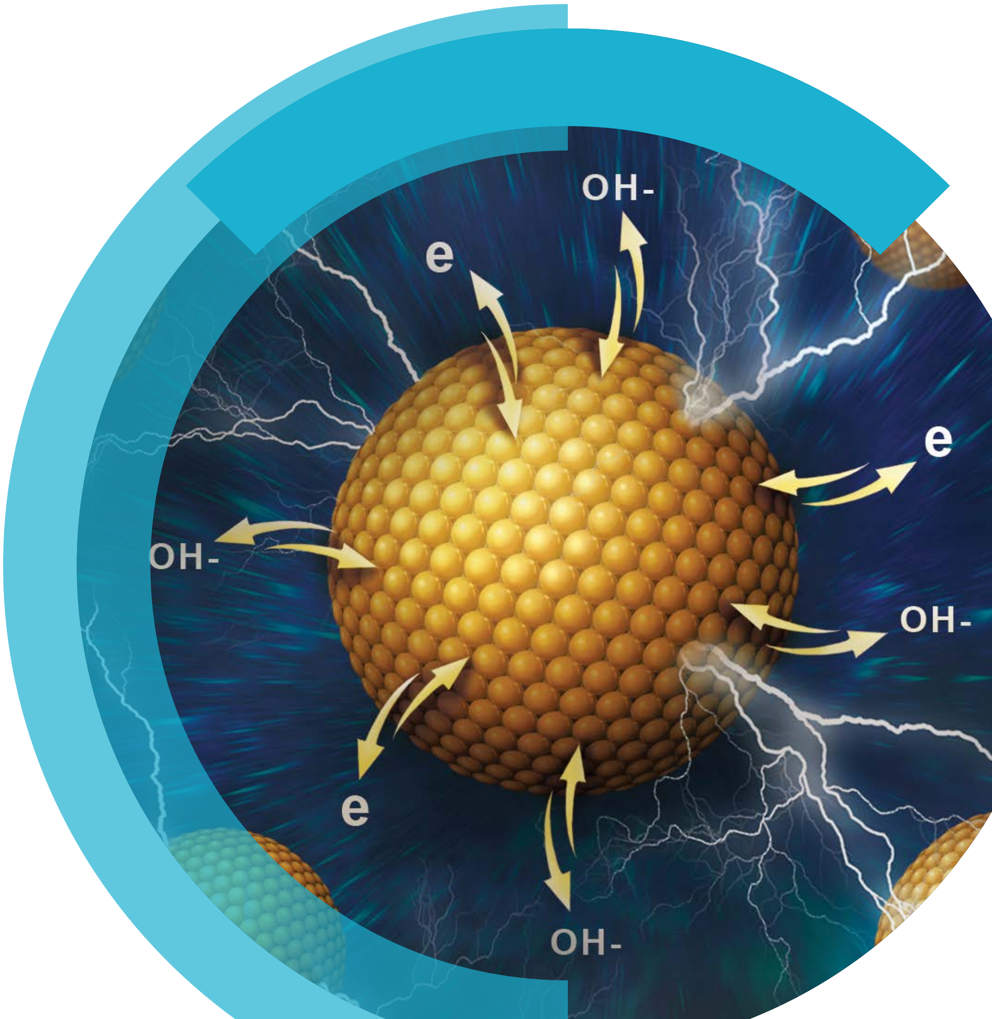
ROYAL SOCIETY OF CHEMISTRY | CELEBRATING IYPT 2019

24 September 2019, Tianjin, China

International Symposium on Inorganic Chemistry Frontiers and Interdisciplinary Sciences

2019年9月24日， 天津



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Welcome from the Organizing Committee

On behalf of the organizing committee, we would like to offer a warm welcome to all of you to the International Symposium on Inorganic Chemistry Frontiers and Interdisciplinary Sciences. The symposium is held at Tianjin Saixiang hotel, Tianjin, China on 24 September 2019. Inorganic Chemistry Frontiers International Symposia are a series of conferences sponsored by *Inorganic Chemistry Frontiers* (ICF), a collaborative journal developed by the Chinese Chemical Society, Peking University and the Royal Society of Chemistry. Previous meetings were held in London (2016), Nanjing (2017), and Sendai, Japan (2018). This symposia are devoted to the recent advances and new trends in inorganic chemistry as well as interdisciplinary studies at the interfaces between inorganic chemistry and other subjects like nano technology, materials science, energy, catalysis and biochemistry etc.

This year's ICF symposium is financially supported and organized by *Inorganic Chemistry Frontiers* and the Key Laboratory of Advanced Energy Materials Chemistry, Ministry of Education in Nankai University. Under the chairmanship of Prof. Jun Chen at Nankai University, the local organizing committee has put together a one-day event with 10 invited lectures from ICF Editorial Board members and invited local speakers, who are leading experts in the field. Topics includes synthesis and properties of metal complexes, hydrogen production, photo- and bio-catalysis, as well as inorganic materials and their applications.

We would like to encourage graduate students and postdoctoral fellows to participate in this symposium, which will offer opportunities to interact with these scientists. We hope that this symposium can provide an ideal forum for the exchange of ideas and experiences, fostering new research collaborations between Chinese inorganic chemists and international experts.

This symposium is freely open to all delegates.

Prof. Jun Chen
Organizing Committee

Introduction of College of Chemistry at Nankai University

College of Chemistry was found in April 1995, originated from the Department of Chemistry founded in 1921 by Prof. Zongyue Qiu.

