

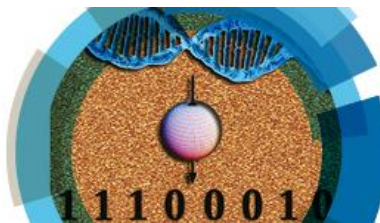
The 2nd Inorganic Chemistry Frontiers International Symposium

14 March 2017, Nanjing, China

School of Chemistry and Chemical Engineering, Nanjing University
(南京大学化学化工学院)

Register now

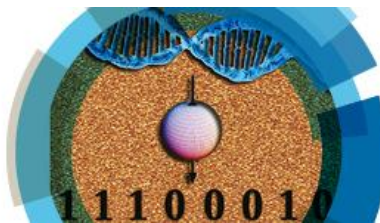
rsc.li/icfis17



Programme

School of Chemistry and Chemical Engineering, Nanjing University (南京大学化学化工学院)

Time	Event	Session Chair
08:50-09:00	Openning Remarks Jinglin Zuo (左景林), Nanjing University Daping Zhang (张大平), Royal Society of Chemistry	
09:00-09:30	Zijian Guo (郭子建), Nanjing University Functionalization of Platinum Anticancer Complexes	Chair of Session 1 John McGrady Oxford University
09:30-10:00	Qiangbin Wang (王强斌), Suzhou Institute of Nano-Tech and Nano-Bionics, CAS Ag ₂ S Quantum Dot: A New Near-Infrared-II Fluorescence Nanoprobe for In Vivo Bioimaging	
10:00-10:30	Ling Huang (黄岭), Nanjing Tech University Luminescent Rare Earth Nanomaterials and Applications	
10:30-10:50	Coffee & Tea (20 min)	
10:50-11:20	Zhiping Zheng (郑智平), University of Arizona Transition Metal Clusters as Novel Platforms for Chemical Transformations and Materials Development	Chair of Session 2 Zijian Guo (郭子建) Nanjing University
11:20-11:50	John McGrady , Oxford University Metallo-Silicon Clusters: A Computational Chemist's Playground	
11:50-12:20	Oleg V. Ozerov , Texas A&M University New Chemistry With Boron In and Out of Pincers	
12:20-13:40	Lunch (80 min)	
13:40-14:10	Yi Xie (谢毅), University of Science and Technology of China Design of the Ultrathin 2D Electrocatalysts for Promoting CO ₂ Reduction	Chair of Session 3 Hiroki Oshio University of Tsukuba
14:10-14:40	Yaqian Lan (兰亚乾), Nanjing Normal University The Application of Polyoxometalate-based Composite Materials in Energy Storage and Conversion	
14:40-15:10	Yong Cui (崔勇), Shanghai Jiaotong University Design of Chiral Covalent Organic Frameworks for Enantioselective Processes	
15:10-15:30	Coffee & Tea (20 min)	
15:30-16:00	Hiroki Oshio , University of Tsukuba Metal complexes with bistability	Chair of Session 4 Oleg V. Ozerov Texas A&M University
16:00-16:30	Hiroshi Kitagawa , Kyoto University Dimensional Crossover in Coordination Chemistry	
16:30-17:00	Song Gao (高松), Peking University Ferroelectric molecular magnets and single-ion magnets	
17:00	Closing Remarks Song Gao (高松), Peking University	



Zijian Guo

郭子健

**School of Chemistry and Chemical
Engineering, Nanjing University, Nanjing
210023, China**

—

Email: zguo@nju.edu.cn

Zijian Guo was born in Hebei, China in 1961. After receiving his PhD degree from the University of Padua in 1994, he worked as a postdoc fellow at the University of London, the University of British Columbia and the University of Edinburgh successively. He joined Nanjing University as a professor in 1999 and served as the director of the State Key Laboratory of Coordination Chemistry from 2000 to 2009 and the dean of the School of Chemistry and Chemical Engineering from 2006 to 2014. He is currently the Changjiang professor in the same school of Nanjing University. His research interests include the metal-based anticancer complexes, fluorescent sensors for biorelated metal cations, and metal-based artificial nucleases and proteases.

Functionalization of Platinum Anticancer Complexes

Zijian Guo

School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210023, China

Platinum-based antitumor drugs play an important role in the treatment of various malignancies such as colorectal and testicular cancers. Functionalization of platinum anticancer complexes with nanoparticles, fluorescent tags, or MRI contrast could potentially leads to multi-modal systems for cancer therapy and diagnosis.

In the last few years, our lab has been focusing on the molecular design of platinum-based antitumor complexes with novel functional models. For example, the combination of a red light PDT agent and a Pt(II)-based chemotherapeutic drug gives conjugated complexes which maintain the intrinsic functions of each unit. By conjugating cisplatin with superparamagnetic nanoclusters a high drug loading capacity and pH-responsive controlled release system was obtained. Maghemite nanoparticles can be modified with cisplatin to lead a conjugate which is highly cytotoxic toward MCF-7 and Hela cells. The diagnostic capability and tumor-specific accumulation of the conjugate under in vitro and in vivo conditions are verified by the time-dependent negative-contrast enhancement effect in MRI using MCF-7 cells and tumor-bearing mice, respectively. Theranostic potential can be achieved by linking Gd-DTPA MRI contrast agent with cisplatin units.

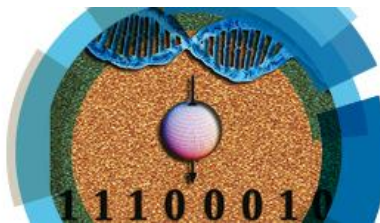
In another approach, we designed a nanocarrier system which can synergistically release platinum anticancer drugs and O₂ in an H₂O₂-responsive manner. Such a system combines the advantages of chemotherapy and oxygen therapy and demonstrated improved therapeutic efficacy against cisplatin resistant cell lines which often appear to be in hypoxia. Using similar strategy, we devised a nano-composite composed of photosensitizer and catalase in the aqueous core, black hole quencher in the polymeric shell, and functionalized with a tumor targeting ligand c(RGDfK). Such a nano-system can be selectively taken up by αvβ₃ integrin-rich tumor cells, generation of O₂ and release of photosensitizer can be realized at the same time.

