the production of CB. Hence, in recent decade, researchers have paid more attention on the new reinforcing fillers, which could be the partial substitution of CB, and also environmental-friendly and inexpensive. Lignocellulose is a natural fiber composed of cellulose, lignin, hemicelluloses and extractives. To be the reinforcing filler, the cellulose and lignin have been applied widely in the rubber industry. To our knowledge, there were few literatures on the reinforcing effect of lignocellulose in the natural rubber (NR) composites. The modified natural rubber (NR) composites with varied ratio of modified lignocellulose and carbon black (CB) have been prepared. The mechanical property, cure characteristic, morphology and thermal stability of the modified NR composites were studied via various testing techniques. The results revealed that the vulcanizate containing 15 phr modified lignocellulose and 35 phr CB in hybrid system exhibited the optimized mechanical properties. The optimum curing time (T_{90}) of vulcanizates increased, whereas the scorch time (T_{10}) decreased with increasing modified lignocellulose. The modified lignocellulose dispersed well in the rubber matrix, showing the firmly bonding interfaces. It was indicating that the treatment used in our experiments was proper and effective. The thermo-degradation of NR was accelerated in the initial stage while improved the thermal stability at high temperature in the presence of modified lignocellulose.

Keywords: *Natural rubber, Carbon black, Lignocellulose, Morphology, Curing property*

^{lviii} Email: dgx480@163.com

Study the synthesis of AmPAM and discuss response factors

Rongchun Nie*, and Yulong Sun

*College of Chemical Engineering, Anhui University of Science & Technology, Huainan 232001,
Anhui Province, P.R. China*

ABSTRACT

In this work, amphoteric polyacrylamide (AmPAM) was synthesized via photoinitiator as initiator, with the raw material of acrylamide (AM), anionic monomer acrylic acid sodium (AANa) and cationic monomer acryloyl oxygen ethyl trimethyl ammonium chloride (DMC). The result indicates that when monomer ratio of n(AM): n(AANa): n(DMC) was 1: 0.7: 0.2, the intrinsic viscosity of the product was 882 mL/g, the degree of cationic is 10.53%, the degree of anion is 36.84%. FT-IR was evaluated for the synthesized AmPAM and examined for slime water. The results show that the product effect of flocculation experiment is better than other types of polyacrylamide.

Keywords: AmPAM, Photopolymerization, Flocculation effect

*Email: rchnie@aust.edu.cn, Fax: +86-554-6668540

The structure feature of HNbWO₆@ZnO nanocomposite and its photocatalytic activity

Lifang Hu, Yuan Wang, Jie He^{lix}

School of Chemical Engineering, Anhui University of Science and Technology, Huainan, 232001 P. R. China

ABSTRACT

HNbWO₆@ZnO nanocomposite was prepared by exfoliation-restacking method through HNbWO₆ nanosheet and ZnO nanoparticle sol. The as-prepared materials were characterized by means of X-ray powder diffraction (XRD), scanning electron microscopy (SEM), Thermo-gravimetric analysis (TG), Fourier transform infrared (FT-IR) spectroscopy, and UV-visible diffuse reflectance spectroscopy (UV-vis DRS). The photocatalytic activity of the as-prepared materials was evaluated by degradation for methylene blue under visible light irradiation. The results show that there is an obvious interaction and synergistic effect between host HNbWO₆ nanosheets and guest oxide ZnO nanoparticles. Due to this synergistic effect, the host-guest crosslinking had an effect on electronic coupling and the transfer of photo-generated electron in the photocatalytic process, and result to the catalysts had good photocatalytic activity for degradation of methylene blue visible light irradiation.

Keywords : HNbWO₆ nanosheet; ZnO nanoparticle; Structural features; synergistic effect; Photocatalytic activity

^{lix}E-mail: jhe@aust.edu.cn , Tel.: +86 554 6668520, Fax: +86 554 6668520;

Preparation and adsorption properties of fly ash/graphene composites

Qingping Wang, Jiali Liu, Fanfei Min, Jinbo Zhu

School of Materials Science and Engineering, Anhui University of Science and Technology, Huainan 232001, China

ABSTRACT

Fly ash/graphene composites were synthesized by hydrothermal method and sintering process using graphene and KH-550 modified fly ash. Composition, crystal structure and morphology were characterized by X-ray diffraction(XRD), field emission scanning electron microscopy(FESEM), Raman spectrum and FTIR methods. The adsorption degradation of methylene blue was studied by U-V spectrophotometry. The results showed that when pH was 6, the concentration of methylene blue was 100mg/L, the dosage of the composites was 0.10g, the degradation rate of methylene blue by fly ash/graphene composites was the largest.

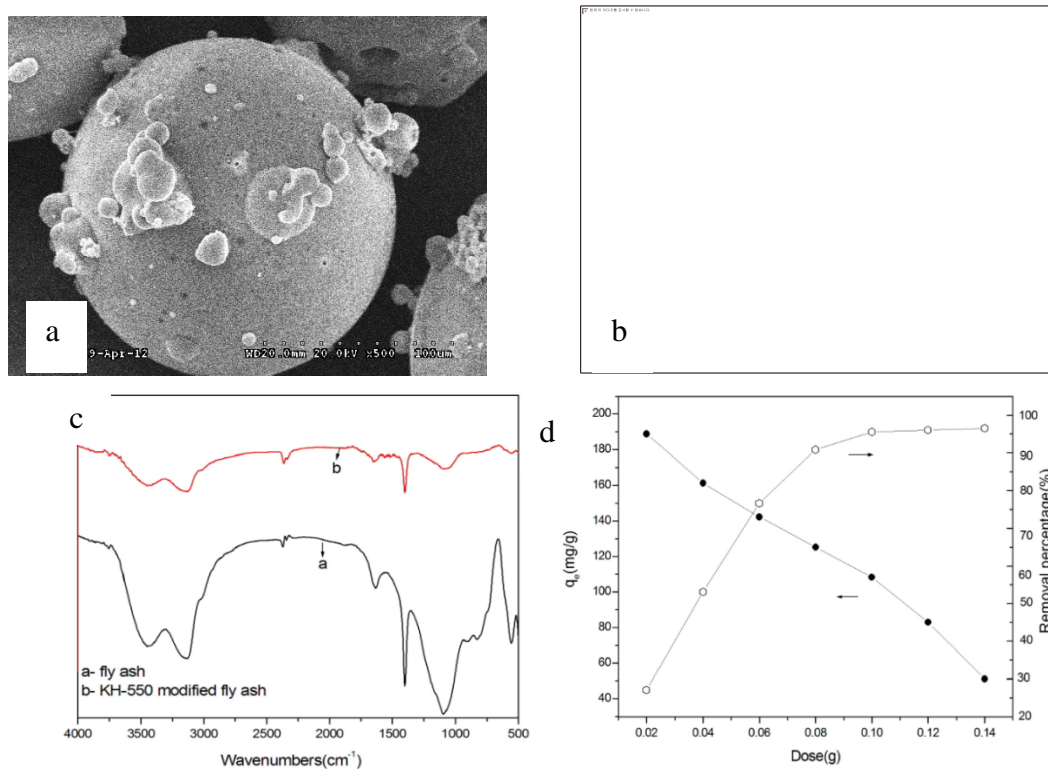


Fig1. (a)SEM image of fly ash (b)SEM image ofKH-550 modified fly ash (c) FT- IR spectra of fly ash (d)The composites dosage on the adsorption effect

Research on preparation of coal waste-based geopolymer and its solidification of heavy metals

Zifang XU,^{lx} Xiuxiang DAI, Juan CHEN

School of Materials Science and Engineering, Anhui University of Science & Technology, Huainan, Anhui, CHINA

ABSTRACT

The limitation of Silica-Alumina raw materials of traditional geopolymers has restricted the development of the immobilization technology of heavy metals. therefore, the performance and mechanism of stabilization/solidification of heavy metals by coal-waste-based geopolymer on were investigated in this paper. Low-calcium fly ash and metakaolin were substituted by coal waste, activated by alkali, the geopolymer with high performance was prepared, and its immobilization of various heavy metals (Co^{2+} , Cr^{3+} , Zn^{2+} , Ni^{2+}) were studied. The results showed that with room temperature of $20^{\circ}\text{C}\sim 25^{\circ}\text{C}$ and the relative humidity of 90%~95%, the optimized ratio of raw materials was that: the ratio of activated coal gangue to high-calcium fly ash was 7:4, mixed with 6.8% of micro-silica fume. The gangue and fly ash were closely surrounded by amorphous polymers. Plenty of scaly products were formed upon the surface of solidified matrix, interlaced with one layer to another, which makes the structure more dense. Synthesizes the compressive strength and the leaching toxicity, the optimum immobilization amounts of Co^{2+} , Cr^{3+} , Zn^{2+} and Ni^{2+} were 1.6%, 2.6%, 2.3% and 1.8%, respectively, with effective immobilization, good stability and long-term safety.

Key words: coal gangue; fly ash; geopolymer; immobilization; heavy metals ions

^{lx}Email: zhfxu@aust.edu.cn , Tel: +86 554 6668649, Fax: +86 554 6668643,

Investigation of material flow and industrial trend of domestic zinc

Kwang-yong Jeong,^a Jin-Koo Han,^a Jar-Myung Koo,^a Kyung-Wan Koo,^b and Soon-Jik Hong^{a, lxi}

^a*Division of Advanced Materials Engineering, Kongju National University*

^b*Department of ICT Automotive Engineering, Hoseo University*

ABSTRACT

Recently, Zinc in various fields of high-tech products, such as industrial and automotive IT is widely used, it has a feature that can improve the performance and quality of the product even with a small amount there is an increasing demand year.