So far, College of Chemistry has two departments (namely Department of Chemistry and Department of Chemical Biology), three institutes (Research Institute of Elemento-organic Chemistry, Institute of Polymer Chemistry and Institute of Applied Chemistry), as well as two research centers (Research center of Analytical Science and National Engineering Research Center of Pesticide(Tianjin)).

Chemical discipline of Nankai University has basically formed a relatively stable discipline layout and research directions. The chemical discipline is geared to the needs of both the international academic frontiers and the national development strategies. After a long period of academic accumulations, continuous optimization of scientific layout, discipline construction strengthening, and the development of burgeoning interdisciplines, College of Chemistry runs two Ph.D. programs, one for Chemistry (the first-level national key discipline) and the other for Pesticide Science (the second-level national key discipline). Scientific research and teaching platform, including Collaborative Innovation Center of Chemical Science and Engineering(Tianjin), State Key Laboratory of Elemento-Organic Chemistry, State Key Laboratory of Medicinal Chemical Biology, the National Engineering Research Center of Pesticide(Tianjin), the Key Laboratory of Functional Polymer Materials (Ministry of Education), the Key Laboratory of Advanced Energy Materials Chemistry (Ministry of Education) and Engineering Research Center for (Ministry of Education), is not only one of the earliest "National Basic Scientific Research and Teaching Personnel Training Base (Chemical)", but also a base for Wisdom Absorption for Discipline Innovation in "111 Program". At present, College of Chemistry of Nankai University has become leading national bases for research and education in chemistry.

Currently, the College of Chemistry has a strong faculty of 349 members. There are 113 professors and 70 associate professors, including five academicians of Chinese Academy of Science, one academician of Chinese Academy of Engineering, eight endorsed professors by Yangtze River Scholar Award program, eighteen winners of National Science Fund for Distinguished Young Scholars, two Innovative Research Group of National Science Foundation and two Yangtze River Innovative Teams of Ministry of Education. At present, the College of Chemistry has 1114 undergraduates, 667 master-level graduate students and 469 PhD-level graduate students.

International Symposium on Inorganic Chemistry Frontiers and Interdisciplinary Sciences

Tianjin Saixiang Hotel, Tianjin, China (天津赛象酒店)
24 September 2019

Time	Event	Session Chair
09:00 - 09:10	**Opening remarks** Jun Chen, Nankai University（陈军, 南开大学） Wenjun Liu, Royal Society of Chemistry（刘文君，英国皇家化学会）	
09:10 - 09:40	Yi Lu, University of Illinois **Designing Functional Metalloenzymes and their Applications in Biocatalysis for Renewable Energy**	**Chair of Session 3** Maochun Hong, Fujian Institute of Research on the Structure of Matter,CAS 洪茂椿 中科院福建物质结构研究所
09:40 - 10:10	Zhiping Zheng, Southern University of Science and Technology（郑智平，南方科技大学） **Hydrogen Production by Aqueous-phase Reforming of Methanol Promoted by Grubbs and Hoveyda-Grubbs Catalysts**	
10:10 - 10:30	Coffee break (20 min)	
10:30 - 11:00	John E. McGrady, University of Oxford **Metal clusters on the localized/delocalized borderline**	**Chair of Session 2** Hongjie Zhang changchun institute of applied chemistry 张洪杰 中科院长春应用化学研究所
11:00 - 11:30	Hiroki Oshio, University of Tsukuba **A Metal complexes with multi-accessible electronic state**	
11:30 - 12:00	Fangyi Cheng, Nankai University（程方益，南开大学） **Mild, Controllable Synthesis of Transition Metal Oxide/Hydroxide Electrodes**	
12:00 - 14:00	Lunch (120 min)	
14:00 - 14:30	Shu-Hong Yu, University of Science and Technology of China（俞书宏，中国科技大学） **Bio-Inspired Synthesis and Self-Assembly of Functional Materials**	**Chair of Session 3** Jihong Yu, Jilin University 于吉红 吉林大学
14:30 - 15:00	Xianran Xing, University of Science and Technology Beijing（邢献然，北京科技大学） **Local structure and negative thermal expansion in nano solids**	
15:00 - 15:30	Tong-Bu Lu, Tianjin University of Technology（鲁统部，天津理工大学） **Artificial Photosynthesis Catalysts**	
15:30 - 15:50	Coffee break (20 min)	
15:50 - 16:20	Paula Diaconescu, University of California, Los Angeles **Redox switchable ring opening copolymerization**	**Chair of Session 4** Song Gao, South China University of Technology 高松 华南理工大学
16:20 - 16:50	Oleg V Ozerov, Texas A&M University **Bond activation reactions by boryl pincer complexes**	
16:50 - 17:00	**Closing remarks** Song Gao, South China University of Technology（高松，华南理工大学）	

Chair Biography

Jun Chen
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Jun Chen obtained his B.Sc. and M.Sc. degrees from Nankai University in 1989 and 1992, respectively, and his Ph.D. from Wollongong University (Australia) in 1999. He held the NEDO fellowship at National Institute of AIST Kansai Center (Japan) from 1999 to 2002. He has been working as a full professor in Nankai University since 2002. He has been Cheung Kong Professor in College of Chemistry at Nankai University since 2005 and is now serving as Vice President of Nankai University from 2019. He has been elected as Chairman of Chinese Society of Electrochemistry and a Fellow of the Royal Society of Chemistry (UK) in 2015.

