

## Curriculum Vitae of Shubin Yang

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### Affiliation

Institute for Catalysis, Hokkaido University

### Personal Data

Sex: Female

Date of Birth: June 24, 1987

Place of Birth/Nationality: Shandong Prov., P. R. China / Chinese

### Education

2012. 10 – 2015. 9 Shizuoka University, Japan, **PhD. in Nanovision Technology**

2012. 9 – 2015. 7 Institute of Plasma Physics, CAS, **PhD. in Chemistry**

2010. 9 – 2012. 9 Institute of Plasma Physics, CAS, **M.S. in Chemistry**

2006. 9 – 2010. 7 Shandong Agricultural University, **B. S. in Applied Chemistry**

### Awards

- Special prize for excellent student of Director's scholarship of Institute of Plasma Physics, CAS in 2015
- Student Award in AEPSE 2015 international conference
- Excellent PhD student of Shizuoka University in 2015
- CAS President Award in 2015
- Excellent Doctoral Student Scholarship of CAS Zhu Liyuehua Award in 2014
- Excellent student of Director's scholarship of Institute of Plasma Physics, CAS in 2014
- Merit student of CAS in 2012-2013
- First class of the seventh excellent paper in natural science of Anhui province
- Shandong Provincial Outstanding Graduate in 2010.
- The National Scholarship of Chinese Ministry of Education in 2008-2009

## **Experiences**

- 2010.7 – 2011.1: Design and fabrication of nanomaterial for the study of environmental physicochemical behavior of heavy metal ions and organic pollutants management with Prof. Xiangke Wang in Institute of Plasma Physics, CAS, Hefei, China.
- 2010.12 – 2011.7: Study on the electrode materials for supercapacitor with Prof. Anwu Xu in University of Science and Technology of China
- 2011.10 – 2012.7: Learn quantum chemistry program Gaussian 03 and carry out theoretical studies on mechanism of the adsorption of heavy metal ions of by graphene oxide with Prof. Dongqi Wang in Institute of High Energy Physics, CAS, Beijing, China.
- 2012.9 – 2015.9: Study and design new adsorbents by low-temperature plasma modification for removal of cesium ions with Prof. Nagatsu Masaaki in Shizuoka University as DDP student of the Institute of Plasma Physics (China, Prof. Xiangke Wang) and Shizuoka University (Japan, Prof. Masaaki Nagatsu).
- 2015.10 – 2016.3: Construct rhodium(IV)-doped TiO<sub>2</sub> composites with high photocatalytic performance: A combined experimental and theoretical study with Prof. Bunsho Ohtani as post doctor researcher.

## **Research Interests**

- Construct novel photocatalysis nanomaterial for high visible-light photocatalytic performance
- Application of nanotechnology in pollution management and nuclear waste management etc.
- Theoretical studies on mechanism of the adsorption of heavy metal ions, organic pollutants and uranyl ions, etc.

## **Publications:**

- 1) S.B. Yang, N. Okada, and M.Nagatsu. The highly effective removal of Cs<sup>+</sup> by low turbidity chitosan-grafted magnetic bentonite, *J. Hazard. Mater.*, 301, 8-16, 2016.
- 2) X. Wang, S.B. Yang,\* W. Shi, J. Li, T. Hayat, X. Wang, Different Interaction Mechanisms of Eu(III) and <sup>243</sup>Am(III) with Carbon Nanotubes Studied by Batch, Spectroscopy Technique and Theoretical Calculation, *Environ. Sci. Technol.*, 49, 11721-11728, 2015.
- 3) S.B. Yang, D.D. Shao, X.K. Wang, G.S. Hou, M. Nagatsu, X.L. Tan, X.M. Ren and J.T. Yu, Design of Chitosan-Grafted Carbon Nanotubes: Evaluation of How the -OH Functional Group Affects Cs<sup>+</sup> Adsorption, *Mar. Drugs.*, 13(5), 3116-313, 2015.
- 4) S.B. Yang, Y. Chen, C.L. Chen, J.X. Li, D.Q. Wang, X.K. Wang, and W.P. Hu, Competitive