References

1. Z.Z. Zhu, Z.H. Wang, Y.G. Hao, C.C. Zhu, Y. Jiao, H.C. Chen, Y.M. Wang, J. Yan, Z.J. Guo, X.Y. Wang, *Chem. Sci.*, **2016**, 7, 2864.
2. Y.F. He, Y. Ding, D. Wang, W.J. Zhang, W.Z. Chen, X.C. Liu, W.J. Qin, X.H. Qian, H. Chen, Z.J. Guo, *Chem. Sci.*, **2015**, 6, 2074.
3. H.C. Chen, J.W. Tian, W.J. He, Z.J. Guo, *J. Am. Chem. Soc.*, 2015, 137, 1539.
4. X.Y. Wang, X.H. Wang, Z.J. Guo, *Acc. Chem. Res.*, **2015**, 48, 2622.
5. Z.Z. Zhu, X.Y. Wang, T.J. Li, S. Aime, P.J. Sadler, Z.J. Guo, *Angew. Chem. Int. Ed.*, **2014**, 53, 13225.
6. Y.F. He, J. Yuan, Y.C. Qiao, D. Wang, W.Z. Chen, X.C. Liu, H. Chen, Z.J. Guo, *Chem. Commun.*, **2015**, 51, 14064.
7. H.C. Chen, W.J. He, Z.J. Guo, *Chem. Commun.*, **2014**, 50, 9714.
8. N. Muhammad, Z.J. Guo, *Curr. Opin. Chem. Biol.*, **2014**, 19, 144.

Acknowledgements

We thank the financial supports from the National Science Foundation of China and the Ministry of Science and Technology of China



Qiangbin Wang

王强斌

Suzhou Institute of Nano-Tech and Nano-Bionics, Chinese Academy of Sciences,
Suzhou 215123, China

—

Email: gbwang2008@sinano.ac.cn

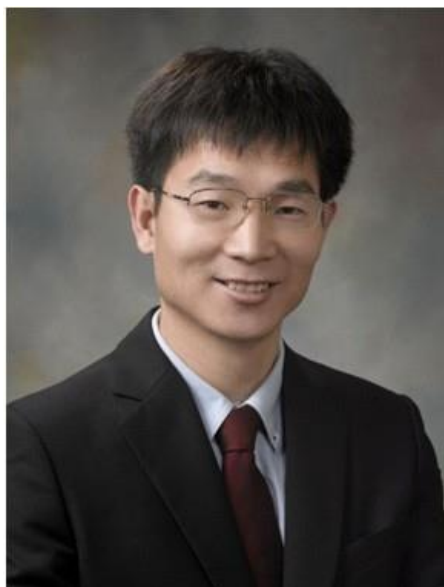
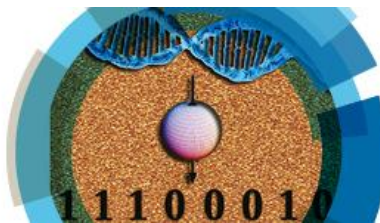
Qiangbin Wang received his B.S. and Master degree in Chemistry from Petroleum University of China in 1996 and 1999, respectively. He got his Ph.D. in Material Sciences from East China University of Science and Technology in 2002, and then joined Shanghai Jiaotong University as a Research Associate. From 2004 to 2008, he worked as a Postdoctoral Associate and an Assistant Research Professor at Arizona State University. In July of 2008, he joined Suzhou Institute of Nano-Tech and Nano-Bionics (SINANO), Chinese Academy of Sciences. He is now a Professor in the Division of Nanobiomedicine at SINANO and Director of the Key Laboratory of Nano-Bio Interface, Chinese Academy of Sciences. He is the recipient of National Science Fund for Distinguished Young Scholars and Japanese Chemical Society for Distinguished Lectureship Award. His main research interests lie at the Nano-Bio interface, with a particular emphasis on in vivo bioimaging with fluorescence in the second near-infrared window.

Ag₂S Quantum Dot: A New Near-Infrared-II Fluorescence Nanoprobe for In Vivo Bioimaging

Qiangbin Wang

CAS Key Laboratory of Nano-Bio Interface, Suzhou Institute of Nano-Tech and Nano-Bionics, Chinese Academy of Sciences, 398 Ruoshui Road, Suzhou, 215123, China

Fluorescent imaging in the second near-infrared window (NIR-II, 1.0~1.4 μm) is appealing due to minimal autofluorescence and negligible tissue scattering in this region, affording maximal penetration depth for deep tissue imaging with high feature fidelity. Herein, for the first time, we reported a new type of NIR-II QDs-Ag₂S QDs and executed a series of bioapplication studies by using Ag₂S QDs. The results show that, by using Ag₂S QDs, the tissue penetration length can reach 1.5 cm, and the spatial and temporal resolution of the in vivo imaging can down to 25 μm and 50 ms, respectively, which are improved several to dozens of times in comparison with those using conventional fluorescence nanoprobes in the visible emission region. Further, this advanced NIR-II fluorescence of Ag₂S QDs was employed for high signal to noise ratio detection of tumor in vivo, dynamical monitoring the tumor angiogenesis, stem cell tracking and regeneration in vivo, and imaging-guided drug delivery and surgery of glioma, *etc.*



Ling Huang

黄岭

Institute of Advanced Materials (IAM),
Nanjing Tech University

—

Email:

iamlhuang@njtech.edu.cn

Dr. **Ling HUANG** received his Ph.D. degree in Chemistry from Nanjing University in 2001. He then pursued post-doctoral research at the University of California, Berkeley (Gabor A. Somorjai), Florida State University (Seunghun Hong), and Northwestern University (Chad A. Mirkin). After that, he worked as a senior research scientist at the Biochemical Division of Corning Incorporated in 2008 and then joined Nanyang Technological University in Singapore as an associate professor since 2009. Starting from August of 2012, Dr. Huang worked as a professor and deputy director of the Institute of Advanced Materials (IAM), at Nanjing Tech University, China. His current research focuses on design, synthesis, and tuning of the optical properties of lanthanide-doped nanocrystals and their related nanocomposites. He has published over 80 scientific research articles in *Nature*, *Science*, *J. Am. Chem. Soc.*, *Angew. Chem. Int. Ed.*, *Adv. Mater.*, *Small*, *Chem. Commun.*, *Nanoscale* and so on, with a total citation of more than 2500 times.

Scandium-Based Luminescent Nanomaterials

Ling Huang

Institute of Advanced Materials (IAM), Nanjing Tech University

In the past decades, rare earth-based upconversion luminescent nanomaterials have drawn greatly increased attention due to their superior optical properties including narrow emission bandwidth, large anti-Stokes shifts, high photostability, long life-time, deep tissue penetration, and low cytotoxicity.