His research activities focus on solid-state materials, nanostructured materials, and energy materials chemistry. He received the State Natural Science Award (the 2nd Grade) in 2011 because of his contribution in H/Li/Mg storage and batteries.

Session Chairs Biography

Song Gao
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Song Gao got his BS and PhD in chemistry at Peking University (PKU) in 1985 and 1991, and then worked at PKU till now. He was a Humboldt Research Fellow in TH Aachen from 1995 to 1997. He has been Cheung Kong Professor in College of Chemistry and Molecular Engineering at Peking University since 2002, and served as dean of this college in 2006-2010. He is now PKU Provost and deputy director of Beijing National Laboratory for Molecular Sciences. He received State Natural Science Award (the 2nd Grade) in 2006 because of his contribution in magnetic coordination polymers and molecular nanomagnets. He was elected as member of Chinese Academy of Sciences in 2007. In the same year, he became a Fellow of the Royal Society of Chemistry (UK). He is member of Editorial Advisory Board for Chem. Soc. Rev., Chemical Science, and Inorganic Chemistry etc., and Editor-in-Chief of Inorganic Chemistry Frontiers.

His research interests are magnetic ordered coordination polymers, molecular nanomagnets, molecular and crystal engineering, and multifunctional molecular materials.

Maochun Hong
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Maochun Hong, an academician of Chinese Academy of Sciences and an academician of TWAS, graduated from the Fuzhou University in 1978 and received his M.S. degree from the Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences in 1981. In 1985-1987, he was a research fellow at Department of Chemistry of the Michigan University and the Illinois University at Chicago in the United States. Since 1994, he has been full professor of Chemistry at the Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences. During this period, he worked as a JSPS visiting professor in Japan in 1998, and obtained his Ph.D degree from Nagoya University.

His research interests are focused on new materials and devices, inorganic functional materials and inorganic-organic hybrid functional materials.

Session Chairs Biography

Hongjie Zhang
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Hongjie Zhang received his PhD in Solid State Chemistry and Material Sciences at Universite de Bordeaux I, Laboratoire de Chimie du Solide du CNRS (France) in 1993. He joined Changchun Institute of Applied Chemistry, CAS, as a professor in 1994.

His current research interests involve lanthanide organic–inorganic hybrid materials, electroluminescent devices, functional nanomaterials and the structure and properties of rare earth magnesium alloys. He has published over 350 papers in peer-reviewed international journals.

Jihong Yu
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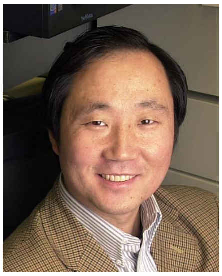
Jihong has been a full professor at Jilin University since 1999, having also completed her BS, MS and PhD there. Between 1996 and 1998 she undertook positions as a post-doctoral researcher at the University of Science and Technology, Hong Kong and as a JST-CREST researcher at Tohoku University in Japan. She is a Fellow of the Royal Society of Chemistry, Secretary-General of the International Zeolite Association (IZA) and in 2015 was officially elected as Academician by the Chinese Academy of Sciences.

Her research group focuses on three main areas, including synthesis of new types of inorganic microporous materials, investigating new routes to the synthesis of inorganic microporous materials, and working toward the rational design and synthesis of inorganic microporous materials.

Biography notes of speakers



Yi Lu
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Dr. Yi Lu received his B.S. degree from Peking University in 1986, and Ph.D. degree from University of California at Los Angeles in 1992 under Professor Joan S. Valentine. After two years of postdoctoral research in Professor Harry B. Gray group at the California Institute of Technology, Dr. Lu started his own independent career in the Department of Chemistry at the University of Illinois at Urbana Champaign in 1994. He is now Jay and Ann Schenck Professor of Chemistry in the Departments of Chemistry, Biochemistry, Bioengineering and Materials Science and Engineering. He is also a member of the Center for Biophysics and Computational Biology and Beckman Institute for Advanced Science and Technology. His research interests lie at the interface between chemistry and biology. His group is developing new chemical approaches to provide deeper insight into biological systems. At the same time, they take advantage of recently developed biological tools to advance many areas in chemistry. Specific areas of current interests include a) design and engineering of functional metalloproteins as environmentally benign catalysis in renewable energy generation and pharmaceuticals; b) Fundamental understanding of DNAzymes and their applications in environmental monitoring, medical diagnostics, and targeted drug delivery; and c) Employing principles from biology for directed assembly of nanomaterials and its applications in photonics and sensing. Dr. Lu has received numerous research and teaching awards, including the Fellow of the American Association for the Advancement of Science (2007), Early Career Award, Society of Biological Inorganic Chemistry (2007), Howard Hughes Medical Institute Professor Award (2002), Camile Dreyfus Teacher-Scholar Award (1999), Alfred P. Sloan Research Fellowship (1998), Research Corporation Cottrell Scholars Award (1997), and the Beckman Young Investigators Award (1996).

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Zhiping Zheng received his B.S. (1987) and M.S. (1990) degrees in chemistry from Peking University, China, and his Ph.D. from UCLA in 1995 with Professor M. Frederick Hawthorne. After conducting postdoctoral research with Professor Richard H. Holm at Harvard University, he joined the faculty of the University of Arizona in 1997, where he is now Professor of Chemistry. His current research interests include the synthetic and structural chemistry of cluster compounds of both lanthanide and transition metal elements.