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- Adsorption of Pb(II), Ni(II) and Sr(II) Ions on Graphene Oxides: A Combined Experimental and Theoretical Study, *ChemPusChem*, 80, 480-484, 2015.
- 5) Y.B. Sun, S.B. Yang, Y. Chen, C.C. Ding, W.C. Cheng, and X.K. Wang, Adsorption and desorption of U(VI) on functionalized graphene oxide: A Combined Experimental and Theoretical study, *Environ. Sci. Technol.* 49, 4255-4262, 2015 (co-first author)
  - 6) S.B. Yang, C. Han, X.K. Wang and M. Nagatsu. Characteristics of Cesium Ion Sorption from Aqueous Solution on Bentonite- and Carbon Nanotube-based Composites, *J. Hazard. Mater.*, 274, 46-52, 2014.
  - 7) S.B. Yang, D.D. Shao, X.K. Wang and M. Nagatsu. Localized In-situ Polymerization on Carbon Nanotube Surfaces for Stabilized Carbon Nanotube Dispersions and Application for Cobalt(II) Removal, *RSC Advances*, 4, 4856-4863, 2014.
  - 8) S.B. Yang, X.L. Wu, C.L. Chen, H.L. Dong, W.P. Hu, and X.K. Wang, Spherical  $\alpha$ -Ni(OH)<sub>2</sub> nanoarchitecture grown on graphene as advanced electrochemical pseudocapacitor materials, *Chem. Commun.*, 48, 2773-2775, 2012.
  - 9) S.B. Yang, J. Hu, C.L. Chen, D.D. Shao, and X.K. Wang, Mutual Effects of Pb(II) and Humic Acid Adsorption on Multiwalled Carbon Nanotubes/Polyacrylamide Composites from Aqueous Solutions, *Environ. Sci. Technol.* 45, 3621-3627, 2011.

## Academic achievements

### Publications:

- 1) S.B. Yang, N. Okada, and M. Nagatsu. The highly effective removal of Cs<sup>+</sup> by low turbidity chitosan-grafted magnetic bentonite, *J. Hazard. Mater.*, 301, 8-16, 2016.
- 2) X. Wang, S.B. Yang,\* W. Shi, J. Li, T. Hayat, X. Wang, Different Interaction Mechanisms of Eu(III) and <sup>243</sup>Am(III) with Carbon Nanotubes Studied by Batch, Spectroscopy Technique and Theoretical Calculation, *Environ. Sci. Technol.*, 49, 11721-11728, 2015.
- 3) S.B. Yang, D.D. Shao, X.K. Wang, G.S. Hou, M. Nagatsu, X.L. Tan, X.M. Ren and J.T. Yu, Design of Chitosan-Grafted Carbon Nanotubes: Evaluation of How the -OH Functional Group Affects Cs<sup>+</sup> Adsorption, *Mar. Drugs.*, 13(5), 3116-313, 2015.
- 4) S.B. Yang, Y. Chen, C.L. Chen, J.X. Li, D.Q. Wang, X.K. Wang, and W.P. Hu, Competitive Adsorption of Pb(II), Ni(II) and Sr(II) Ions on Graphene Oxides: A Combined Experimental and Theoretical Study, *ChemPusChem*, 80, 480-484, 2015.
- 5) Y.B. Sun, S.B. Yang, Y. Chen, C.C. Ding, W.C. Cheng, and X.K. Wang, Adsorption and desorption of U(VI) on functionalized graphene oxide: A Combined Experimental and Theoretical study, *Environ. Sci. Technol.* 49, 4255-4262, 2015 (co-first author)
- 6) S.B. Yang, C. Han, X.K. Wang and M. Nagatsu. Characteristics of Cesium Ion Sorption from Aqueous Solution on Bentonite- and Carbon Nanotube-based Composites, *J. Hazard. Mater.*, 274, 46-52, 2014.
- 7) S.B. Yang, D.D. Shao, X.K. Wang and M. Nagatsu. Localized In-situ Polymerization on Carbon Nanotube Surfaces for Stabilized Carbon Nanotube Dispersions and Application for Cobalt(II) Removal, *RSC Advances*, 4, 4856-4863, 2014.
- 8) S.B. Yang, X.L. Wu, C.L. Chen, H.L. Dong, W.P. Hu, and X.K. Wang, Spherical  $\alpha$ -Ni(OH)<sub>2</sub> nanoarchitecture grown on graphene as advanced electrochemical pseudocapacitor materials, *Chem. Commun.*, 48, 2773-2775, 2012.
- 9) S.B. Yang, J. Hu, C.L. Chen, D.D. Shao, and X.K. Wang, Mutual Effects of Pb(II) and Humic Acid Adsorption on Multiwalled Carbon Nanotubes/Polyacrylamide Composites from Aqueous Solutions, *Environ. Sci. Technol.* 45, 3621-3627, 2011.