But Zinc has a problem around the world that supply is very limited or, the only store some countries, such as China, Latin America and Africa.

Accordingly, the phenomenon of lack of demand for the Zinc is occurring and has established a variety of related institutions and policies to secure the stockpiles.

In this study, Changes in the resources to the measurement of the consumption and production patterns of the resource through the MFA (material flow analysis), the basic material of zinc, the primary processing products, intermediate products, final products and waste materials collection and recycling irradiation overall It investigated the zinc material flow in Korea.

Due to the MFA (material flow analysis) quantitative analysis of the material flow of national, regional, industry zinc and improves the productivity of resources is expected to be utilized usefully to establish a resource recycling system.

^{lxi} Email: hongsj@kongju.ac.kr

Investigation of material flow and industrial trend of domestic tungsten

Jin-Koo Han,^a Kwang-yong Jeong,^a Ho-Jun Lee,^a Jeong-Gon Kim,^b Soon-Jik Hong^{a,lxii}

^a*Division of Advanced Materials Engineering, Kongju National University*

^b*Department of Advanced Materials Science and Engineering, Incheon National University*

ABSTRACT

It has recently semiconductor, automotive, communications equipment, shipbuilding, petrochemical, machinery, etc. These are all high dependence on common property resources by industries that make the most out of Korea's export manufacturing industry.

Korea has relied on imports for most of the resources, as affected by price fluctuations in the world market as a resource mitigate the effects of the crisis in the industry according to the depletion of resources and establishment parties and the institutions and policies.

Reduce resource consumption of processes within the industry to improve resource productivity in the industry, and the need to promote the recycling of waste material supply resources, and through the institutions and policies are utilized in the industry to be prepared for problems.

In this study, Investigate the overall tungsten is used in a lot of raw materials and basic materials, primary processed products, intermediate products, final products, waste collection and recycling resources industry surveys in Korea.

This makes it possible to efficiently through use and management of resources, and expected to be useful to build the system in the Korea industry.

^{lxii} Email: hongsj@kongju.ac.kr

Measurement of the planar thermal conductivity in the ultrathin thermal sheets

Ju Yong Cho¹, Justin Solomon Manong'a¹, Won Kweon Jang^{1*}

¹Department of Electronic Engineering, Hanseo University, Seosan, 356-706, Korea

ABSTRACT

Recently the thickness of thermal sheet in various mobile devices such as the cellular phone and gear watch are being thinner to be applied to more convenient appliance. Thermal conduction in the core communication devices is getting more important because the larger data processing with higher frequency consumes higher power. The planar thermal conductivity is an important property factor in characterizing thermal sheet capacity.

Various portable devices demand higher thermal conductivity of ultrathin thermal sheet in x-y plane to avoid the device heating up and degradation. Thermal generation from electronic components can be minimized with thermal sheets such as copper, aluminium and graphite sheet which have the high thermal properties. Graphite sheet of ultrathin thickness has been reported as the outstanding thermal conduction in x-y plane direction. However, there is not a proper instrument for the ultrathin thermal sheets to evaluate the quantitative thermal property. The conventional method has not been used for thinner than 100 micron

In this paper, the direct contacted type has been studied to measure the thermal conductivity of ultrathin thermal sheet in the x-y plane direction based on Resistance Temperature Detector(RTD). To exclude the convection effect the sample sheet placed in vacuum. To prove the liability of the proposed algorithm, we compared the thermogram with measured RTD result of the sample.

Key words: planar thermal conductivity, thermal sheet, ultrathin

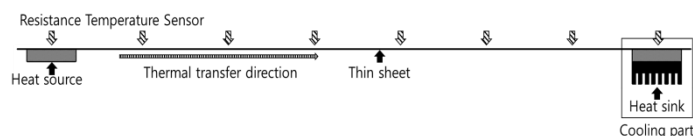


Figure 1. direct contacted algorithm for analysis of thermal property of the thin sheet (side view)

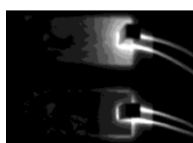


Fig. 2. Thermogram of graphite (upper) and copper sheets (lower)

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*Email: jwk@hanseo.ac.kr; Fax: +82-41-688-3448

Feasibility study of night-soil sludge to use as a fuel and evaluation of its combustion characteristics

Jin Chae Jeong, Sung Bae Jung, Cheol Gyu Kim^{lxiii}

Dept. of Civil and Environmental Engineering, Hanbat National University, Daejeon, 34158, Korea

ABSTRACT

The feasibility study on the night-soil sludge to use as a fuel and its combustion characteristics were carried out in this study.

For this purpose, the analyses of basic properties, such as the element analysis, proximate analysis and analyses of calorific value and the contents of heavy metals were performed. In addition, the isothermal TGA/DTA to identify the combustion characteristics were carried out by using thermal analyzer, and then their activation energy were estimated by using Kissinger, Friedman and Ozawa model. The combustion reaction kinetic equation was also formulated from a reaction order (n) and frequency factor (A) which were derived from the Friedman model equation.

As a result of the feasibility test to use as a fuel, the calorific value of night-soil sludge was approximately 3,500 kcal/kg, implying the ability as a solid refuse fuel source. From the heavy metal content analysis, it was found that it met the quality standard for the solid refuse fuel (SRF) regulation. For volatile matters and combustion index, it showed the value between coal and wood pellet as it had low content of carbon.

To identify the combustion behavior of night-soil sludge, isothermal gravimetric analysis was carried out by measurements of TGA with the various heating rate (5, 10, 15, 20 °C/min) in the air atmosphere. It showed the weight loss by drying in the initial temperature 45-200 °C, then the weight loss by evaporation and burning of volatile matters at 200-400 °C, further weight loss by burning of char at 400-550 °C. Finally the combustion reaction ended at 550-600 °C.

As a result of research on combustion reaction parameters, the activation energy was calculated using the Kissinger, Friedman, Ozawa model equation. The maximum activation energy showed 80.55 kcal/mol, 206.79 kcal/mol, and 199.32 kcal/mol at the temperature of 400-450 °C, respectively. In addition, when the combustion behavior region was divided into two parts as shown in DTG graph, region 1 200-400 °C and region 2 400-550 °C. The reaction order (n) and frequency factor (A) were obtained using Friedman model, it showed that the reaction order (n) was 12.81, and the frequency factor (A) was 4.61×10^{12} in region 1 while the reaction order (n) was 13.63 and the frequency factor (A) was 1.08×10^{18} in region 2, respectively.

Consequently, the night-soil sludge used in this study could be used as a solid refuse fuel. Also, the combustion behavior of night-soil sludge was identified by using isothermal gravimetric analysis, and its combustion reaction parameters were also derived properly in the purpose of this research.

^{lxiii} Email: cgkim@hanbat.ac.kr

Simple and sensitive colorimetric assay system for heavy metals detection in drinking water using microfluidic paper-based analytical devices

Benjawan Ninwong^{lxiv} Sunisa Mohsani and Aseesah Doloh

Department of Chemistry, Faculty of Science and Technology, Nakhon Si Thammarat Rajabhat University, Nakhon Si Thammarat 80280, Thailand

ABSTRACT

The development of a simple, portable assay system using microfluidic paper-based analytical devices (μ PADs) coupled with colorimetric detection for rapid measurements of heavy metals in drinking water was reported. The analytical device constructed by solid wax printing on filter paper. The Fe(II) was detected via reaction of Fe(II) with 1,10-phenanthroline in the red/orange ferriox complex $[\text{Fe}(\text{phen})_3]^{2+}$ formed. For the Ni(II) determination, dimethylglyoxime (DMG) was used to produce bright pink Ni-DMG. In term of the Al(III) detection, analyzed by using cyanidin extracted from red cabbage. The colors in detection zone were immediately changed after dropping the three ions, and the colors changing depended on their concentrations. The color intensities were analyzed by using ImageJ software in gray mode. Under the optimum conditions, the linear range between the color intensity and the concentration of Ni(II), Al(III) and Fe(II) were found to be 1–15 mg/L ($R^2=0.9985$) 0.05–15 mg/L ($R^2=0.9952$) and 0.005–1.0 mg/L ($R^2=0.9975$), respectively. In addition, the limits of detection (LOD) for Ni(II), Al(III) and Fe(II) were found at 1.0, 0.05 and 0.005 mg/L, respectively. It is therefore evident that the developed method can be successfully applied to the determination of metal ions for drinking water samples which the recoveries were in the range of 84–120%. Moreover, the procedure provides rapid, sensitive and selective for metal ions detection in water samples, minimal reagent usage, low cost, and is especially suitable for on-site environmental monitoring.