His contributions in research and teaching have been recognized by a number of awards, including the US National Science Foundation CAREER Award, International Junior Research Award from the European Rare Earths and Actinide Society, the IUPAC Young Observer, and Teaching Excellence from the Honors College, University of Arizona. He serves on the Advisory Board of Crystal Growth and Design, and is also an Overseas Managing Editor for the Journal of Rare Earths.

Biography notes of speakers

John McGrady
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John McGrady gained a BA in chemistry from the University of Oxford in 1990, and then pursued doctoral studies at the Australian National University, Canberra. Following postdoctoral positions in the UK, France and Australia, he took up his first academic post at the University of York in 1997and then moved to the University of Glasgow as WestCHEM chair of chemistry in 2006. 1n 2009 he took up his current position at the University of Oxford, where he is Professor of Computational Inorganic Chemistry and a Fellow of New College.

His research interests revolve around the use of quantum mechanics to explore the properties of inorganic molecules and solids, particularly those containing paramagnetic transition metal ions.

Hiroki Oshio
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Hiroki Oshio graduated from Kyushu University in 1977 and obtained his Ph.D. in 1982. After a postdoctoral fellowship at Marquette University between 1982 and 1984, he was appointed as a research associate at the Institute for Molecular Science (Okazaki, Japan) in 1985. In 1992 he moved to Tohoku University as an Associate Professor, before he was appointed as a Professor at the University of Tsukuba in the Graduate School of Pure and Applied Sciences in 2001.

His research has focused on molecular magnetism, including bistable and spin-crossover systems. He has received an award of The CSJ Award for Creative Work (2005) and has accumulated over 200 peer-reviewed research publications.

Biography notes of speakers

Fangyi Cheng
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Fangyi Cheng received his B.S. (2003) and Ph.D. (2009) from Nankai University, where he was appointed as an assistant professor in 2009 and has been a full professor since 2016. During 2015-2016, he was a visiting scholar at UCLA. His research interests encompass design, synthesis and mechanistic studies of functional materials (particularly 3d transition metal oxides) for electrochemical energy storage and conversion. He has co-authored more than 100 peer reviewed journal papers, owning citations over 16,000 and an H-index of 65 as of August 2019. He is among 2018 Clarivate Highly Cited Scientists and Elsevier Most Cited Chinese Researchers. His honors and awards include Chinese Chemical Society Young Chemist Award, National Natural Science Award (2nd rank, co-winner), etc.

Shu-Hong Yu
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Shu-Hong Yu completed PhD in inorganic chemistry in 1998 from University of Science and Technology of China. From 1999 to 2001, he worked in Tokyo Institute of Technology as a Postdoctoral Fellow, and was awarded the AvH Fellowship (2001-2002) in the Max Planck Institute of Colloids and Interfaces, Germany. He was appointed as a full professor in 2002 and the Cheung Kong Professorship in 2006. He serves as the Director of the Division of Nanomaterials and Chemistry, Hefei National Laboratory for Physical Sciences at Microscale. He is a senior editor for Langmuir and an associate editor for Sci. China Mater. and EnergyChem, and on the editorial board or advisory board of journals Accounts of Chemical Research, Chemistry of Materials, Chemical Science, Materials Horizons, Research, Nano Research, Matter, Trends in Chemistry, and ChemNanoMat.

His research interests include bio-inspired synthesis of inorganic nanostructures, self-assembly of nanoscale building blocks, nanocomposites, their related properties and applications. His research work has been cited more than 45,000 citations (H index 119), named as a Highly Cited Researcher from 2014 to 2018.

Biography notes of speakers

Xianran Xing
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Xianran Xing is Changjiang professor at University of Science and Technology Beijing (USTB), and Fellow of the Royal Society of Chemistry. He received his BS degree in chemistry from Anqing Teachers College (1988), and his Ph.D from Department of Physical Chemistry USTB (1994). His research interests focus on the solid state chemistry, involving syntheses strategy, crystal structure and chemical design for functional materials. The systematic work is done to determine the average structures and local structures of solids.

He leads a group to work on the negative thermal expansion (NTE) in perovskite compounds and related materials, which could be used to tailor thermal expansion coefficients and physical properties. The NTE mechanism is being understood by proposed “spontaneous volume ferroelectrostriction”, which is a new concept, but very common phenomena in ferroelectrics. More than 200 peer-reviewed papers were published in the journals.

Tong-Bu Lu
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Tong-Bu Lu graduated in Chemistry from Lanzhou University in 1993, and then moved to Sun Yat-Sen University as a Postdoctor. He joined to the Faculty member in the same University, and became Professor of Chemistry in 2000. He moved to Tianjing University of Technology in 2016. He worked as a postdoctor in F. Albert Cotton’s group at Texas A&M University in 1998 and 2002. His research interest is coordination chemistry, including macrocyclic chemistry and MOFs. Currently he focuses on the study on artificial photosynthesis, including homogeneous and heterogeneous photo-/electro-catalysts for water splitting and CO2 reduction. He obtained the National Natural Science Foundation for Distinguished Youth Scholar in 2006. He has over 250 scientific publications with H-index of 46. Now, he is a fellow of Royal Society of Chemistry (FRSC), the Editorial Advisory Board of the Journal of CrystEngComm, Current Green Chemistry, Current Pharmaceutical Design, and co-editor of the Journal of Acta C.