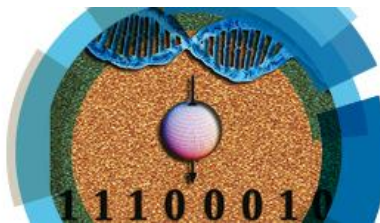
However, majority of the studies have been focused on Y- and lanthanide-based nanomaterials while quite few attention has been paid on Scandium-based nanomaterials while on the other side, Sc sits at the junction between the top of the rare earth column and the beginning of the transition metal row, which has imparted unique chemical and physical properties to Sc and its compounds. For example, both the chemical compositions and the crystal structures of $\text{Na}_x\text{ScF}_{3+x}$ are very sensitive to the synthesis experimental conditions, they also emit strong red upconversion luminescence, different from those of the hexagonal phase nanomaterials of Y- and lanthanide-based fluorides, which usually generate strong green upconversion luminescence.¹⁻⁵

21 Sc 钪 3d ¹ 4s ² 44.96	22 Ti 钛 3d ² 4s ² 47.87	23 V 钒 3d ³ 4s ² 50.94	24 Cr 铬 3d ⁵ 4s ¹ 52.00	25 Mn 锰 3d ⁵ 4s ² 54.94
39 Y 钇 4d ¹ 5s ² 88.91				
57-71 La-Lu 镧系				

Fig. 1. Position of Sc in the periodic table.

References

1. Teng, X.; Zhu, Y.; Wei, W.; Wang, S.; Hu, W.; Tok, A. I. Y.; Han, Y.; Zhang, Q.; Fan, Q.; Huang, W.; Capobianco, J. A.; Huang, L. *J. Am. Chem. Soc.* **2012**, 134, 8340-8343.
2. Ding, Y.; Teng, Pei, W.; Zhu, J. J.; Huang, L.; Huang, W. *Nanoscale* **2013**, 5, 11928-11932.
3. Wang, X.; Chang, H.; Xie, J.; Huang, L.; Huang, W. *Coord. Chem. Rev.* **2014**, 273-274, 201-212.
4. Pei, W.-B.; Chen, B.; Teng, X.; Lau, R.*; Huang, L.*; Huang, W., *Nanoscale* **2015**, 7, 4048-4054.
5. Zhao, B.; Xie, X.; Xu, S.; Pan, Y.; Yang, B.; Guo, S.; Wei, T.; Su, H.; Wang, H.; Chen, X.; Dravid, V. P.; Huang, L.; Huang, W. *Adv. Mater.* **2016**, 28, 6665-6671.



Zhiping Zheng

郑智平

**Department of Chemistry and
Biochemistry, The University of Arizona,
Tucson, Arizona 85721, USA**

—

Email: zhiping@email.arizona.edu

Zhiping Zheng received his BS (1987) and MS (1990) degrees in Chemistry from Peking University, China, and his PhD from University of California (Los Angeles) 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 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.

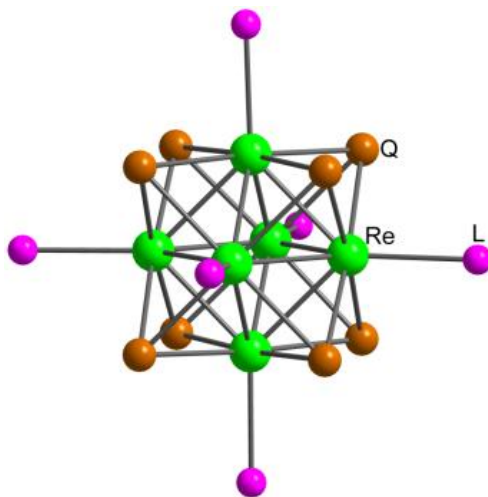
His current research interests include the synthetic and structural chemistry of cluster compounds of both lanthanide and transition metal elements.

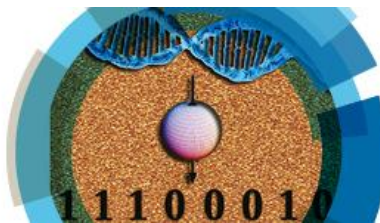
Transition Metal Clusters as Novel Platforms for Chemical Transformations and Materials Development

Zhiping Zheng

Department of Chemistry and Biochemistry, the University of Arizona, Tucson, Arizona 85721, USA

Transition metal clusters are a unique class of chemical substances. Not only do they have well-defined molecular structures, they also exhibit interesting and potentially useful properties that are inherent to metal-metal bonded species. To be presented are highlights of our research in developing synthetic methodologies necessary to bring a cluster system out of the limited sphere of fundamental cluster chemistry and into general synthetic applicability. Specifically, the design and synthesis, structural characterization, and synthetic uses of judiciously chosen cluster complexes of the $[\text{Re}_6(\mu_3\text{-Se})_8]^{2+}$ core (see figure) will be discussed. Key findings in three areas of research will be detailed. In the first area, we explore the uses of site-differentiated cluster complexes as stereospecific building blocks for supramolecular construction. A great variety of cluster-supported molecular and supramolecular architectures have been realized, some of which display rather interesting electronic and spectroscopic properties. In the second area, we pursue the activation of small-molecule ligands (MeCN, CO) by the Lewis acidic cluster core and subsequent chemical transformations, with an eye on developing novel catalytic schemes. Along a third and distinct direction of research, we develop cluster-containing functional materials, for light-emitting or optical limiting applications. Together, these results mark the beginning of what promises to be an exciting new chapter in cluster chemistry and materials.





John E. McGrady

Department of Chemistry, University of
Oxford, OX1 3QZ, United Kingdom

—

Email: john.mcgrady@chem.ox.ac.uk

John McGrady graduated with a BA in Chemistry from the University of Oxford in 1990, and then studied for a PhD at the Australian National University in Canberra (graduated 1994). Following academic appointments at the Universities of York and Glasgow, he was appointed as Professor of Computational Inorganic Chemistry at the University of Oxford in 2009.