Keywords: *Metals, Paper-based microfluidic device, Drinking water.*

^{lxiv} Email: ben-benone@hotmail.com; Tel. +66-7537-7443, Fax +66-7537-7443

Numerical simulation on the influence of solidification rate on mechanical properties of semi-crystalline thermoplastic composites

Chol-Ho Hong,¹ and Byeong Sam Kim^{2,lxv}

¹ School of Mechanical Engineering, Hoseo Univ., Asan 31499, Korea

² School of Automotive Engineering, Hoseo Univ., Asan 31499, Korea

ABSTRACT

As with the consolidation time, the cooling rate applied during the solidification stage of the composite processing cycle influences the total processing cycle time, as well as the mechanical performance. By controlling the solidification rate, changes in the matrix morphology and crystallinity can be achieved, and hence different mechanical properties may be obtained. Control of the solidification rate is also important in order to control the level and distribution of internal stresses generated within the part during processing. These stresses may cause the composite to warp, resulting in unsatisfactory part quality, and can lead to premature failure of the part, necessitating costly repair or replacement. Therefore, this chapter emphasizes the necessity of controlling the solidification rate, and examines its influence on the mechanical properties and the dimensional stability of composites based on CF/PA12 commingled yarns. The influence of solidification rate on crystallinity, morphology, and resulting mechanical properties of thermoplastic composites has become the subject of many research investigations over the last decade. Transverse tensile tests were performed to examine the influence of the solidification rate on the mechanical properties of the CF/PA12 laminates based on commingled yarns. In order to study the influence of solidification rate on interlaminar fracture toughness, mode I interlaminar fracture tests were carried out using the double cantilever beam (DCB) method, interlaminar fracture toughness.

Keywords: Mechanical properties, Solidification stage, Numerical simulation, Thermoplastic composites.

^{lxv} Email : kbs@hoseo.edu, Tel: +81-41-540-5814

Simulations on the effect of urea-SCR system on NO_x reduction in diesel engine for responding the EURO-6C

Kyoungwoo Park,^{1,lxvi} Gildong Kim,² Jonghoon Park,² Seong Joon Moon,³ and Ho Kil Lee³

¹*School of Mechanical Engineering, Hoseo University, Asan 31499, Korea*

²*Graduate School of Hoseo University, Asan 31499, Korea*

³*Korea Automotive Technology Institute (KATECH), Cheonan 31214, Korea*

ABSTRACT

In general, diesel engines have higher efficiency but emit more pollutants such as nitrogen oxides (NO_x) and particular matter (PM) than gasoline engines. As the urea water solution (UWS) is injected into the exhaust gas of diesel engine, the understanding of control mechanism of it is become very important research field. Therefore, the studies on the reduction of NO_x emissions from diesel engines have been paid attention in the past decade both numerical and experimental methods. In the present study, major design parameters concerning urea solution injection in front of SCR are optimized by using a CFD analysis and Taguchi method. The computational prediction of internal flow and spray characteristics in front of SCR was carried out by using STAR-CCM+ code that used to evaluate NH₃ uniformity index (NH₃ UI). The adopted design variables (i.e., the number and diameter of the nozzle, injection directions (upper and horizontal), and penetration length) are optimized by using the L₁₆ orthogonal array and small-the-better characteristics of the Taguchi method. As the results of the study, the optimal solutions are obtained both for minimizing the activation time and maximizing the NH₃ uniformity. In addition, we propose a method to minimize wall-wetting around the urea injector in order to prevent injector blocks caused by solid urea loading.

Keywords: *EURO-6C, Diesel engine, Urea water solutions (UWS), Urea-SCR System, Computational fluid dynamics (CFD), Activation time, NH₃ uniformity index, Chemical reactions, Taguchi method.*

^{lxvi} *Email: kpark@hoseo.edu, Tel: +81-41-540-5804*

Numerical simulation on the effect of diffuser on thermal stratification of a thermal storage tank

Gildong Kim¹, Jonghoon Park¹, Chol-Ho Hong², and Kyoungwoo Park^{2,lvii}

¹Graduate School of Hoseo University, Asan 31499, Korea

²School of Mechanical Engineering, Hoseo University, Asan 31499, Korea

ABSTRACT

Efficient and reliable thermal energy storage (TES) system is a key element in solar energy applications and it is well known that the thermal stratification phenomenon in a thermal storage tank (TST) of TES systems has a significant positive effect on its efficiency. For this reason, much research has paid attention to an accurate prediction of heat transfer characteristics in a TST. In the present work, CFD simulations for three-dimensional, transient, and mixed convective heat transfer in a cylindrical-shaped thermal storage tank have been carried out to predict the thermal stratification phenomena and investigate the effects of diffuser configurations and operating conditions on the performance of a solar energy system. The governing equations are solved by using the STAR-CCM+ for turbulent, mixed convection flow based on the Boussinesq approximation. In this simulation, the numerical results on the flow patterns and temperature distributions in a liquid storage tank for various diffuser specifications and mass flow rates are presented. In addition, to quantify the degree of thermal stratification, the thermocline thickness (δ_{th}) and the volume ratio for high temperature region (V_h) are introduced in this work. The results show that a diffuser can enhance the thermal stratification in a thermal storage tank and the performance of the solar energy system is improved compared to that of no-diffuser as a result. It is also shown that the optimum design of diffuser is proposed for the best performance of the TST.

Keywords: Thermal energy storage (TES) system, Diffuser, Thermal stratification, Computational fluid dynamics(CFD), Mixed convective heat transfer, Boussinesq approximation

^{lvii} Email: kpark@hoseo.edu, Tel: +81-41-540-5804

Prediction of the effect of moving conditions on printing quality of a digital textile printing system

Gildong Kim¹, Jonghoon Park¹, Gilwon Lee¹, Kyung Shin², and Kyoungwoo Park^{3, lxxviii}

¹⁾ Graduate School of Hoseo University, Asan 31499, Korea

²⁾ Research Institute, Pyungan FA Co., Daegu 42720, Korea

³⁾ School of Mechanical Engineering, Hoseo University, Asan 31499, Korea

ABSTRACT

Printing quality of a shear-type piezoelectric inkjet printhead is influenced by the nozzle shape, the substrate movement, and distance between nozzle exit and substrate in a high speed of single-pass type DTP (digital textile printing) system. It is also well known that the printing quality is generally dependent on the volume and velocity of main and satellite droplets and break-up time. Therefore, in the present work, the droplet behavior of a piezoelectric actuator is investigated numerically. The transient three-dimensional conservation equations of mass and momentum are solved by the computational fluid dynamics (CFD). The continuous surface force (CFS) model is used in order to predict the effect of surface tension force in the free surface flow. The volume-of-fluid method with the piecewise linear interface construction (PLIC) scheme is employed for tracking the interfacial movement and reconstructing the interface between ink and air. The interaction between the air flow induced by droplet drag and the Couette flow entrained from the substrate movement is also investigated as well as the effect of distance between nozzle exit and substrate.

Keywords: DTP(Digital textile printing), Single-pass type, Shear-mode piezoelectric actuator, Droplet behavior, Computational fluid dynamics (CFD), Two-phase flow, Moving boundary condition, Couette flow

^{lxxviii} Email: kpark@hoseo.edu, Tel: +81-41-540-5804

Aquathermolysis of vacuum residual oil

Hoo-Cheol Lee, Jin Young Ko and Seung-Kyu Park^{lxi}

Department of Chemical Engineering, Hoseo University, Asan 336-795, Korea

ABSTRACT

Heavy crude oil is the oil that has viscosity typically greater than about 100 cP and density greater than 930 kg/m³. Vacuum residual oil has similar viscosity properties since it has high fraction of resins and asphaltenes. The key challenge for upgrading the VR is its viscosity — with viscosities often in the hundreds of thousands and millions of cP, it does not readily flow from the reservoir to the surface. Steam stimulation (huff and puff) is the most popular and effective technology to recover heavy oil in the world. In the steam injection process, the viscosity reduced according to its viscosity–temperature characteristic properties, reduce the flowing resistance through the pore media of reservoir, and increase the yield and production rate [1-4]. Aquathermolysis reactions are relatively non-destructive, as compared to the higher temperature thermal cracking process [4-6]. We have conducted the aquathermolysis reaction of VR at the temperature range of 200-350 °C at above 20 psi pressure.

Key words: *Vacuum Residual Oil (VR), Aquathermolysis, Viscosity reduction*

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^{lxi} Email: skpark@hoseo.edu, Tel : +82 41 5409686, Fax : + 82 41 5405758,

Synthesis of 2-amino-2-methylpropanol

Dong Ho Park, Jin Young Ko, and Seung-Kyu Park^{lxx}

Department of Chemical Engineering, Hoseo University, Asan 336-795, Korea

ABSTRACT

Recently, global warming resulting from the emission of greenhouse gases, especially CO₂, has become a big worldwide concern. Even though various CO₂ capture technologies have been proposed, chemical absorption using aqueous alkanolamine solutions is proposed to be the most applicable technology. Particularly, for the post-combustion power plants, elimination of CO₂ by neutralization reaction with aqueous amine solution seems the most suitable one [1-3]. Currently, mostly common aqueous alkanolamine solutions used in industry are monoethanolamine (MEA), diethanolamine (DEA), 2-di-propanolamine (DIPA), and methyl-diethanolamine (MDEA), etc. Among them, 2-Amino-2-methylpropanol (AMP) is spotlighted for the fast desorption process [2,3]. In this work, we have synthesized AMP by Henry reaction by the reaction of formaldehyde and nitropropanol. 2-Nitro-2-methyl propanol (2-NMP) formed as an intermediate in the Henry reaction. And then consecutive reduction results in the formation of AMP successfully. We are reporting the experimental results in the conference.