### International Conferences

- 1) Shubin Yang, Naoya Okada, Xiangke Wang, and Masaaki Nagatsu, Cesium Ion Capture by Magnetic Bentonite Particles with Low Turbidity Enhanced by Plasma-Induced Graft Chitosan, AEPSE 2015, Jeju, Republic of Korea: 2015.9.20-24 (Oral and poster, Student Award)
- 2) Shubin Yang, Naoya Okada, Xiangke Wang, and Masaaki Nagatsu, Synthesis of Chitosan-coated Magnetic Bentonite by Plasma-Induced Graft Chitosan and Its Application in Cs<sup>+</sup> Capture, 2015 International Symposium toward the Future of Advanced Researches in Shizuoka University, Hamamatsu, Japan: 2015.1.27-28 (Oral and poster)
- 3) Shubin Yang, Okada Naoya, Xiangke Wang, Masaaki Nagatsu, Understanding the Sorption of

- Cesium ion on bentonite by Plasma Jet, ISPlasma2014 / IC-PLANTS 2014, Nagoya: 2014, 3. 2-6 (poster)
- 4) Shubin Yang, Chou Han, Xiangke Wang, Masaaki Nagatsu, Removal Mechanism of Cesium Ion from Aqueous Solution with Bentonite- and Carbon Nanotube-based Composites, ICRP-8/SPP-31, Fukuoka: 2014, 2. 3-7 (poster)
  - 5) Shubin Yang, Chou Han, Xiangke Wang, Masaaki Nagatsu, Sorption Mechanism of Cesium Ions from Aqueous Solution by Chitosan-grafted Carbon Nanotubes and Bentonite by Plasma-induced Grafting Method, MRS-J, Yokohama: 2013, 12. 9-11 (poster)
  - 6) Shubin Yang, Chou Han, Xiangke Wang, Masaaki Nagatsu, Removal of Cs ion from aqueous solution using plasma functionalized chitosan-grafted graphite-encapsulated magnetic nanoparticles, APCC-12, Chiba: 2013. 7.14-19 (poster)

### **Domestic Conferences**

- 1) Shubin Yang, Naoya Okada, Masaaki Nagatsu, Study of Adsorption and Desorption of Cs<sup>+</sup> Ions on Chitosan-Grafted Magnetic Bentonite, The 62nd JSAP Spring Meeting, 2015, 3.11-14 Shibuya, (Oral).
- 2) Shubin Yang, Naoya Okada, Xiangke Wang, and Masaaki Nagatsu, Synthesis and characterization of bentonite-based composites by plasma-induced graft chitosan for separation of cesium ions from waste solutions, 306th Monday Morning Forum, 2014. 12.15, Hamamatsu, Japan (Oral).
- 3) Shubin Yang, Naoya Okada, Xiangke Wang, Masaaki Nagatsu, Characteristics of cesium ion sorption from aqueous solution on plasma-induced chitosan grafted magnetic bentonite composites, Plasma Conference, 2014.11.18-21, Niigata (Oral and poster).
- 4) Shubin Yang, Xiangke Wang, Masaaki Nagatsu, Study of the Sorption of Cobalt(II) Ion on Magnetic Carbon Nanotubes by Atmospheric Pressure Plasma Jet, The 61nd JSAP Spring Meeting, 2014, 3.17 -20 Sagamihara, (Poster).
- 5) Shubin Yang, Chou Han, Xiangke Wang, Masaaki Nagatsu "Study on the Sorption Mechanism of Cesium ion by Chitosan-grafted Nanomaterials", JSPF Annual Meeting, 2013.12.3-6, Tokyo (Poster).