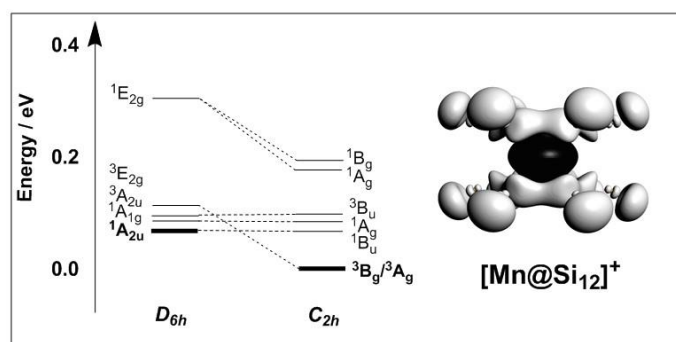
His research interests lie in the electronic structure and properties of inorganic compounds, with a particular emphasis of systems with open electron shells.

Metallo-Silicon Clusters: A Computational Chemist's Playground

John E. McGrady

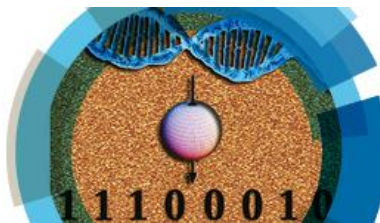
Department of Chemistry, University of Oxford, OX1 3QZ, United Kingdom

The structures and electronic properties of endohedral clusters of the tetrel elements Si, Ge, Sn, Pb, $M@E_n$, are of great interest to both the physics and chemistry communities. To a physicist, clusters such as $M@Si_n$ clusters represent the smallest conceivable models for metal impurities in bulk silicon, and designing systems which retain the characteristic magnetic properties of the encapsulated metal is an important target. From a chemical perspective, the Wade-Mingos rules provide an important framework for understanding the structure of clusters, although the emphasis is firmly on the bonding within the cluster rather than between the cluster and the metal. A coordination chemist might, in contrast, regard the cluster as a pseudo ligand, donating and potentially accepting electron density from the metal. Our recent work on clusters containing first-row transition metals suggests that open-shell character is in fact dominant in many cases, particularly in the middle of the period, and this has profound effects on the structural and spectroscopic properties of the clusters. Using a combination of unrestricted DFT and *ab initio* techniques, I will try to develop a consistent model that captures the properties of this diverse class of compounds.¹



References

1. V. Arcisauskaite, D. Fijan, M. Spivak, C. de Graaf and J. E. McGrady, *PhysChemChemPhys* **2016**, 8, 24006.



Oleg V. Ozerov

Department of Chemistry, Texas A&M
University, College Station, TX 77845,
USA

—

Email: ozеров@chem.tamu.edu

Oleg V Ozerov 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 Professor Folami Ladipo on the chemistry of titanium complexes supported by calix[4]arene-derived aryl oxides. After receiving his PhD degree (2000), Oleg spent two years as a Postdoctoral Associate in the group of Professor Ken Caulton at Indiana University. He spent his time there investigating new chemistry of ruthenium and rhenium in a pincer ligand context. In 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 2009, Oleg relocated to Texas A&M University where he is now Professor of Chemistry and Coordinator of Graduate Recruiting. 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).

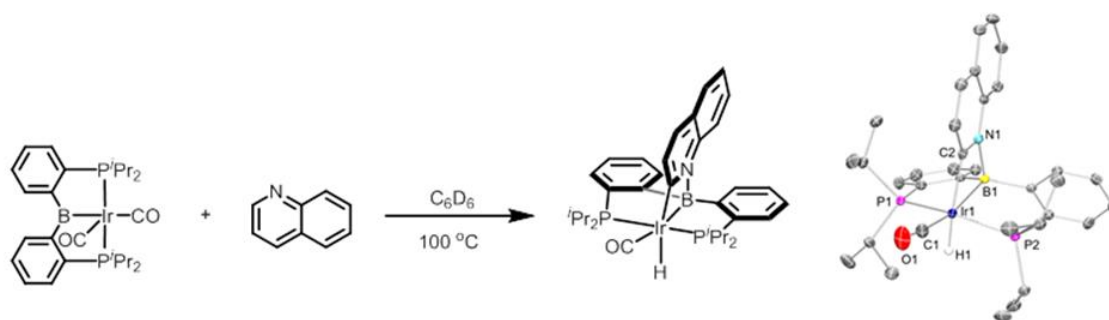
His research interests are in synthetic organometallic chemistry and its diverse applications in catalysis and energy-related problems.

New Chemistry with Boron In and Out of Pincers

Oleg V. Ozerov

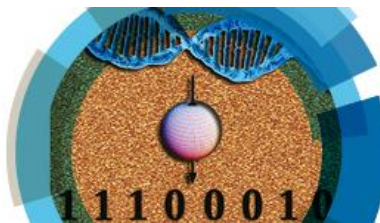
Department of Chemistry, Texas A&M University, College Station, TX 77845, USA

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^{1,2} and arenes.³ 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.⁴ We have discovered that activation C-H and other bonds of heteroatom-containing substrates is possible with unique selectivities relying on coordination of the heteroatom to the metal-bound boryl donor. The current efforts are focused on optimizing this type of reactivity for catalytic applications.



References

1. "Catalytic Dehydrogenative Borylation of Terminal Alkynes by a SiNN Pincer Complex of Iridium", Lee, C.-I.; Zhou, J.; Ozerov, O. V. *J. Am. Chem. Soc.* **2013**, 135, 3560-3566.
2. "Ligand Survey Results in Identification of PNP Pincer Complexes of Iridium as Long-lived and Chemoselective Catalysts for Dehydrogenative Borylation of Terminal Alkynes", Lee, C.-I.; DeMott, J. C.; Pell, C. J.; Christopher, A.; Zhou, J.; Bhuvanesh, N.; Ozerov, O. V. *Chem. Sci.* **2015**, 6, 6572-6582.
3. "High-Turnover Aromatic C-H Borylation Catalyzed by POCOP-type Pincer Complexes of Iridium", Press, L. P.; Kosanovich, A. J.; McCulloch, B. J.; Ozerov, O. V. *J. Am. Chem. Soc.* **2016**, 138, 9487-9497.
4. "Facile Insertion of Rh and Ir into a Boron-Phenyl Bond, Leading to Boryl/Bis(phosphine) PBP Pincer Complexes", Shih, W.-C.; Gu, W.; MacInnis, M. C.; Timpa, S. D.; Bhuvanesh, N.; Zhou, J.; Ozerov, O. V. *J. Am. Chem. Soc.* **2016**, 138, 2086-2089.