Keywords: AMP, NMP, CO₂, Greenhouse

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^{lxx}Email: skpark@hoseo.edu, Tel : +82 41 5409686, Fax : + 82 41 5405758,

Antioxidant effect, according to the extraction time of Pu-erh tea

Jin Young Park, Hye Seon Kim, Hee Su Chae, and Seung-Kyu Park^{lxxi}

Department of Chemical Engineering, Hoseo University, Asan 336-795, Korea

ABSTRACT

Pu-erh tea is a form of black tea which undergoes a special fermentation process for some certain period of time [1-4]. Depending on the fermentation periods, usually for 30 to 40 days or sometimes for years or even for decades, the tea provides a unique flavor and some potential health benefits. Many research results have been reported that the antioxidant actions of pu-erh tea may increase the anti-oxidation effect to human body and then potentially improve the inhibition of tumor growth through a variety of mechanisms. In this work, we are reporting the anti-oxidant effects of pu-erh tea which are prepared by solvent extraction process. We have studied four different anti-oxidation experiments. The antioxidant activity of the pu-erh tea extracts were measured using *in vitro* assays including the reducing power assay and the assay evaluating the free radical scavenging capacity such as the hydroxyl. In this study, we reported an experimental study on the *in vitro* antioxidant activity of various extracts of pu-erh tea depending on different extraction time and methods.

Key words: *Pu-erh tea, Catechin, DPPH, DMPD, ABTS, FRAP*

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^{lxxi} Email: skpark@hoseo.edu, Te : +82 41 5409686, Fax: + 82 41 5405758,

Core-shell structure with color shell for color polymer dispersed liquid crystal device

Jae Yoon Lee and Chul Gyu Jhun^{lxxii}

Department of Display Engineering, Hoseo University, Asan 336-795, Korea

ABSTRACT

Polymer dispersed liquid crystal (PDLC) device can be applied to the switchable windows and other light shutter device. The PDLC has also several advantages such as no polarizer, fast response time, easy fabrication process. However, in PDLC, the materials are usually operated between a transparent state and a scattering state [1]. Therefore, color realization is limited. In this paper, we fabricated liquid crystals droplets by microencapsulation method [2]. Liquid crystal materials of our proposed device are confined in droplets with polymer shell by complex coacervation method using a gelatine aqueous and gum arabic aqueous. Coacervation is the separation into two liquid phases in colloidal systems. It is caused by the interaction of two oppositely charged colloids. In this experiment, we fabricated coloured core-shell structure with the gelatine aqueous and colour pigment in the shell materials [3]. We demonstrate color characteristics of the proposed device.

Key words: *Polymer dispersed liquid crystal, Core-shell structure, Color*

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^{lxxii} Email: cgjhun@hoseo.edu, Tel: +82 41 5405899, Fax: + 82 41 5405618,

Metal-organic-framework-derived two-dimensional ultrathin mesoporous hetero-ZnFe₂O₄/ZnO nanosheets with enhanced lithium storage properties for Li-ion batteries

Linrui Hou*, Hui Cao, Siqi Zhu, and Changzhou Yuan

Anhui University of Technology, Ma'anshan Anhui, P. R. China, 243002

ABSTRACT

Mesoporous hetero-structures have drawn tremendous attentions with inherently unprecedented advantages for advanced Li-ion batteries (LIBs). In this study, we smartly developed a facile metal-organic-framework-engaged synthetic methodology to large-scale fabrication of two-dimensional (2D) mesoporous hetero-ZnFe₂O₄/ZnO nanosheets (ZFOZ NSs) with homogeneously dispersed hetero-nanodomains of spinel ZnFe₂O₄ and ZnO. When evaluated as promising anode for high-performance LIBs, the resultant ultrathin mesoporous hetero-ZFOZ NSs exhibited extraordinary electrochemical Li-storage performance with long-cycling behavior and large reversible capacities at high rates for next-generation LIBs applications, thanks to intriguing synergetic contributions from ultrathin mesoporous architecture and electroactive bi-component hetero-interfaces. More encouragingly, the electrode concept we developed here can be easily generalized to rational design and synthesis of other mesoporous hetero-hybrids with excellent lithium capacities for LIBs. would be a powerful electrode platform for advanced next-generation supercapacitors.

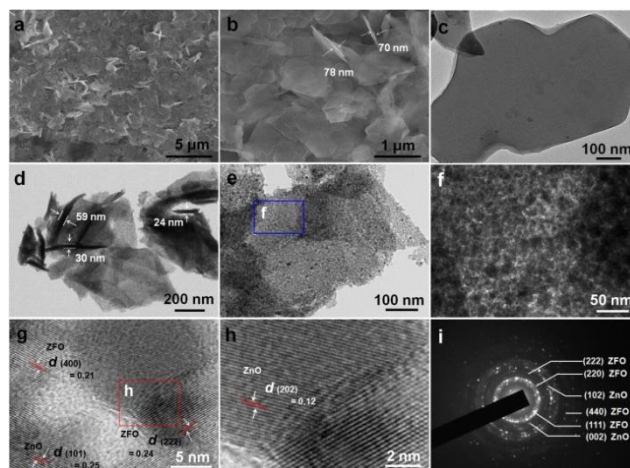


Fig. 1. FESEM (a, b) and TEM (c) images for the ZF-MOFs. TEM (d-f), HRTEM (g, h) images and SAED pattern (i) of the as-obtained mesoporous hetero-ZFOZ NSs

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*Email: houlr629@163.com

Magnesium ammonium phosphate-halloysite/epoxy polymer nanocomposites: synthesis and synergistic flame retardancy

Yanmao Dong,^{1,2,3} Dan Zhao,¹ Xing Zhou,¹ Hao Wu,³ Joseph H Koo³

¹ Suzhou University of Science and Technology, School of Chemistry, Biology and Materials Engineering, 1 Kerui Road, Suzhou, JS 215009, China

²Jiangsu Key Laboratory for Environment Functional Materials, 1 Kerui Road, Suzhou, JS 215009, China

³The University of Texas at Austin, Materials and Science Program, Austin, TX 78712, USA

ABSTRACT

To recycle the nitrogen (N) and phosphorus (P) from waste water, the magnesium ammonium phosphate-halloysite (MAP-HNT) was synthesized using simulated waste water as raw materials. The adsorption-chemical precipitation method was employed to synthesize target products and the optimal conditions for synthesis of MAP-HNT were obtained. The FT-Infrared (FTIR) spectroscopy, Energy Dispersive Spectrometer (EDS), Scanning Electron Microscope (SEM), Transmission Electron Microscopy (TEM) and Thermal Gravity Analysis (TGA) were conducted to characterize the samples. The MAP-HNTs and Exolit[®] OP 1230 (OP) were introduced into epoxy (EP) to prepare the polymer nanocomposites. The Heat Release Rate (HRR) and flammability of epoxy composites were tested by Micro-scale Combustion Calorimetry (MCC) and UL-94 instruments. The mechanical properties of EP composites also were tested by tension testing system. Results indicated that the flame retardancy and mechanical properties of epoxy composites were improved by MAP-HNT. The addition of MAP-HNT and OP gave rise to an evident reduction of HRR and prolonged burning time for epoxy. The EP/MAP-HNT/OP passed the UL 94 V-0 rating. The analysis of the char revealed the synergy of MAP-HNT and OP in reducing the flammability and enhancing the mechanical property of epoxy. Conclusions of this work show a potential application in the wastewater treatment and N/P recycling.

Keywords: *Magnesium ammonium phosphate, Halloysite, Epoxy, Nanocomposites, Flame retardancy*

Bionic titania coating carbon multi-layer material derived from natural leaf and its superior photocatalytic performance

Feng Chen,¹ Zhi-Gang Chen,^{1, lxxiii} Jun-Chao Qian,¹ Cheng-Bao Liu,¹ and Zheng-Yin Wu¹

¹*School of Chemistry, Biology and Materials Engineering, Suzhou University of Science and Technology, Suzhou, China*

ABSTRACT

In recent years, the photocatalytic processes utilized in waste water control, indoor air purifying, dye-sensitized solar cells and other applications have attracted extensive interest among researchers. In this study, bionic titania coating carbon multi-layer material was fabricated by employing canna leaves as a substrate and carbon precursor. Titania nanocrystals were assembled and coated on the natural film, and carbonation treatment under a pure N₂ atmosphere yielded the ultrathin multi-film hybrid material. The novel composite layer structure was fabricated by 8-10 nm titania particles and a carbon layer that was hundreds of nanometers thick. The carbon composite material possessed a highly specific surface area of 248.3 m²·g⁻¹. Under air atmosphere, the natural template transformed entirely into CO₂ and H₂O, and the photocatalytic ability of pure titania is lower than that of the hybrid material. Examination using UV-visible spectrophotometer (UV-vis) of the hydrogen production by photocatalytic splitting of water under visible light irradiation showed that the band gap of the multi-layer material was reduced to 2.75 eV. The H₂ production was about 302 μmol·g⁻¹ and about three times greater than that of the pure bionic TiO₂.