Biography notes of speakers

Paula Diaconescu
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Paula Diaconescu joined the Chemistry & Biochemistry Department of University of California, Los Angeles, in 2005, after spending two years as a postdoctoral fellow in the group of Professor Robert Grubbs at the California Institute of Technology. She obtained her PhD degree under the supervision of Professor Christopher Cummins at Massachusetts Institute of Technology, working on arene-bridged complexes of uranium. Her earlier education was completed in Romania, where she obtained her BS from the University of Bucharest and worked on coordination complexes of transition metals and lanthanides at the University Politehnica of Bucharest. Besides awards received from UCLA, she received an Alfred P. Sloan Fellowship (2009), a Friedrich Wilhelm Bessel Research Award from the Alexander von Humboldt Foundation (2014), and a Guggenheim Fellowship (2015).

Her research group is interested in various aspects of metal-ligand cooperation as stem from using ferrocene-based supporting ligands with applications ranging from small molecule activation to the formation of biodegradable polymers. Specific focuses of the group are redox switchable catalysis and biodegradable polymer synthesis.

Oleg Ozerov
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Oleg Ozerov was born in Novosibirsk, Russia in 1976 and spent his formative years there, and in Moscow, Russia. He received his undergraduate training at the Higher Chemical College of the Russian Academy of Sciences. In 1996, Oleg moved to the United States to attend graduate school at the University of Kentucky where he worked with Prof. Folami Ladipo on the chemistry of titanium complexes supported by calix[4]arene-derived arylooxides. After receiving his Ph.D. degree in 2000, Oleg spent two years as a postdoctoral associate in the group of Prof. Ken Caulton at Indiana University investigating new chemistry of ruthenium and rhenium in a pincer ligand context. In the summer of 2002, Oleg joined the Department of Chemistry at Brandeis University as an assistant professor of chemistry and earned promotion to associate professor with tenure in 2006. In January of 2009, Oleg relocated to Texas A&M University where he is now Professor of Chemistry and Coordinator of Graduate Recruiting.

His research interests are in synthetic organometallic chemistry and its diverse applications in catalysis and energy-related problems. Oleg has been honored with the Alfred P. Sloan Research Fellowship (2006), the Camille Dreyfus Teacher-Scholar Award (2007), the ACS Award in Pure Chemistry (2012), and the Norman Hackerman Award in Chemical Research (2012).

Designing Functional Metalloenzymes and their Applications in Biocatalysis for Renewable Energy

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Abstract: Metalloenzymes play critical roles in renewable energy, such as in photosynthesis, biofuel cells and water splitting or oxidation. Designing metalloenzymes is an ultimate test of our knowledge about metalloenzymes and can result in new biocatalysts for practical applications.1 Despite decades of efforts by numerous scientists, most designed metalloenzymes or synthetic model compounds display much lower activity than those of native metalloenzymes. In this presentation, I will provide three examples to demonstrate that, while reproducing the primary coordination sphere may be good enough to make structural models of metalloenzymes, careful design of the non-covalent secondary coordination sphere interactions is required to create functional metalloenzymes with high activity.1 In the first example, we have met a key challenge in fuel cell catalysis for oxygen reduction reaction (ORR), which uses precious metals (e.g., Pt) and has a high overpotential. We show that the presence of waters as part of new hydrogen-bonding network is necessary to confer ORR activity in reducing O2 to water with minimum release of other reactive oxygen species using earth abundant metal ions (e.g., Fe and Cu), with activity similar to that of native enzymes.2 In the second example, we have addressed a major issue in energy research in that most active catalysts work at a high cost of overpotentials and it is difficult to carry out reactions at minimal or zero overpotential without sacrificing the activity. We have been able to demonstrated that the fine-tuning of reduction potentials of azurin, a member of cupredoxin family that are involved in long-range electron transfers (ET) in many biological processes such as photosynthesis, to span the entire physiological potential range of ~2 V, through carefully design of hydrophobicity and hydrogen bonding networks around the primary coordination sphere.3 A combination of the above approach with rational tuning of redox potentials have recently resulted in new ORR catalyst with a very low over-potential.4 In the last example, we have been able to computationally design a complex heme-[4Fe-4S] center to structurally and functionally mimic sulfide reductase, which play a major role in global sulfur cycle, with activity similar to that of native enzyme.5 Recent results and their implications for designing novel biocatalysts for alternative energies will be discussed.

References:

1. a) Y. Lu, et al., Nature 460, 855 (2009); b) E. N. Mirts, A Bhagi-Damodaran, and Y. Lu, Acc. Chem. Res. 52, 935–944 (2019).
2. a) K. D. Miner, et al., Angew. Chem., Int. Ed. 51, 5589 (2012); b) Yang Yu, et al., J. Am. Chem. Soc. 137, 11570–11573 (2015).
3. a) N. M. Marshall, et al., Nature 462, 113 (2009); b) Parisa Hosseinzadeh, et al., Proc. Natl. Acad. Sci. USA 113, 262-267 (2016).
4. A Bhagi-Damodaran, J. Am. Chem. Soc. 136, 11882-11885 (2014).
5. E. N. Mirts, Science 361, 1098-1101 (2018).