Yi Xie

谢毅

Collaborative Innovation Center of
Chemistry for Energy Materials,
University of Science and Technology of
China, Hefei, , 230026, P. R. China

Email: yxie@ustc.edu.cn

Dr Yi Xie received her BS in Xiamen University (1988) and PhD at University of Science and Technology of China (1996). She was appointed as the Cheung Kong Scholar Professor of inorganic chemistry in 2000, and is also a recipient of many awards, including China Young Scientist Award (2002), China Young Female Scientist Award (2006) and IUPAC Distinguished Women in Chemistry/Chemical Engineering Award (2013). She is now a Principal Investigator of the Department of Nanomaterials and Nanochemistry at Hefei National Laboratory for Physical Sciences at Microscale and a Full Professor of Chemistry at the University of Science and Technology of China.

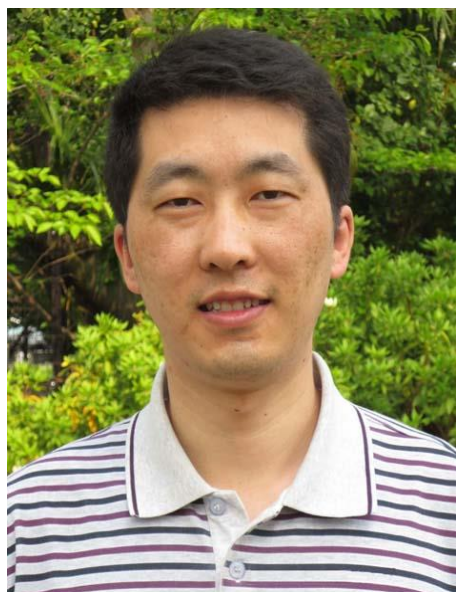
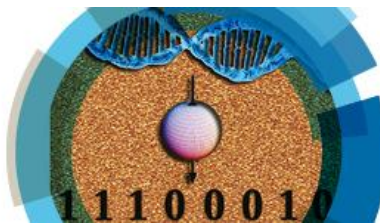
Her research interests are in solid state and materials chemistry.

Design of the ultrathin 2D electrocatalysts for promoting CO₂ reduction

Yi Xie

Hefei National Laboratory for Physical Sciences at the Microscale, Collaborative Innovation Center of Chemistry for Energy Materials, University of Science and Technology of China, Hefei, Anhui, 230026, P. R. China

This study firstly reviews our group's recent advances in the controllable synthesis, fine structure and defect characterization, and electronic structure modulation of ultrathin 2D semiconductors. The optimized electronic/phonon structures with efforts to achieve enhanced photocatalytic and thermoelectric efficiencies, finally enabled these ultrathin semiconductors promising opportunities for harvesting solar energy to generate chemical energy or for converting waste heat into electricity. For instance, to achieve promoted CO₂ electroreduction performances, we proposed that ultrathin 2D electrocatalysts can offer ultralarge fraction of active sites, high electric conductivity and superior structural stability, which holds great promise for designing efficient and robust catalysts for CO₂ electroreduction. Specifically, we construct an ideal model of metal atomic layer with its native oxide to evaluate CO₂ reduction in two well-defined catalytic sites. The result show both the atomic-scale structure and the presence of oxide help to change the underlying paths of CO₂ electroreduction which enable the partially oxidized cobalt atomic layers with much improved activity and selectivity. These findings point to novel opportunities for manipulating and improving the CO₂ electroreduction properties with 2D ultrathin materials with different surface modification, as well as throwing lights into the fundamental understanding of CO₂ activation mechanism.



Ya-Qian Lan

兰亚乾

**Northeast Normal University, 210023,
Nanjing**

—

Email: yqlan@njnu.edu.cn

Ya-Qian Lan was born in 1978 in Jilin, P. R. China. He received his B.S. and Ph.D. degree (2009) from Faculty of Chemistry, Northeast Normal University under the supervision of Prof. Zhong-Min Su. In 2010, he joined Prof. Qiang Xu's group as a JSPS (Japan Society for the Promotion of Science) postdoctoral fellow at AIST (National Institute of Advanced Industrial Science and Technology). Since the end of 2012, he has been a Professor of Chemistry at Nanjing Normal University.

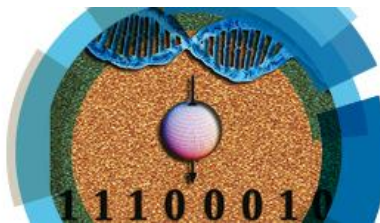
His current research interests focus on the application of polyoxometalate-based composite materials in energy storage and conversion and porous metal-organic frameworks for applications in catalysis and proton conduction

The application of polyoxometalate-based composite materials in energy storage and conversion

Ya-Qian Lan

Northeast Normal University, 210023, Nanjing

Polyoxometalates (POMs) possess excellent acidity, redox ability, and specific molecular structure. POMs are promising electrode materials for energy storage and conversion, but the superb solubility in water makes it becomes a challenge to separate and recycle in application. To solve the above problem, our group developed two major strategies. One strategy is combining POMs with metal-organic frameworks (MOFs) to carry out the research of POM-based MOFs (POMOFs). On the basic of POMOFs crystal materials, we synthesized POMOFs composites and porous carbon-based nanocomposites. Another strategy is to prepare two-dimensional porous materials derived from polyoxometalate/conductive polymer/graphene precursors, which are prepared taking advantage of the redox ability of POMs. Conductive polymer can anchor POMs and improve the conductivity of materials. The introduction of POMs can prevent graphene from aggregating and increase the specific surface area of composites. The synthesized POMOFs composites, PCG two-dimensional porous materials and their derivatives are applied as electrode materials and/or electrocatalyst for Li-ion batteries, Na-ion batteries and hydrogen evolution reaction. Our work provides theoretical and experimental basis for the research and development of POM-based composites in energy storage and conversion.



Yong Cui

崔勇

**School of Chemistry and Chemical
Engineering, Shanghai Jiao Tong
University, Shanghai, 200240, China**

—

Email: yongcui@sjtu.edu.cn

Yong Cui received a Ph.D in chemistry in 1999 from Fujian Institute of Research on the Structural of Matter, Chinese Academy of Sciences. He conducted postdoctoral research at the University of Science and Technology of China (1999–2000), at the University of North Carolina (2001–2002) and at the University of Chicago (2003–2005). He was appointed as the Cheung Kong Scholar Professor in 2013 and became a Fellow of the Royal Society of Chemistry in 2015. He is now a full professor Shanghai Jiao Tong University.

His research focuses on coordination chemistry and chiral chemistry.