Keywords: *Bionic multi-layer, Titania, Carbon, Photocatalytic performance*

^{lxxiii} Email: czj@usts.edu.cn, Tel: +86-0512-6737-4120, Fax: +86-0512-6737-4120

The effecton analysis of subzero grinder construction to nylon powder granularity

Difang Zhao,* Ming Ding, and Junjun Huang

Department of Chemical and Materials Engineering, Hefei University, Hefei 230601, P.R. China

ABSTRACT

One of the important processing technologies is the deep underzero grinding. Polyamid 12 is the most difficult to process material through mechanical milling. An experimental study was carried out to understand the influence of deep underzero gringder's physical construction on the powder granularity and particle size distribution of polyamide 12. The polyamid 12 powder is produced by anchor type (AT) grinding tool, turbin type (TT) grinding tool and cornona type crushing tool miller. The results indicate that the cornona type(CT) crushing tool miller particles has the high aspect ratio , fine sphericity and low flakiness ratio. The scanning electron microscopy (SEM) images demonstrated that the CT particle shape of the polyamide 12 powder has the smooth edge and potato-like morphology.

Key words: *Deep subzero grinder, Polyamide 12, Particle distribution, Aspect ritio, Sphericity*

Facile controllable synthesis and photocatalytic properties of assembled hierarchical AgBr/Fe₃O₄ microspheres

Jinsong Xie,* Mingxing Nie, Shihao Yin, Junjun Huang, Chengliang Han, Difang Zhao, and Ming Ding

Department of Chemistry and Materials Engineering, Hefei University, Hefei, 230601

ABSTRACT

In the paper, the magnetic Fe₃O₄ microspheres with its average diameter in 200-300 nm assembled from hierarchical structure of 10 nm particles, have been prepared through hydrothermal method by sodium acetate and FeCl₃·6H₂O as raw materials, using glycol as solvent. Then, the AgBr/Fe₃O₄ composite powder was been obtained by ultrasonic precipitation method, by adding hexadecyltrimethyl ammonium bromide (CTAB) and silver nitrate solution into the above formed Fe₃O₄ solution under ultrasonic treatment. Finally, the structures and morphologies of AgBr/Fe₃O₄ composite catalysts were characterized by X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM) analysis. The photocatalytic experimental results show that the composite catalyst has good catalytic degradation ability of methyl orange under visible-light irradiation.

Key words: *AgBr/Fe₃O₄ microspheres, Composite catalyst, Hydrothermal synthesis*

Structural studies on the binary solvent mixture: propionic acid-water system

Young-Min Kwon,¹ Hui Zhang,² Daming Gao,² and Chang Kyung Kim^{1,*}

¹Department of Chemistry and Chemical Engineering, Center for Design and Applications of Molecular Catalysts, Inha University, 100 Inharo, Nam-gu, Incheon 22212, Korea

²The Chemical and Material Engineering Department, Hefei University, 373 Huangshan Road, Hefei, China

ABSTRACT

Propionic acid, one of the smallest carboxylic acids, is widely used in industry. It is a very useful reactant for production of various chemicals such as amide, ester, and halide derivatives. It has a good solubility with water. In pure solvent, a number of small clusters exist in the liquid phase including a stable dimer. When propionic acid is mixed with water to form a binary solvent system, the number of homo- and hetero-clusters increases rapidly. The structures of these clusters are quite diverse. In particular, the clusters of solvent molecules can influence various physical and chemical properties of the solvent. Therefore, it is necessary to understand the cluster structures in order to study chemical reaction and physical phenomena in a binary mixture.

In this work, several clusters in the propionic acid-water binary system were studied using the B3LYP/6-31+G(d) level of theory. Especially, we calculated all the possible isomers of homo-dimers and -trimers of propionic acid and water, respectively, and hetero dimers and trimers of propionic acid-water mixture. All calculations were performed by using the Gaussian 09 package.

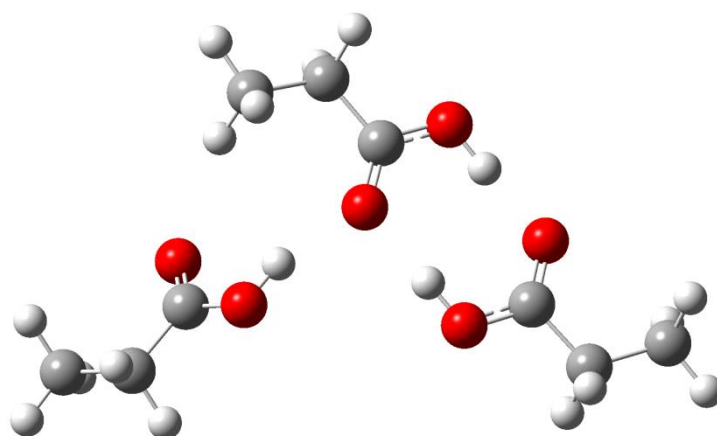


Fig. 1. Propionic acid trimer

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Detection of oxygen species generated of C₇₀-Ag₂Se heterojunction photocatalysts

Ze-Da Meng, Shou-Qing Liu, Feng Chen, Zhi-Gang Chen

Provincial Key Laboratory of Environmental Science and Engineering, College of Chemistry, Bioengineering and Material Engineering, Suzhou University of Science and Technology, Suzhou 215009, China

ABSTRACT

Reactive oxygen species (ROS) can be produced by interactions between sunlight and light-absorbing substance in natural water environment and can completely destroy various organic pollutants in wastewaters. In this study, a novel Ag₂Se-C₇₀ heterojunction photocatalysts were successfully prepared. Surface area and pore volumes of the Ag₂Se-C₇₀ samples showed decrease due to deposition of Ag₂Se. The generations of reactive oxygen species were detected through the oxidation reaction from DPCI to DPCO. The photocurrent density and the PGO effect increase in the case with the modified C₇₀. The PGO effect of the C₇₀ modified with Ag₂Se composites is increased significantly due to the synergetic effect between the C₇₀ and the Ag₂Se nanoparticles.

Keywords: Nanostructures, fullerenes, chemical synthesis, Optical properties, TEM, Catalytic properties

Inhibition studies of α -amylase and α -glucosidase with capsaicin using a molecular docking

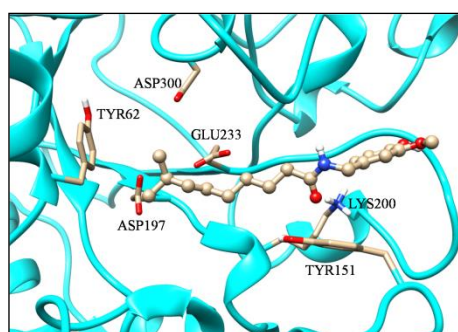
Kultida Thongnum, Saksit Chanthai and Khatcharin Siriwong^{lxxiv}

Materials Chemistry Research Center, Department of Chemistry and Center of Excellence for Innovation in Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand

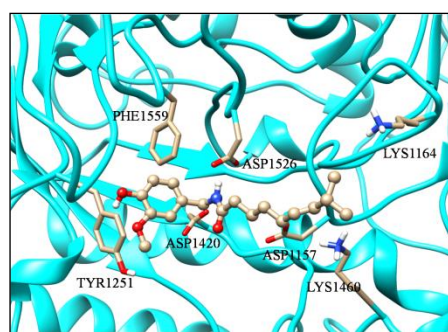
ABSTRACT

Diabetes has become a dangerous disease killing many people. One of therapeutic approach for diabetes disease is to control the blood sugar level by inhibiting the carbohydrate hydrolyzing enzymes which are α -amylase and α -glucosidase. This work aims to investigate the inhibitory activity of capsaicin, which is one of capsaicinoid compounds, on these enzymes using a molecular docking and quantum calculation. Acarbose, a commercial diabetes drug, was also investigated for comparison. The docking results revealed that acarbose yields better inhibition efficiency with binding free energy ($\Delta G_{\text{binding}}$) of about -8.2 to -11.9 kcal/mol, and inhibition constant (K_i) of about 0.0002 to 0.4 μM , whereas capsaicin provided the $\Delta G_{\text{binding}}$ of -5.5 to -6.0 kcal/mol and K_i of 42.3 to 88.2 μM . The summation of binding energies ($\Delta E_{\text{binding}}$) between each inhibitor and amino acids in active site of enzyme obtained from quantum calculation with MP2/6-31G(d,p) level is in agreement with the $\Delta G_{\text{binding}}$, i.e. the total $\Delta E_{\text{binding}}$ of acarbose was larger negative than that of capsaicin. The amino acids interacting with inhibitor as hydrogen bonds mainly contribute to the total binding energy. Nevertheless, it could be concluded that capsaicin has a potential to be developed as an alternative drug for diabetes disease.