Hydrogen Production by Aqueous-phase Reforming of Methanol Promoted by Grubbs and Hoveyda-Grubbs Catalysts

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Abstract: Hydrogen gas is a promising sustainable energy carrier. However, practical applications are hampered by its low volumetric energy density. Efforts have therefore been focused on the development of advanced storage methods, of which the exploration of liquid organic hydrogen carriers (LOHCs) has received much recent interest. Hydrogen gas can be generated upon chemical reactions of an LOHC which is otherwise stable and can be easily handled and transported. Aqueous solution of methanol is one such system of interest due to its high hydrogen content and ready accessibility from biomass or industrial sources. In 2013, the groups of Beller and Grützmacher independently reported the first attempts using ruthenium complexes as catalysts in aqueous-phase reforming of methanol to produce hydrogen.1,2 Several other catalysts for a similar purpose were reported in the years that followed. Progress notwithstanding, the number of catalysts for effective aqueous-phase reforming of methanol remains small. We have recently explored the use of Grubbs and Hoveyda-Grubbs catalysts along the same line of interest. In this talk, our findings will be presented, along with the experimental and theoretical studies of a mechanism possibly responsible for the observed catalysis.

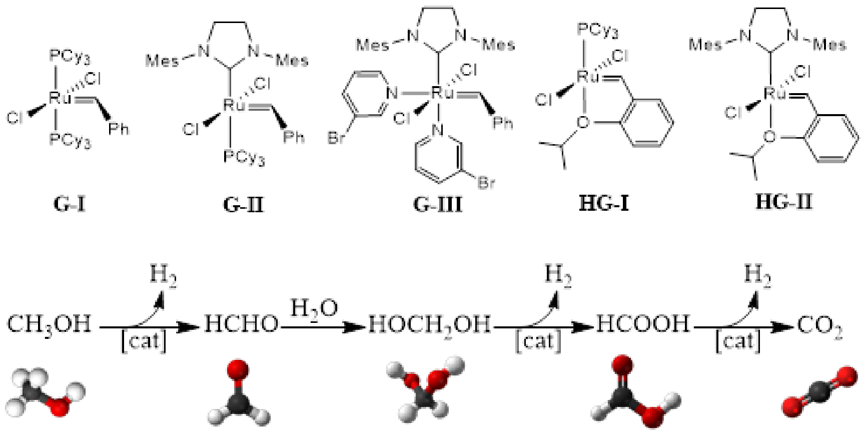

Figure 1. Hydrogen production by reforming an aqueous solution of methanol using Grubbs (G-I, G-II, and G-III) and Hoveyda-Grubbs (HG-I and HG-II) catalysts.

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Metal clusters on the localized/delocalized borderline

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Abstract: Transition metal clusters traditionally fall into one of two distinct classes: covalent, or exchange coupled. The former is typically the province of organometallic chemistry, classic examples being carbonyl clusters such as Ru3(CO)9 where covalent metal-metal bonds are integral to stability. The metal ions in exchange coupled systems, in contrast, are not linked by direct covalent bonds but rather by super-exchange interactions mediated by bridging ligands. Quite distinct theoretical paradigms have evolved to deal with these two distinct classes: molecular orbital theory, with its emphasis on delocalized bonding, is generally applied to covalent clusters whilst the language of valence bond theory is more appropriate for exchange coupled systems. In this presentation, I will explore the electronic structure of systems that lie at the intersection of these two apparently quite distinct regimes, and show how their properties are remarkably dependent on subtle perturbations to their environment.[1,2,3] Perhaps unsurprisingly, an accurate treatment of electron-electron repulsion is absolutely essential for a balanced treatment, and the choice of density functional proves to be critical. Here, we tension the results of DFT against correlated ab initio methods (CASPT2) and highlight the factors that control the balance between the localized and delocalized regimes.

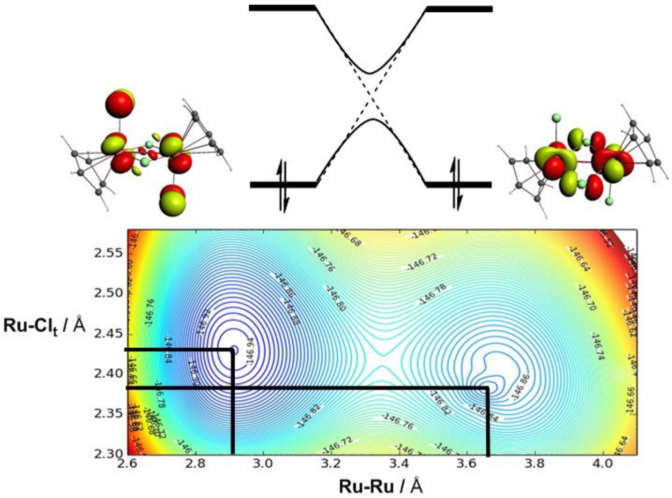

Figure 1: Two-dimensional potential energy surface for $CpClRu(\mu\text{-}Cl)_2RuCpCl$, highlighting the double minima corresponding to covalent and exchange coupled limits.

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3. J. E. McGrady, Angew. Chem., Int. Ed., 2000, 39, 3077.