Design of Chiral Covalent Organic Frameworks for Enantioselective Processes

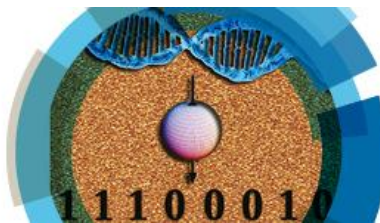
Yong Cui*, Xing Han, Jie Zhang

Shanghai Jiao Tong University, Shanghai, 200240, China

Covalent organic frameworks (COFs) are an emerging class of crystalline polymers that allow precise integration of organic building blocks into two-dimensional (2D) or three-dimensional (3D) networks with tunability of composition, structure, and function, similar to those found in metal-organic frameworks (MOFs). Synthetic control over chirality and function is the crowning achievement for MOFs, however, the same level of control has not been achieved for COFs. COF crystallization is inherently less controllable than MOFs crystallization, and there are only several CCOFs having been reported. Enantioselective processes based on CCOFs still remain relatively unexplored. We will report that homochiral CCOFs can be obtained by direct synthesis or chiral induction and their application in asymmetric catalysis and enantioseparation.

References

1. A. P. Côte, A. I. Benin, N. W. Ockwig, M. O'Keeffe, A. J. Matzger, O. M. Yaghi. *Science* **2005**, 310, 1166.
2. S. Kandambeth, A. Mallick, B. Lukose, M. Mane, T. Heine, R. Banerjee. *J. Am. Chem. Soc.* **2012**, 134, 19524.
3. D. N. Bunck, W. R. Dichtel. *J. Am. Chem. Soc.* **2013**, 135, 14952.
4. X. Wang, X. Han, J. Zhang, X. Wu, Y. Liu, Y. Cui. *J. Am. Chem. Soc.* **2016**, 138, 12332.



Hiroki Oshio

University of Tsukuba, Chemistry
Department, Tennodai 1-1-1, Tsukuba
305-8571, Japan

—

Email: oshio@chem.tsukuba.ac.jp

Hiroki Oshio graduated from Kyushu University in 1977 and obtained his PhD 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. He has received an award of The CSJ Award for Creative Work (2005) and has accumulated over 200 peer-reviewed research publications.

His research has focused on molecular magnetism, including bistable and spin-crossover systems.

Metal Complexes with Bistability

Hiroki Oshio

University of Tsukuba, Chemistry Department, Tennodai 1-1-1, Tsukuba 305-8571, Japan

Molecules may have flexible structures with easily controlled electronic states. When molecules have several stable electronic states and their structures are flexible upon state changes, such molecular systems can be promising candidates for molecular switching devices. Spin crossover (SCO) and mixed valence (MV) complexes rest in two spin states and two valence states, respectively. Multi-component molecules, in which each component possesses several states due to spin conversion and electron transfer, are expected to show synergistic behaviors with stepped and/or selective state conversions. In this lecture, multi-component systems showing variety of functions¹⁻⁵ such as selective spin state conversion, photo-induced SCM, and lability controlled cluster syntheses, will be presented.

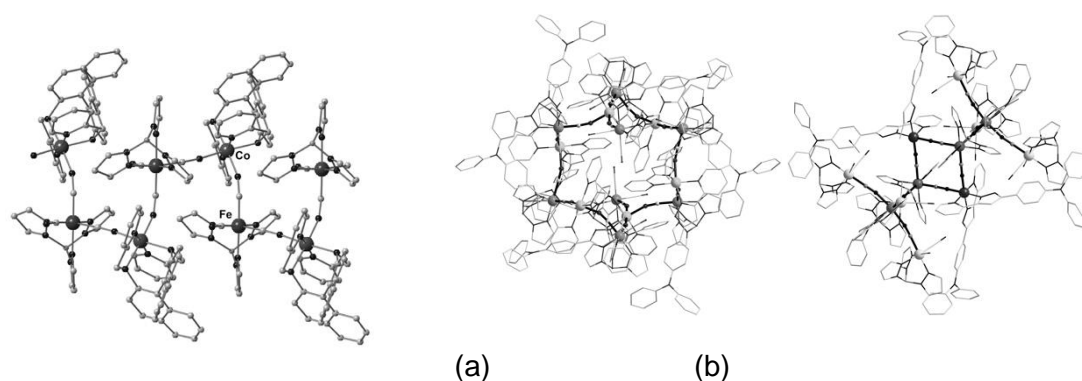
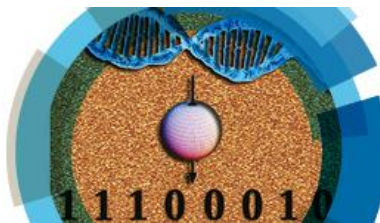


Figure 1 Cyanide bridged 1D and discrete complexes showing photo-induced SCM (left) and clusters generated from different electronic states (right), respectively.

References

1. T. Matsumoto, G.N. Newton, T. Shiga, S. Hayami, Y. Matsui, H. Okamoto, R. Kumai, Y. Murakami, H. Oshio, *Nat. Commun.* **2014**, 5, 3865/1.
2. N. Hoshino, F. Iijima, G.N. Newton, Y. Yoshida, T. Shiga, H. Nojiri, A. Nakao, R. Kumai, Y. Murakami, H. Oshio, *Nat. Chem.* **2012**, 4, 921.
3. Newton, G. N.; Mitsumoto, K.; Wei, R.-J.; Iijima, F.; Shiga, T.; Nishikawa, H.; Oshio, *Angew. Chem.* **2014**, 53, 2941.
4. M. Nihei, Y. Yanai, I.-J. Hsu, Y. Sekine, H. Oshio, *Angew. Chem.* **2017**, 56, 591-594.
5. R.-J. Wei, T. Shiga, G.N. Newton, D. Robinson, S. Takeda, H. Oshio, *Inorg. Chem.* R.-J. Wei, T. Shiga, G.N. Newton, D. Robinson, S. Takeda, H. Oshio, *Inorg. Chem.* **2016**, 55, 12114-12117, 55, 12114-12117



Hiroshi Kitagawa

Division of Chemistry, Graduate School
of Science, Kyoto University

Kitashirakawa-Oiwakecho, Sakyo-ku,
Kyoto 606-8502, Japan

Email: kitagawa@kuchem.kyoto-u.ac.jp

Hiroshi Kitagawa finished his Ph.D course in 1991 and received his Ph.D. from Kyoto University in 1992. He moved to Institute for Molecular Science as an assistant professor in 1991, Japan Advanced Institute of Science & Technology as an assistant professor in 1994, University of Tsukuba as an associate professor in 2000, and Kyushu University as a professor in 2003. In 2009, he returned back to the original laboratory at Kyoto University. He held a visiting appointment at Davy-Faraday Research Laboratory, Royal Institution of Great Britain (1993-1994). He was a chair of the 5th Chemical Sciences and Society Summit, 2013. He is also engaged at Japan Science & Technology Agency as a Research Director of ACCEL and a Research Supervisor of Science and Creation of Innovative Catalysts, PRESTO. His research fields are solid-state chemistry, coordination chemistry, nano-science, low-dimensional electron system, and molecule-based conductors.