Keywords: *Molecular Docking, α -Amylase, α -Glucosidase, Capsaicin, Acarbose.*



α -amylase–capsaicin



α -glucosidase–capsaicin

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^{lxxiv} Email: skhatcha@kku.ac.th, Tel. +66 8 5000 7543, Fax: +66 43 202373

Characterization of bimetallic CoFe supported on HZSM-5 zeolites and their catalytic performance on methanol conversion

Waenkaew Pantupho,¹ Siriphorn Buttha,¹ Arthit Neramittagapong,² Jatuporn Wittayakun,³ and Sirinuch Loiha^{1, lxxv}

¹Materials Chemistry Research Center, Department of Chemistry, Faculty of Science, Khon Kaen University, KhonKaen 40002, Thailand

²Department of Chemical Engineering, Faculty of Engineering, Khon Kaen University, Khon Kaen 40002, Thailand

³Material Chemistry Research Unit, School of Chemistry, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima 30000, Thailand

ABSTRACT

Zeolite ZSM-5 is widely used as catalyst support for petrochemical process due to its intrinsic properties of high thermal stability and shape selectivity. However, the drawback of high acidic strength of the zeolite is observed on the process by observing of high carbon deposition on the catalyst surface with long time operation. This research focus on modification the ZSM-5 based catalysts by addition of iron (Fe) and cobalt (Co) oxides to reduce acidic strength of the parent zeolite. The iron and cobalt oxides are reported as active species for dehydration reaction. The catalytic performance on methanol dehydration to produce dimethyl ether (DME) is investigated. Influenced of metal structure and metal-support interaction on the catalytic performance are interested. Monometallic Fe/HZSM-5 catalysts were synthesized by impregnation (IMP) and hydrothermal (HYD) methods. The bimetallic catalysts of CoFe/HZSM-5_IMP and CoFe/HZSM-5_HYD were prepared using sequential impregnation. The catalyst structures and physicochemical properties were characterized using XRD, FT-IR, N₂-adsorption desorption isotherm and NH₃-TPD techniques. Metal structures on the zeolite were investigated using UV-Vis and EXAFS techniques. The catalytic performance on methanol dehydration was carried on under fixed-bed flow reactor with varying reaction temperature and time. Coke production after long reaction time of 24 h was investigated. The crystalline structure of ZSM-5 zeolite was maintained after FeCo loading. No metal oxide phases of Fe and Co were observed. This result indicated good dispersion of the metal oxides on the zeolite structure. Comparing with the monometallic Fe/HZSM-5, the micropore area and total surface area of CoFe/HZSM-5 were not significantly decreased indicating no micropore blocking by Co loading. Lower acidic amount of the CoFe/HZSM-5 than Fe/HZSM-5 was observed. Different cobalt structures were observed on CoFe/HZSM-5_IMP and CoFe/HZSM-5_HYD. The tetrahedral and octahedral cobalt oxide species were mainly observed on CoFe/HZSM-5_HYD and CoFe/HZSM-5_IMP, respectively. The catalytic performances on methanol dehydration of Fe/HZSM-5 were improved by cobalt loading. Moreover, the structural effect of cobalt on the catalytic selectivity to DME was discovered. The cobalt oxide in tetrahedral form on CoFe/HZSM-5_HYD showed higher selectivity to DME formation than octahedral form on CoFe/HZSM-5_IMP. Both of bimetallic CoFe/HZSM-5 had lower carbon content than monometallic one. Therefore, the bimetallic CoFe/HZSM-5 not only improves the catalytic performance of methanol dehydration but also reduce deactivation.

Keywords: CoFe/HZSM-5, Methanol dehydration, Dimethyl ether, Cobalt structure

^{lxxv} Email: sirilo@kku.ac.th

Cobalt-based 2D and 3D metal-organic frameworks for efficient heterogeneous catalysts of epoxidation and dye photodegradation

Jintana Othong, Jaurusup Boonmak and Sujittra Youngme^{lxxvi}

*Materials Chemistry Research Center, Department of Chemistry and Center for Innovation in Chemistry,
Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand.*

ABSTRACT

Three cobalt-based metal-organic frameworks were successfully synthesized and the synthetic methods play important roles in the formation of complexes with diverse structures. These compounds were characterized by single-crystal X-ray diffraction, IR spectrometry, powder X-ray diffraction, solid-state diffuse-reflectance UV-vis spectrometry and thermogravimetric analysis. Structural determination reveals that compounds **1** and **2** exhibit 2D coordination framework while **3** displays 3D coordination framework with the difference in structural architectures. All compounds were used as heterogeneous catalysts for the aerobic epoxidation of alkene using tert-butyl hydroperoxide (*t*-BuOOH) as oxidant, and the results show that these materials exhibit high catalytic activity as well as good stability. After the reaction, the catalysts can be reused quite easily without loss of its catalytic performance for five cycles. Furthermore, the photodegradation performance of compound **3** with lowest energy band gap was also evaluated for the photodegradation of methylene blue under UV-light.

Keywords: *Metal-organic framework, Epoxidation of alkenes, Heterogeneous catalysis, Cobalt(II), Photodegradation, Methylene blue*

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^{lxxvi} Email: sujittra@kku.ac.th

Single-crystal-to-single-crystal transformation and dyes adsorption of copper metal-organic frameworks

Siriporn Phengthaisong, Jaursup Boonmak, and Sujitra Youngme^{lxxvii}

Materials Chemistry Research Center, Department of Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand.

ABSTRACT

Two new metal-organic frameworks containing Cu(II), 3-sulfobenzoate and 4,4'-bipyridine ligands, were synthesized by solvent diffusion method. Synthetic investigations and structural analyses reveal that compounds **1** and **2** show distinct frameworks with remarkable solvent-directed feature. Compound **1** shows 1D chain structure and these chains are further linked by π - π stacking interactions and hydrogen bonds to form a 3D supramolecular framework. **2** exhibits two-independent infinite 1D polymeric chains that are also linked by hydrogen bonds and C-H \cdots π interactions to form a 3D supramolecular framework. Interestingly, when compound **1** was immersed in water, the structure of **1** transformed to **2** with the color changes from deep blue to violet through the single-crystal-to-single-crystal transformation. However, compound **2** was also prepared directly in aqueous solution by solvent evaporation method. Furthermore, the organic dyes adsorption properties of compound **2** were evaluated and found that compound **2** has a high potential application for Congo red adsorption.

Keywords: *Metal-organic Frameworks, Dyes adsorption, 3D supramolecular, Congo red, Single crystal*

^{lxxvii} Email: sujitra@kku.ac.th

Anions-dependent assemblies of two new cationic Cu-MOFs based on 3,5-diaminobenzoic acid: Syntheses and structures

Theanchai Wiwasuku, Jaurusup Boonmak, and Sujittra Youngme^{lxxviii}

Materials Chemistry Research Center, Department of Chemistry and Center of Excellence for Innovation in Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand

ABSTRACT

Two new cationic metal-organic frameworks (MOFs) (**1**) and (**2**) based on Cu(II) and tridentate aminobenzoic ligand, namely 3,5-Diaminobenzoic acid (3,5-Hdaba) were constructed. Compounds **1** and **2** were obtained by the similar method from the reaction of 3,5-Hdaba ligand with Cu(II) ion containing different counteranions. The structure analyses reveal that compound **1** presents three-dimensional (3D) structure which contains Cu(II) trinuclear secondary building units (SBUs). These SBUs are bridged by 3,5-daba ligands in the $\mu_3\text{-}\eta^2\text{:}\eta^1\text{:}\eta^1$ and $\mu_3\text{-}\eta^1\text{:}\eta^1\text{:}\eta^1$ coordination modes resulting in 3D framework in which counter anions NO_3^- were located in the lattice of framework. Compound **2** exhibits two-dimensional (2D) layer in which Cu(II) ion centers are linked by 3,5-daba ligand in a $\mu_3\text{-}\eta^1\text{:}\eta^1\text{:}\eta^1$ coordination mode forming 2D layers with SO_4^{2-} as counter anions. The difference in structures between **1** and **2** is attributed to the effects of counter anion and the different coordination modes of the organic ligand. Moreover, this study reports the new $\mu_3\text{-}\eta^2\text{:}\eta^1\text{:}\eta^1$ coordination mode found for the 3,5-daba ligand.

Keywords: Metal-organic framework, 3,5-Diaminobenzoic acid, Cu-MOF, Anion, Cationic MOFs

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^{lxxviii} E-mail: Sujittra@kku.ac.th

Synthesis, structural and optical characterization of $\text{Al}_x\text{Zn}_{1-x}\text{O}$ semiconductors

Janvaphon Buaphang, Nithima Khaorapapong, and Sujitra Klinsrisuk^{lxxix}

Materials Chemistry Research Center, Department of Chemistry and Center of Excellence for Innovation in Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand

ABSTRACT

$\text{Al}_x\text{Zn}_{1-x}\text{O}$ ($x = 0.00, 0.05, 0.10, 0.25, 0.50$) semiconductors were synthesized by a simple sol-gel autocombustion method using metal nitrates of zinc and aluminum. Structural and optical properties of the $\text{Zn}_{1-x}\text{Al}_x\text{O}$ samples annealed at 450 °C were characterized by using X-ray diffraction (XRD) spectroscopy, transmission electron microscopy and UV-Visible spectroscopy. The XRD patterns of ZnO semiconductor were assigned to hexagonal Wurtzite structure. The crystallinities of the Al-doped ZnO samples were decreased with the increase of the Al^{3+} content. The spectral absorption analysis showed that the optical band gap energy (E_g) for the $\text{Zn}_{1-x}\text{Al}_x\text{O}$ semiconductors were in the range of 2.98–3.61 eV and increased with the increasing of Al dopant.