## Abstract of past research

### 1) The individual and competitive adsorption of metal ions on graphene oxides (GOs) studies by experimental and DFT calculation

The heavy metal ions can be accumulated in living tissues, so they must be removed from polluted water. Graphene oxides (GOs) are considered as the ideal adsorbent material because the large quantities of oxygen-containing functional groups strengthen their hydrophilicity and adsorption capacity towards the heavy metal ions and positively charged organic molecules besides the high specific surface area like graphene. However, different metal ions often coexist in the wastewaters and aquatic environment rather than single metal ions. Although, much work focuses on the single metal ion adsorption on GOs, there are few reports on the competitive adsorption of coexisting metal ions on GOs. In addition, the theoretical calculation for investigating the interaction between metal ions and GOs is scarce. In the context of wastewaters, the information of competitive adsorption of coexisting metal ions on GOs is important and useful for improving the absorption capacity of GOs towards specific metal ions.

In my study, the individual and competitive adsorption of Pb(II), Ni(II) and Sr(II) on GOs were investigated by experimental and DFT studies. We have successfully explained the experimental observations by DFT calculation. In this work, we have revealed that (1) among the ions Pb(II), Ni(II), or Sr(II), which one is much easier to react with graphene oxides; (2) which group, -OH, -COOH or -COO, is mainly responsible for the adsorption of metal ions; (3) how do the adsorption and desorption reactions carry out; and (4) Pb(II) can easily abstract the OH groups from graphene oxides (GOs) to form much more stable Pb(OH)-GO complex. For the first time, we proposed the OH-abstracting mechanism for the excellent adsorption property of graphene oxide, and to understand the interaction of different heavy metal ions with graphene oxides from experiments and DFT calculations.

## **2) Design and fabrication of nanomaterials by low-temperature plasma modification and their application in the removal of cesium ions from aqueous solutions.**

With the rapid increase industrialization in many countries, the pollution load on the environment is increasing. Radioactive caesium is of serious social and environment concern as it can be easily dissolved in water and has a high fission yield, long half-life. Although many research groups have made important contributions to search the high-efficiency sorbent for  $\text{Cs}^+$  ions, and the mechanisms of  $\text{Cs}^+$  adsorption are proposed, the detailed adsorption mechanisms still remain unclear. To search a high-efficiency adsorbent to remediate  $\text{Cs}^+$  ions from contaminated water is an issue that needs to be addressed urgently. Therefore, an accurate and detail mechanism is required and calls for contribution to understand the adsorption process in order to facilitate the development of more efficient adsorbent.

In order to understand effect of cation exchange and the hydroxyl exchange on  $\text{Cs}^+$  sorption and whether the sorption capacity of the material can be improved by increasing the amount of hydroxyl groups, we designed the chitosan-grafted carbon nanotubes (CS-g-CNTs) and chitosan-grafted bentonite (CS-g-bentonite) by plasma-induced method as the models of low and high cation exchange capacity materials, respectively. We found the sorption of  $\text{Cs}^+$  is significantly affected by cation exchange in monovalent Group I and divalent Group II. The cation-exchange mechanism is much more effective than the hydroxyl group exchange. The effect of hydroxyl groups is dependent on the property of the matrix. The  $\text{Cs}^+$  adsorption capacity of material cannot be improved only by increasing the amount of hydroxyl groups in any case. The spatial structure and the cation-exchange capacity of the material are important factors for  $\text{Cs}^+$  removal from radioactive waste water. Our findings are important for estimating and optimizing the sorbents for  $\text{Cs}^+$  ions and give the future directions of new and selective adsorbents for the removal of  $\text{Cs}^+$  ions in groundwater or wastewater.