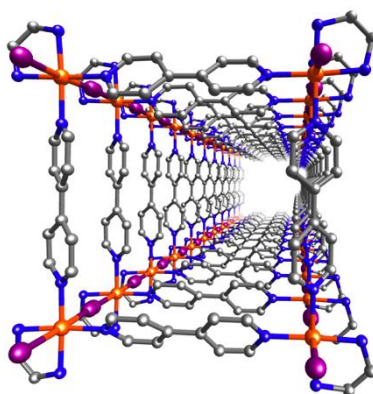
Dimensional Crossover in Coordination Chemistry

Hiroshi Kitagawa

Division of Chemistry, Graduate School of Science, Kyoto University Kitashirakawa-Oiwakecho, Sakyo-ku, Kyoto 606-8502, Japan

Recently, we have developed a bottom-up approach for the fabrication of well-defined dimensional-crossover nano-architectures with high tunability using metals and organic molecules as building blocks or linkers [1-8]. We succeeded in rationally constructing assemblies; (1) ladders and tubes which are located in dimensional-crossover region between 1D and 2D, (2) surface metal-organic frameworks (SurMOFs) which are located in dimensional-crossover region between 2D and 3D, and (3) nanoparticles coated with MOFs or polymers which are located in dimensional-crossover region between 0D and 3D.

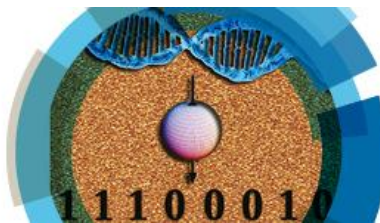
We have demonstrated several square prism-shaped metal-organic nanotubes with aside of 0.3 - 2 nm. Several uniform 1D channels were fabricated inside the tube, and H₂O and alcohol can be selectively adsorbed. Their optical gaps are around 1 eV of semiconductive region, and X-ray and theoretical studies revealed their unique electronic structures of charge-density-wave (CDW) quartets. In addition, their electronic states can be successively controlled by exchanges of structural components and guest molecules. These results show a rational route to the creation of nanotubes with high tunability of structures and electronic states, and might also offer valuable insights into multifunctional nanomaterials. In addition, our recent study on proton transport properties is presented and proton diffusion in a confined water-nanotube of hydrophobic nanochannel is discussed in details by a pulse field gradient NMR study.



References

1. S. Sakaida, K. Otsubo, O. Sakata, C. Song, A. Fujiwara, M. Takata, H. Kitagawa, *Nature Chemistry*, **2016**, 8, 377.
2. G. Li, H. Kobayashi, J. M. Taylor, R. Ikeda, Y. Kubota, K. Kato, M. Takata, T. Yamamoto, S. Toh, S. Matsumura, H. Kitagawa, *Nature Materials*, **2014**, 13, 802.

3. K. Otsubo, Y. Wakabayashi, J. Ohara, S. Yamamoto, H. Matsuzaki, H. Okamoto, K. Nitta, T. Uruga, H. Kitagawa, *Nature Materials*, **2011**, 10, 291.
4. R. Makiura, S. Motoyama, Y. Umemura, H. Yamanaka, O. Sakata, H. Kitagawa, *Nature Materials*, **2010**, 9, 565.
5. R. Makiura, T. Yonemura, T. Yamada, M. Yamauchi, R. Ikeda, H. Kitagawa, K. Kato, M. Takata, *Nature Materials*, **2009**, 8, 467.
6. T. Yamada, K. Otsubo, R. Makiura, H. Kitagawa, *Chem. Soc. Rev.*, **2013**, 42, 6655
7. K. Otake, K. Otsubo, K. Sugimoto, A. Fujiwara, H. Kitagawa, *Angew. Chem. Int. Ed.*, **2016**, 55, 6448.
8. K. Otsubo and H. Kitagawa, *CrystEngComm*, **2014**, 16, 6277.



Song Gao

高松

**College of Chemistry and Molecular
Engineering, Peking University, Beijing
100871, China.**

—

E-mail: gaosong@pku.edu.cn

Song Gao got his BS and PhD in chemistry at Peking University (PKU) in 1985 and 1991, and still works at PKU 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 from 2006-2010. He is now PKU Provost and Deputy Director of Beijing National Laboratory for Molecular Sciences. He received the State Natural Science Award (the 2nd Grade) in 2006 because of his contribution in magnetic coordination polymers and molecular nanomagnets. He was elected as a member of Chinese Academy of Sciences in 2007 and in the same year he became a Fellow of the Royal Society of Chemistry (UK).

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

Ferroelectric Molecular Magnets and Single-Ion Magnets

Song Gao

Beijing National Laboratory for Molecular Sciences, State Key Laboratory of Rare Earth Materials Chemistry and Applications, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China.

Some ammonium metal formate frameworks (AMFFs) with ABX₃ perovskite architecture (A = organic amine cation, B = transition metal ion, X = formate) exhibit a rich variety of structural phase transitions and physical properties, especially coexistence or synergy of magnetic and electric orderings [1-5].

After the milestone discovery of the first single-molecule magnets (SMMs) Mn₁₂ac, many new SMMs were structurally and magnetically characterized. The most studied systems are mainly conventional coordination compounds with polynuclear structures. From 2011, we explored a series mononuclear lanthanide or transition-metal organometallic molecules, which behave as a single-ion magnets (SIMs) [6-17]. It opened a door of SMMs to the chemists in organometallic chemistry. We hope these systems can provide new understandings of slow magnetic relaxation and new clues on the design and synthesis of molecular nanomagnets [18].