Keywords: *Semiconductors, Wurtzite structure, Sol-gel autocombustion, Band gap energy*

^{lxxix} Email: sujitra_kn@kku.ac.th

An iodine supplementation of chilli pepper and/or tomato fruits coated with an edible film of the iodide/iodate-doped chitosan

Nunticha Limchoowong,^a Phitchan Sricharoen,^a Mongkol Konkavan,^a Suchila Techawongstien,^b and Saksit Chanthai^{a,lxxx}

^aMaterials Chemistry Research Center, Department of Chemistry and Center of Excellence for Innovation in Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand

^bDepartment of Plant Science and Agricultural Resources, Faculty of Agriculture, Khon Kaen University, Khon Kaen 40002, Thailand

ABSTRACT

In general, the risk of numerous thyroid cancers inevitably increases among people with iodine deficiencies. An iodide-doped chitosan (CT-I) solution was prepared for dipping tomatoes to coat the fresh surface with an edible film (1.5 μm), thereby providing iodine-rich fruits for daily intake. Characterization of the thin film was conducted by FTIR and SEM. Stability of the CT-I film was studied via water immersion at various time intervals, and no residual iodide leached out due to intrinsic interactions between the cationic amino group of chitosan and iodide ions. Moreover, the iodide supplement exhibited no effect on the antioxidant activity of tomatoes. The iodine content in the film-coated tomato was determined by ICP-OES. The tomato coating with 1.5% (w/v) CT-I contained approximately 0.4 μg iodide per gram fresh weight. In addition, the freshness and storability of iodine-doped tomatoes were also maintained for shelf-life concerns. Alternatively, the present study was also designed for an iodine supplement as an edible thin film of an iodate-doped chitosan (CS-IO₃), a potential approach to prevent thyroid cancers for public health. Chilli pepper fruits were of choice to coat its fresh skin with the iodate thin film. The iodate-rich film is certainly ready-to-eat serving valuable nutrients as well. Stability of the CS-IO₃ film was also studied using the water dipping method, resulting in no leaching of an iodate ion due similarly to strong electrostatic interactions. Characterization of the iodate doped thin film was also conducted as mentioned above. The iodate-rich coating film showed no change in their antioxidant activity. The iodate concentration in the film treated hot chilli peppers was spectrophotometrically determined at 620 nm selectively based on the developed decolorization method of malachite green. It was found that the iodate contents in the chilli pepper fruits coating with 1.5% (w/v) CS-IO₃ were 11.5 mg per gram dry weight of the film sample. Freshness and storability of the iodate-rich chilli peppers were also preserved for shelf life. These results, therefore, demonstrate that the iodine supplementation of such vegetables and fruits coated with an edible thin film of the iodide or iodate-doped chitosan is a subject trend in an advocacy campaign for iodine deficiency in any supplementary food production.

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^{lxxx} Email: sakcha2@kku.ac.th

Manganese(II) ions removal from aqueous media using graphene oxide as adsorbent

Anek Suddai^{lxxxi} Prawit Nuengmatcha and Saksit Chanthai

Department of Chemistry, Faculty of Science and Technology, Nakhon Si Thammarat Rajabhat University, Nakhon Si Thammarat 80280, Thailand.

ABSTRACT

Manganese is known to be a neurotoxic agent, which elevated levels of manganese can result in toxic neurological effects. The present study was thus subject to the adsorption of Mn(II) with graphene oxide (GO) as adsorbent due to its main advantage is consisted of various functional groups on their surface giving anchored sites for metal ions complexation. Adsorption studies of Mn(II) were carried out varying some conditions: the effect of pH, the effect of incubation time and the effect of initial concentration. Manganese (II) ion was analyzed by AAS. It is determined that Mn(II) adsorption follows both Langmuir and Freundlich isotherms. The maximum adsorption capacity for Mn(II) removal from synthetic aqueous wastewater was 41.67 mg/g at pH 5 and their adsorption state was completed within 30 min. The adsorption isotherms of Mn(II) fit well with the Langmuir model. The adsorption kinetics well fitted using a pseudo second-order kinetic model. In thermodynamics diversion, changes in free energy (ΔG°), enthalpy (ΔH°) and entropy (ΔS°) were also evaluated. The overall adsorption process was exothermic and spontaneous in nature. It is demonstrated that GO can also be a highly potential adsorbent for toxic metals.

Keywords: *Graphene oxide, Manganese(II) ions, Adsorption isother, Thermodynamics, Kinetics*

^{lxxxi} Email: chem1_udon@hotmail.com, Tel. +66-7537-7443, Fax +66-7537-7443

Degradation of dye pollutants using ZnO-graphene-TiO₂ as catalyst

Prawit Nuengmatcha^{1,lxxxii} Saksit Chanthai,² and Won Chun Oh,³

¹*Department of Chemistry, Faculty of Science and Technology, Nakhon Si Thammarat Rajabhat University, Nakhon Si Thammarat 80280, Thailand.*

²*Department of Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand.*

³*Department of Advanced Materials Science & Engineering, Hanseo University, Chungnam 356-706, South Korea.*

ABSTRACT

Textile dyeing process is an important source of an environmental pollution. One of the most problems of textile wastewater in addition to both toxic and carcinogenic nature is color effluent. The removals of these dyes are crucial process from both economical and environmental points of view. This research was aimed to study the degradation of dye pollutants using ZnO-graphene-TiO₂ (ZGT) as catalyst via photocatalysis and sonocatalysis processes. ZGT was synthesized by a simple solvothermal method. The as-obtained samples were characterized by X-ray diffraction, transmission electron microscopy and energy dispersive X-ray spectroscopy. The band gap energy of the as-synthesized catalysts was performed by UV-vis diffuse reflectance spectroscopy. For sonocatalysis, the sonocatalytic activities of catalysts were tested by the oxidation of various dyes under ultrasonic irradiation, and compared with ZnO-graphene (ZG), graphene, ZnO and TiO₂, respectively. The results indicated ZGT displayed higher ultrasound activated sonocatalytic activity than other catalysts. The optimum conditions including irradiation time, pH, dye concentration, catalyst dosage and ultrasonic intensity were 120 min, 9, 20 mg/L, 1.00 g/L and 40%, respectively. In addition, the photocatalytic activities of as-obtained catalysts were assessed based on the degradation of both standard and industrial dyes under visible-light irradiation. ZGT exhibited higher visible-light-activated photocatalytic activity than did other samples. It is therefore evident that the ZGT can be applied not only as a highly effective sonocatalyst but also highly performance photocatalyst for dye pollutants.

Keywords: ZnO-graphene-TiO₂, Photocatalysis; Sonocatalysis, Dye pollutants

^{lxxxii} Email: pnuengmatcha@gmail.com, Tel. +66-7537-7443, Fax +66-7537-7443

Role of chromophores/fluorophores in plant pigments highly relates to antioxidant activity of the anthocyanins-rich Mao juice

Thitiva Sripakdee, Ratana Mahachai and Saksit Chanthai^{lxxxiii}

Materials Chemistry Research Center, Department of Chemistry and Center of Excellence for Innovation in Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand

ABSTRACT

Antioxidant and/or anti-aging activities are always lined with people's minds as major potential benefits concerning human health in the recent commercial features for an economic world of foodstuffs and medical uses. Total phenolics including flavonoids and anthocyanins, and ascorbic acid in the Mao juices are closely related to their antioxidant activity. Numerous research approaches on these functional foods, in particular the colored fruits and vegetables, have been investigated. Method validation and determination of the potential compounds have been increasingly developed with highly sensitive and selective procedures and applications including thermal stability of the Mao juice. Their antioxidant activities obtained from different assays related to the contents of both phenolics and ascorbic acid in the anthocyanins-rich Mao juices in Thailand are reported and discussed.

Keywords: *Antioxidant activity, Mao juice, Phenolic compounds, Flavonoids, Anthocyanins, Ascorbic acid*

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^{lxxxiii} Email: sakcha2@kku.ac.th

Synthesis and characterization of magnetic molecularly imprinted polymers of folic acid determination

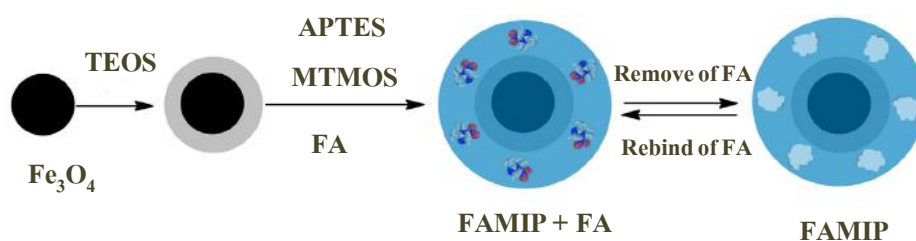
Yonrapach Areerob and Saksit Chanthai^{lxxxiv}

Materials Chemistry Research Center, Department of Chemistry and Center of Excellence for Innovation in Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand

ABSTRACT

A novel core-shell magnetic nanoparticles with surface molecularly imprinted polymer coating was synthesized by sol-gel process. Methyltrimethoxysilane (MTMOS) and 3-aminopropyltriethoxysilane (APTES) were used as functional monomer, tetraethyl orthosilicate (TEOS) as cross-linker with the template folic acid (FA) in porogenic solvent. The synthesized product was characterized by various techniques such as X-ray powder diffraction (XRD) analysis, Fourier transform infrared spectrometer (FT-IR), UV-Visible spectroscopy, scanning electron microscopy (SEM), and transmission electron microscopy (TEM). The TEM image of core shell particles showed that the particles were almost spherical with average diameter of 330 nm, consisting of 70 nm for Fe_3O_4 core and 100 nm of silica shell thickness. The polymer coated on core shell particle, which imprinting layer is estimated to be 20 nm. In addition, MIP showed rapid magnetic separation (10s) and high stability. Subsequently, the MIP was successfully applied for the chemical sensor, antibodies, solid-phase extraction, and other applications.