A Metal complexes with multi-accessible electronic states

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Abstract: Next-generation molecular devices will rely on simple, nanoscale species possessing multiple distinct electronic states which can be reversibly switched under the application of external stimuli.[1] These have long been shown to exhibit an attractive variety of switchable magnetic, electronic and optical properties in response to temperature, light, pressure or guest absorption/desorption.[3] A key advantage of employing such species is their amenability to novel molecular design approaches which allows control over both their structure and composition, but also the potential for fine tuning of their electronic properties by modification of both the inner- (via ligand design),[4] and outer- (via hydrogen-bonding, ani or solvent interactions) coordination spheres.[5]

Recently, the development of pH-responsive systems via multi-dentate ligands which retain an acidic proton – such as free imidazole or pyrazole N H moieties – allow the design of a new class of switchable complexes. We report here metal complexes of which electronic sates can be tuned by protonation/deprotonation of "Brønsted ligands", acting simultaneously as both Brønsted acids and bases.

References:

1. a) O. Kahn, C. J. Martinez, Science 1998, 279, 44-48; b) F. Prins, M. Monrabal-Capilla, E. A. Osorio, E. Coronado, H. S. J. van der Zant, Adv. Mater. 2011, **23**, 1545-1549; c) G. Aromí, D. Aguilà, P. Gamez, F. Luis, O. Roubeau, Chem. Soc. Rev. 2012, **41**, 537-546; d) O. Sato, Nature Chem. 2016, **8**, 644.
2. F. Lambert, C. Policar, S. Durot, M. Cesario, L. Yuwesi, H. Korri-Youssoufi, B. Keita, L. Nadjo, Inorg. Chem. 2004, **43**, 4178-4188.
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Artificial Photosynthesis Catalysts

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Abstract: Global energy shortage and climate deterioration caused by CO2 greenhouse gas emission are two well-known issues that greatly threaten the sustainable development of human beings. The solar-driven reduction of CO2 into chemical fuels/feedstocks represents a potential strategy for solving the above issues of energy crisis and global warming caused by increasing CO2 emission. The critical bottleneck of this project is to develop cheap and stable photocatalysts and electrocatalysts that can selectively and effectively reduce CO2 into a single chemical fuel/feedstock, using water as an electron source.

In this presentation, we will present the investigations on the synthesis and catalytic performance of a series of homogeneous and heterogeneous Artificial photosynthesis catalysts [1-8].

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Bio-Inspired Synthesis and Self-Assembly of Functional Materials

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Abstract: There is a rich and long history of gaining inspiration from nature for the design of practical materials and systems. Biominerals are well-known composites of inorganic and organic materials in the form of fascinating shapes and high ordered structures, which exist in Nature, for example, pearl, oyster shells, corals, ivory, sea urchin spines, cuttlefish bone, limpet teeth, magnetic crystals in bacteria, and human bones, created by living organisms. During the past few decades, it has been one of the hottest research subjects in materials chemistry and its cutting-edge fields to explore new bio-inspired strategies for generation of materials with controlled morphologies, unique structural specialty, and complexity. This lecture will present our recent advances on bio-inspired synthesis of a family of inorganic or inorganic-organic micro-/nano- structural materials and their macroscopic scale assemblies, including bio-inspired molecule induced synthesis of micro-/nano-inorganic materials, bio-inspired interfacial assembly of macroscopic assemblies and functionalization. Especially, we will report our recent effort on how to realize the production of bulk materials, such as synthetic nacre1 and artificial woods,2 spanning all the length scales, either by predesigned matrix-directed mineralization process1 or a bottom-up self-assembly process.3 These macroscopic nanoparticle assemblies are emerging as a new material system1-7, showing enormous application potentials in diverse fields.

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Local structure and negative thermal expansion in nano solids

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Abstract: Most of solids expand upon heating, however, a few of them contract, called negative thermal expansion (NTE). NTE originates from ferroelectrics, spin, magnetic transition, but also from nanosize effects. The lattice deviation between bulk and nanocrystalline in different temperatures provides a new perspective accessing the complicated local structure, which is a great challenge in the field of modern nanoscience. For expample, an atomic insight into the local chemical ordering and lattice strain is particular interesting to recent emerging bimetallic nanocatalysts such as PtNi alloys. Here, we reported the atomic distribution, chemical environment and lattice thermal evolution in full-scale structural description of PtNi alloy nanoparticles (NPs). The different segregation of elements in the well-faceted PtNi nanoparticles is convinced by extended X-ray absorption fine structure (EXAFS). Atomic pair distribution function (PDF) study evidences the co-existence of the face-centered cubic phase and tetragonal ordering phase in the nanoparticles. Further reverse monte carlo (RMC) simulation with PDF data obviously exposed the segregation as Ni and Pt in the centers of {111} and {001} facets respectively. Layer-by-layer statistic analysis up to 6 nm for the local atomic pairs revealed the distribution of local tetragonal ordering on the surface. This local coordination environment facilitates the distribution of heteroatomic Pt-Ni pairs, which plays an important role in the negative thermal expansion of $Pt_{41}Ni_{59}$ NPs. The present study on PtNi alloy NPs from local short-range coordination to long-range average lattice provides a new perspective on tailoring physical properties in nanomaterials.

Keywords: negative thermal expansion (NTE), nanoscaled solid, local structure.