References

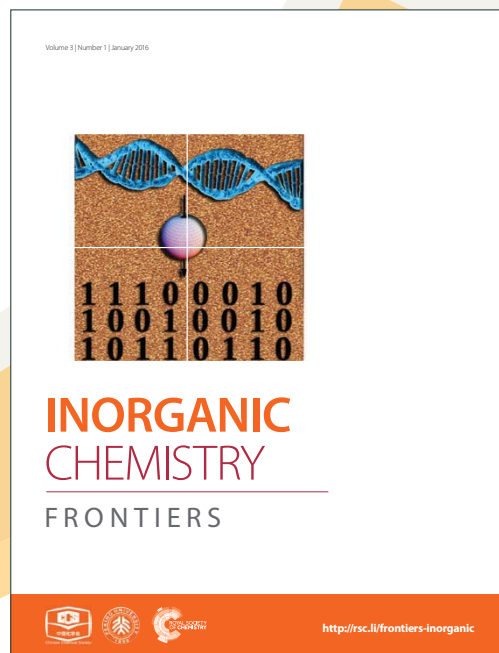
1. G.-C. Xu, X.-M. Ma, L. Zhang, Z.-M. Wang, S. Gao, *J. Am. Chem. Soc.* **2010**, 132, 9588.
2. G.-C. Xu, W. Zhang, X.-M. Ma, Y.-H. Chen, L. Zhang, H.-L. Cai, Z.-M. Wang, R.-G. Xiong, S. Gao, *J. Am. Chem. Soc.* **2011**, 133, 14948
3. S. Chen, R. Shang, B.-W. Wang, Z.-M. Wang, S. Gao, *Angew. Chem. Int. Ed.* **2015**, 54, 11093
4. R. Shang, S. Chen, B.-W. Wang, Z.-M. Wang, S. Gao, *Angew. Chem. Int. Ed.* **2016**, 55, 2097
5. W. Li, Z.-M. Wang, F. Deschler, S. Gao, R. H. Friend, A. K. Cheetham, *Nat. Rev. Mater.* **2017**, 2, 16099.
6. S.-D. Jiang, B.-W. Wang, H.-L. Sun, Z.-M. Wang, S. Gao, *J. Am. Chem. Soc.* **2011**, 133, 4730.
7. S.-D. Jiang, S.-S. Liu, L.-N. Zhou, B.-W. Wang, Z.-M. Wang, S. Gao, *Inorg. Chem.* **2012**, 51, 3079.
8. M.-E. Boulon, G. Cucinotta, S.-S. Liu, S.-D. Jiang, L. Ungur, L. F. Chibotaru, Gao, S. R. Sessoli, *Chem. Eur. J.* **2013**, 19, 13726.
9. M. Perfetti, G. Cucinotta, M.-E. Boulon, F. E. Hallak, S. Gao, R. Sessoli, *Chem. Eur. J.* **2014**, 20, 14051.
10. S.-S. Liu, J.W. Ziller, Y.-Q. Zhang, B.-W. Wang, W.J. Evans, S. Gao, *Chem. Commun.* **2014**, 11418.
11. S.-S. Liu; L. Xu, S.-D. Jiang, Y.-Q. Zhang, Y.-S. Meng, Z.-T. Wang, B.-W. Wang, W.-X. Zhang, Z.-F. Xi, S. Gao, *Inorg. Chem.* **2015**, 54, 5162.
12. Y.-S. Meng, Y.-S. Qiao, Y.-Q. Zhang, S.-D. Jiang, Z.-S. Meng, B.-W. Wang, Z.-M. Wang, S. Gao, *Chem. Eur. J.* **2016**, 22, 4704.

13. Y.-S. Meng, Y.-Q. Zhang, Z.-M. Wang, B.-W. Wang, S. Gao, *Chem. Eur. J.* **2016**, 22, 12724.
14. Y.-S. Meng, C.-H. Wang, Y.-Q. Zhang, X.-B. Leng, B.-W. Wang, Y.-F. Chen, S. Gao, *Inorg. Chem. Front.* **2016**, 3, 828.
15. Y. Bi, C. Chen, Y.-F. Zhao, Y.-Q. Zhang, S.-D. Jiang, B.-W. Wang, J.-B. Han, J.-L. Sun, Z.-Q. Bian, Z.-M. Wang, S. Gao, *Chem. Sci.* **2016**, 7, 5020.
16. Y.-S. Meng, Z.-B. Mo, B.-W. Wang, Y.-Q. Zhang, L. Deng, S. Gao, *Chem. Sci.* **2015**, 6, 7156.
17. X.-N. Yao, J.-Z. Du, Y.-Q. Zhang, X.-B. Leng, M.-W. Yan, S.-D. Jiang, Z.-X. Wang, Z.-W. Ouyang, L. Deng, B.-W. Wang, S. Gao, *J. Am. Chem. Soc.* **2017**, 139, 373.
18. Y.-S. Meng, S.-D. Jiang, B.-W. Wang, S. Gao, *Acc. Chem. Res.* **2016**, 49, 2381.

Acknowledgements

We are grateful to the NSFC, the National Basic Research Program of China for financial support.

About the journal



At *Inorganic Chemistry Frontiers*, we publish research articles, reviews, notes, comments and methods covering all areas of inorganic chemistry. We are delighted to announce a first impact factor of 4.532*, positioning *Inorganic Chemistry Frontiers* in the top 10 of the 'Chemistry, Inorganic & Nuclear' category.

Our scope places particular emphasis on interdisciplinary studies where inorganic chemistry and organometallic chemistry meet related areas, such as catalysis, biochemistry, nanoscience, energy and materials science.

Your paper should report high-quality work of exceptional novelty, which will be of significant interest to the broad readership of the journal.

The Frontiers project

The enterprising *Frontiers* family is a truly international, world-class journal series directed by leading Chinese academic institutions and published in partnership with the Royal Society of Chemistry. With expert Editors-in-Chief appointed from the Chinese partner institutions, the *Frontiers* series has a strong Chinese identity, reflecting an editorial focus and lead from China, but a global reach, reporting the very best science from China, Asia and the rest of the world to an international audience.

The Frontiers series includes *Inorganic Chemistry Frontiers* plus sister journals *Organic Chemistry Frontiers* and *Materials Chemistry Frontiers*.

*Data based on 2015 Journal Citation Reports® (Thomson Reuters, June 2016).

Image reproduced by permission of Alejandro Gaita-Ariño from *Inorg. Chem. Front.*, 2016, **3**, 61.