Keywords: *Molecularly imprinted polymer, Sol-gel method, Folic acid*



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^{lxxxiv} Email: sakcha2@kku.ac.th

Phytochemicals in *Capsicum* oleoresin from different varieties of hot chilli peppers with their antidiabetic and antioxidant activities due to some phenolic compounds

Phitchan Sricharoen, Nattida Lamaiphan, Pongpisoot Patthawaro, Nunticha Limchoowong and

Saksit Chanthai^{lxxxv}

Materials Chemistry Research Center, Department of Chemistry and Center of Excellence for Innovation in Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand

ABSTRACT

Due to its wide use in nutritional therapy, a capsicum oleoresin extraction from hot chilli pepper was optimized using ultrasound assisted extraction. Under optimal conditions, a 0.1 g sample in 10 mL of a 20% water in methanol solution was extracted at 50°C for 20 min to remove phytochemicals consisting of oleoresin, phenolics, carotenoids, flavonoids, capsaicinoids (pungency level), reducing sugars. Antioxidant and antidiabetic activities of the crude extracts from 14 chilli pepper varieties were examined. The antioxidant and antidiabetic activities of some phenolic compounds were also tested individually. The results showed that these chilli pepper samples are a rich source of phytochemicals with antioxidant and antidiabetic activities. High antioxidant activity of the extracts was evaluated using the 2,2-diphenyl-1-picrylhydrazyl, N,N-dimethyl-*p*-phenylenediaminedihydrochloride, 2,2'-azino-bis(3-ethylbenzothiazolin-6-sulfonic acid) and ferric ion reducing antioxidant power assays. The crude extracts had a lower level of sugars induced by the inhibitory effect of α -amylase activity. Thus, their enzymatic inhibitory effect might have resulted from a synergism among the phytochemicals concerned. Therefore, a diet with this type of food may have beneficial health effects.

Keywords: *Phytochemicals, Antidiabetic, Antioxidants, Phenolics, Chilli pepper, Ultrasound assisted extraction*

^{lxxxv} Email: sakcha2@kku.ac.th

Preparation and optical properties of zinc sulfide in DS@CoAl-layered double hydroxide

Sonchai Intachai¹, Nithima Khaorapapong^{1,lxxxvi} and Makoto Ogawa²

¹Materials Chemistry Research Center, Department of Chemistry and Center of Excellence for Innovation in Chemistry, Faculty of Science, Khon Kaen 40002, Thailand

²Department of Chemical Engineering, School of Energy Science and Engineering, Vidyasirimedhi Institute of Science and Technology, Rayong 21210, Thailand

ABSTRACT

Zinc sulfide (ZnS), a type of II-IV semiconductors, has been received much interest owing to its tunable band gap and luminescence properties.¹ The control of size and morphology of ZnS using nanospace of layered host materials is a possible way to tailor its properties. *Here*, the formation of ZnS in the dodecylsulfate (DS) modified CoAl-LDH was investigated. The CO₃²⁻-CoAl-LDH was prepared by precipitation method using urea hydrolysis.²⁻⁵ The organically modified CoAl-LDH was carried out by anion exchange reaction and denoted as DS@CoAl-LDH. The introduction of ZnS in DS@CoAl-LDH was conducted by mixing an aqueous solution of ZnCl₂ and an ethanol suspension of DS@CoAl-LDH under magnetic stirring at room temperature for 24 h and subsequent reaction with an aqueous solution of Na₂S for 24 h. The increase in the basal spacing from 0.76 nm (*d*₀₀₃) for CoAl-LDH to be 2.53 nm for DS@CoAl-LDH, which was consistent with the appearance of the characteristic FTIR bands of the CH₂ (2859 and 2932 cm⁻¹) and CH₃ (2950 cm⁻¹) stretching modes, as well as OSO₃ stretching vibration (985-1220 cm⁻¹) and the loss of the band due to stretching mode CO₃²⁻ (1358 cm⁻¹) revealed the intercalation of DS⁻ ion in CoAl-LDH.⁶ The *d*₀₀₃ of DS@CoAl-LDH was decreased to be 0.78 nm after the *in situ* formation of ZnS in the interlayer space, corresponding to the gallery height of 0.30 nm, indicating the intercalation of ZnS, as well as the partial de-intercalation and re-arrangement of the intercalated DS⁻. TEM image of ZnS/DS@CoAl-LDH showed the distribution of ZnS nanoparticle with the average size of 2.6 nm on nanosheets of CoAl-LDH. The large blue-shifts of the absorption onset from 387 nm for bare ZnS to 340 nm for ZnS/DS@CoAl-LDH and the emission band from 470 nm for bare ZnS to 422 nm for ZnS/DS@CoAl-LDH were thought to be due to the quantum confinement effect.

Keywords: CoAl-layered double hydroxide, Zinc, Sulfide, Dodecylsulfate, Optical properties

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^{lxxxvi} Email: nithima@kku.ac.th

Hollow mesoporous hetero-NiCo₂S₄/Co₉S₈ submicro-spindles: unusual formation, appealing pseudocapacitance and its applications in hybrid supercapacitors

Changzhou Yuan*, Hui Hua, Yaoyao Shi, and Linrui Hou

Anhui University of Technology, Ma'anshan Anhui, P. R. China, 243002

ABSTRACT

Hierarchical hollow porous architectures with intriguing hetero-interfaces are currently of particular interest in emerging energy-related fields. In the investigation, we report a smart template-free methodology to purposefully fabricate high-quality uniform hollow hetero-NiCo₂S₄/Co₉S₈ (NCCS) submicro-spindles with well-dispersed hetero-nanodomains at the nanoscale. High-yield hollow mesocrystal nickel cobalt carbonate spindles are first solvothermally synthesized as the intermediate, and following shape-preserving conversion into hetero-NCCS submicro-spindles *via* hydrothermal anion-exchange reaction occurs. The underlying template-free formation mechanism of hollow structures was tentatively proposed here. When evaluated as promising electrode for supercapacitors, the resultant hollow mesoporous hetero-NCCS electrode with loading mass of 5 mg cm⁻² delivers a fascinating pseudocapacitance of ~749 F g⁻¹ at current rate of 4 A g⁻¹, and holds it approximately 660 F g⁻¹ at 10 A g⁻¹, in virtue of intrinsic synergetic contributions from structural/compositional/componential merits. Furthermore, an asymmetric device based on hollow mesoporous hetero-NCCS achieves an encouraging energy density of around 33.5 Wh kg⁻¹ at a power density of 150 W kg⁻¹, and exceptional cycling behaviors with capacitance degradation of ~0.006% per cycle over 5000 consecutive cycles at 3 A g⁻¹. Comprehensive investigations unambiguously highlight that the unique hollow mesoporous hetero-NCCS submicro-spindles would be a powerful electrode platform for advanced next-generation supercapacitors.

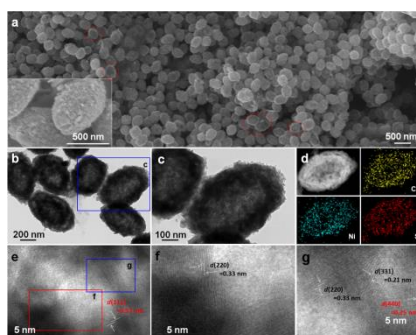


Fig. 1. FESEM image (a), TEM images (b, c), elemental (Co, Ni, S) mapping images (d), and HRTEM images (e-g) of the hollow hetero-NCCS submicro-spindles. The inset in panel (a) for high-magnification FESEM image of the NCCS sample

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*Email: ayuancz@163.com; ayuancz@ahut.edu.cn

Detection of oxygen species generated of Ag₂Se-graphene heterojunction photocatalysts with excellent visible light driven photocatalytic performance

Ze-Da Meng^{*1,2}, Shouqing Liu¹, Zhigang Chen¹ and Won-Chun Oh²

¹*Jiangsu Key Laboratory of Environmental Functional Materials, College of Chemistry and Bioengineering, Suzhou University of Science and Technology, Suzhou 215009, China*

²*Department of Advanced Materials Science & Engineering, Hanseo University, Seosan-si, Chungnam-do, Korea, 356-706*

ABSTRACT

Reactive oxygen species (ROS) can be produced by interactions between sunlight and light-absorbing substance in natural water environment and can completely destroy various organic pollutants in wastewaters. In this study, we used graphene oxide modified Ag₂Se nanoparticles to enhance the photochemically generated oxygen (PGO) species activity. Surface area and pore volumes of the Ag₂Se-graphene (Ag₂Se-G) samples showed a catastrophic decrease due to the deposition of Ag₂Se. The generations of reactive oxygen species were detected through the oxidation reaction from DPCI to DPCO. The photocurrent density and the PGO effect increase in the case with the modified graphene. The PGO effect of the graphene modified with Ag₂Se composites is increased significantly due to the synergetic effect between the graphene and the Ag₂Se nanoparticles. The photocatalytic activity of the sample was evaluated by measuring the degradation of organic pollutants such as methylene blue (MB), and industrial dyes such as Texbrite BA-L (TBA) under visible light.

Keywords: Ag₂Se-graphene, TEM, visible light, FT-IR, Industrial dyes, Texbrite BA-L