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Mild, Controllable Synthesis of Transition Metal Oxide/Hydroxide Electrodes

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Abstract: First row 3d-electron transition metal oxides and hydroxides have been widely investigated as electrode materials for electrochemical energy storage and conversion, because of advantages including high abundance, low cost, and rich redox chemistry.1,2 Their efficient use depends to a large extent on the rational preparation and understanding of the structure-properties relationship. In recent years, we have developed mild synthesis routes for a series of metal oxides and investigated their electrochemical properties.3-15 For example, a solution-based methodology involving oxidation-precipitation and insertion-crystallization at ambient atmosphere and temperatures lower than 200 oC was employed to prepare ultrasmall spinel oxide with controllable cubic/tetragonal phase and composition.3,9,12 We also developed a versitile cathodic electrodeposition of metal hydroxide/oxide hybrid materials by taking advantages of oxyacid anion insertion in graphene layers to enhance deposit/substrate interaction.15 These mild synthetic methodologies allow in situ formation of homogenous oxide/carbon nanocomposites with strong metal-oxygen-carbon coupling or generation of carbonaceous substrate-supported electrode materials, which helps to build robust electron conducting network and to reduce charge transfer barrier. Our electrochemical results indicate the importance of tuning metal valence and nonstoichiometry in enhancing the performance. Particularly, for Mn-based oxides, multivalent Mn and moderate oxygen vacancies are found to favor oxygen electrocatalysis while the Mn deficiency benefits fast and reversible intercalation of Zn ions.4,7,11 Some of our latest results will be discussed in this talk.

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Redox switchable ring opening copolymerization

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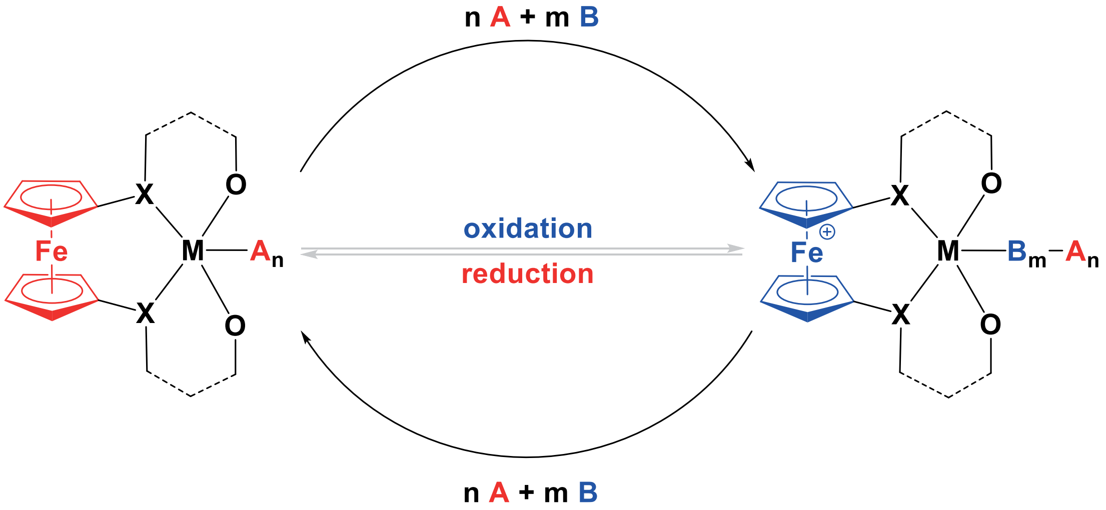
Abstract: Switchable polymerization processes have received increased attention because they hold the promise of mimicking the selectivity exhibited by natural systems. We are studying a chemical method to shuttle between two catalyst states, by switching the oxidation state of iron in ligands containing a ferrocene backbone. This idea is applied to the ring opening polymerization of cyclic esters/ethers catalyzed by transition metal complexes with the goal of forming biodegradable copolymers.



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Bond activation reactions by boryl pincer complexes

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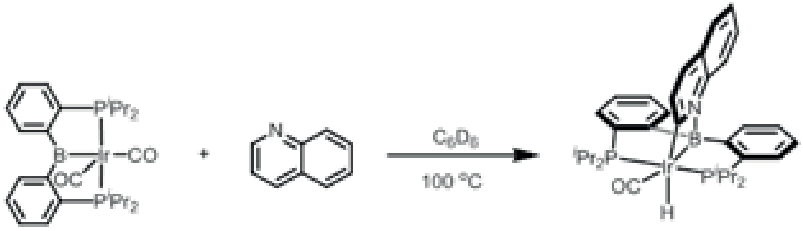
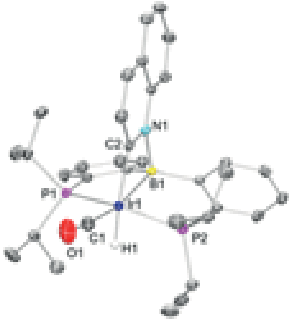
Abstract: Pincer complexes of late transition metals have been widely used in studies of stoichiometric and catalytic activation of carbon-hydrogen and carbon-heteroatom bonds. Our group recently demonstrated the impressive potential of Ir pincer complexes in C-H bond borylation of terminal alkynes and arenes. Studies of transformations that involve metal-boryl intermediates where the boryl group originates from a reagent have led us to consider alternative approaches to bond activation that incorporate boryl donors into supporting pincer ligands. We have discovered that activation C-H and other bonds of heteroatom-containing substrates is possible with selectivity controlled by the coordination of the heteroatom to the metal-bound boryl donor. The presentation will focus on the stoichiometric reactions and on the current efforts to optimize this type of reactivity for catalytic applications.



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