## Preparation and properties of rhodium (IV) and carbon-codoped TiO<sub>2</sub> photocatalyst

### Present research related to research plan

Photocatalysis is an environmentally friendly technology for degradation of target pollutants using solar energy.<sup>1</sup> Up to now, titania (TiO<sub>2</sub>) has been one of the most promising photocatalysts because of its easy availability, low toxicity, high photostability, and high efficiency.<sup>2</sup> However, challenges such as rapid recombination of electron-hole pairs due to TiO<sub>2</sub> wide band gap (ca. 3.0eV) and poor recycling, limit its activity towards the degradation of organic contaminants. Therefore, the development of highly efficient TiO<sub>2</sub>-based photocatalysts with smaller bandgap has become an important research direction. Usually, doping or co-doping of TiO<sub>2</sub> with noble metals, transition metals, and nonmetallic elements can improve photocatalytic activities by creating localized/delocalized states in the band gap.<sup>3</sup>

Recently, rhodium-doped photocatalysts have attracted considerable scientific interest. Because of charge balance and almost the same cation size, four-valent rhodium (Rh(IV)) is expected to readily substitute Ti<sup>4+</sup> in TiO<sub>2</sub>. In previous study, we found that Rh-TiO<sub>2</sub> exhibits high photoelectrochemical properties under visible-light irradiation via a two-photon band-gap excitation mechanism.<sup>4</sup> However, Rh(IV)-doped photocatalysts were prepared by oxidizing Rh<sup>III</sup> to Rh(IV) at high temperature ( $\geq 900^\circ\text{C}$ ) and the complete oxidization of Rh<sup>III</sup> is difficult.

Herein, we propose to dope Rh(IV) ion directly into TiO<sub>2</sub> by hydrothermal method. Combining experimental and density function theory (DFT) studies, we found Rh(IV)-doped TiO<sub>2</sub> composite exhibits an enhanced photocatalytic activity for acetic acid decomposition but a decreased activity for methanol dehydrogenation under UV and visible-light irradiation. DFT calculation indicates that while Rh(IV) is doped into TiO<sub>2</sub>, two new bands appear between valence band ( $VB_{TiO_2}$ ) and conduction ( $CB_{TiO_2}$ ) of TiO<sub>2</sub>. One is a valence band slightly above the  $VB_{TiO_2}$ , which consists of occupied  $T_{2g}$  orbital of Rh(IV) (referred as  $VB_{Rh}$ ). The other one is a conduction band below the  $CB_{TiO_2}$  and composed of empty  $T_{2g}$  orbital of Rh(IV) (referred as  $CB_{Rh}$ ). TD-DFT calculation shows that the Rh(IV) doped TiO<sub>2</sub> has broad absorption in visible light (400 - 700 nm). These absorption are assigned mainly to  $VB_{TiO_2} \rightarrow CB_{Rh}$  transition and partially  $VB_{Rh} \rightarrow CB_{Rh}$  transition. In these transitions, not only the electron at the edge of  $VB_{TiO_2}$  is excited, but also the deep electrons are excited. These high energy  $VB_{TiO_2} \rightarrow CB_{Rh}$  excitations are likely to be responsible for the increased oxidation ability of Rh(IV) doped TiO<sub>2</sub>. However, energy level of  $CB_{Rh}$  is not as high as the reduction potential of water. As a result, the hydrogen reduction ability is reduced significantly.

For practical use, the photocatalyst should have both high oxidation and reduction capabilities. Therefore, increasing the reduction capability is important to improve Rh(IV)-doped TiO<sub>2</sub>. Carbon (C) has been demonstrated to be an effective doping element to promote the dehydrogenation of methanol and the visible light absorption.<sup>5</sup> Kamisaka et al.<sup>6</sup> studied the effect of C-doping by the DFT calculation, and they found that the substitution of oxygen by C is beneficial for the visible light absorption of TiO<sub>2</sub> and does not change its crystal structure. Especially, Ting et al.<sup>7</sup> designed C-doped rutile TiO<sub>2</sub> sample and found high efficiency for the photocatalytic H<sub>2</sub> generation from water. We expect that the additional doping of C into Rh(IV)-doped TiO<sub>2</sub> will improve the reduction capability. Thus, we proposed this research plan of Rh(IV)/C-co-doped TiO<sub>2</sub> photocatalysis.

### Purpose of proposed research

On the basis of these considerations, the present research aims at designing and synthesizing a



novel Rh(IV)/C-co-doped TiO<sub>2</sub> photocatalyst with both high-efficiency photooxidation and photoreduction performance under visible-light irradiation.

### Proposed plan

In my present research, Rh(IV)-doped TiO<sub>2</sub> with different doping concentration of Rh(IV) have been successfully prepared by a novel and easy two-step hydrothermal method. C-doped TiO<sub>2</sub> will also be prepared by hydrothermal method with the same hydrothermal temperature and time. However, considering the strong acidity of the prepared Rh(IV) solution, to find a suitable carbon source for the hydrothermal reaction will be critical. In addition, examining the photocatalytic activity of rhodium (IV) and carbon codoping TiO<sub>2</sub> materials also be the mainly parts we will focus on.

Firstly, various samples of Rh(IV)/C-co-doped TiO<sub>2</sub> particles are prepared. Then XPS and XRD analyses will be carried out to check the successful synthesis of these materials. After that, analysis of action spectrum, light-intensity dependence, photocatalytic activities and the stability tests in various photocatalytic reaction systems will be performed using the Rh(IV)/C-co-doped TiO<sub>2</sub> materials. The photocatalytic activities of the Rh(IV)/C-co-doped TiO<sub>2</sub> materials will be studied by the oxidation decomposition of acetic acid under an aerobic atmosphere and the methanol dehydrogenation under an argon atmosphere with visible light irradiation. The photocatalytic activities of Rh(IV)/C-co-doped TiO<sub>2</sub> materials will be evaluated with a commercial sample (Nippon Aerosil P25) as a reference.

### Expected results and impacts

The Rh(IV)/C-co-doped TiO<sub>2</sub> materials are successfully synthesized by the hydrothermal method and be confirmed by different characterizations. The UV-vis diffuse reflectance absorption spectra of various Rh(IV)/C-co-doped TiO<sub>2</sub> materials will be characterized. The photocatalytic reactions of different organic substrate in presence of only various Rh(IV)/C-co-doped TiO<sub>2</sub> materials will be traced by action spectra. The photocatalytic efficiency, stability and reusability of the Rh(IV)/C-co-doped TiO<sub>2</sub> photocatalysis could also be evaluated by methanol dehydrogenation and acetic acid decomposition under visible light irradiation.

These results are very important for estimating the photocatalytic reactions which performed by Rh(IV)/C-co-doped TiO<sub>2</sub> catalysts, and exploring its potential applications.

### References

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- [2]B. Ohtani, *J. Photochem. Photobiol. C: Photochem. Rev.*, 2010, **11**, 157-178.
- [3]S. O. Sanni and O. G. Idemudia, *J. Nanomater.*, 2014, **2014**, 1-8.
- [4]J. Kunczewicz and B. Ohtani, *Chem. Commun.*, 2015, **51**, 298-301.
- [5]J. Schneider, M. Matsuoka, M. Takeuchi, J. Zhang, Y. Horiuchi, M. Anpo and D. W. Bahnemann, *Chem. Rev.*, 2014, **114**, 9919-9986.
- [6]H. Kamisaka, T. Adachi and K. Yamashita, *J. Chem. Phys.*, 2005, **123**, 084704.
- [7]T. Xia, W. Zhang, J. B. Murowchick, G. Liu and X. Chen, *Adv. Energy Mater.*, 2013, **3**, 1516-1523.