北京大学 RUTGERS

2019 Peking University - Rutgers University Bilateral Symposium

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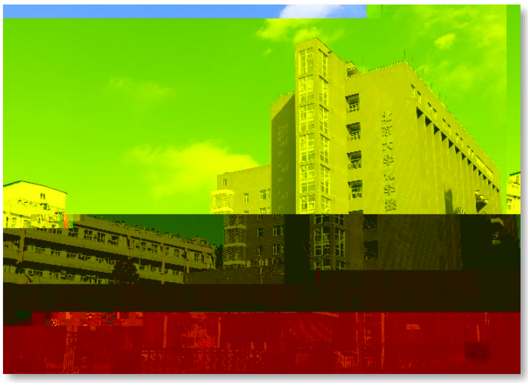
议手册

Sept. 27th – 28th, 2019, Peking University, Beijing, China

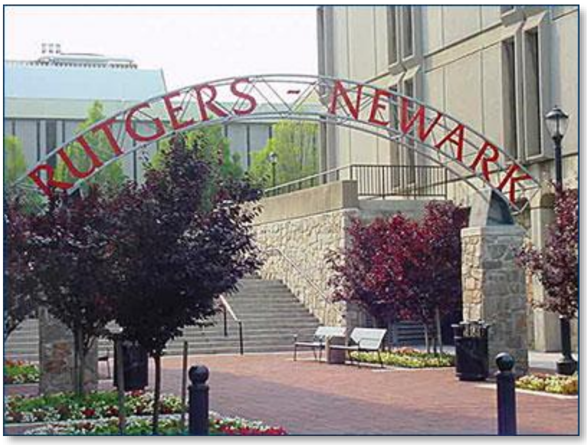
Welcome Address

CCME of PKU



Beijing Graphene Institute (BGI)

Rutgers-Newark



2019 Peking University - Rutgers University Bilateral Symposium

Sept. 27th – 28th, 2019, Peking University, Beijing, China

Sept. 27th, Friday, Lecture Hall (A204), CCME

Time	Lectures
08:30-08:40	**Opening – Prof. Zhongfan LIU, Prof. Piotr PIOTROWIAK**
	Session Chair: Prof. Frieder JÄKLE
08:40-09:10	**Prof. Piotr PIOTROWIAK (Rutgers)**
09:10-09:40	**Prof. Zhenfeng XI (PKU)**
09:40-10:10	**Prof. Zhongfan LIU (PKU)**
10:10-10:30	**Group Photo & Coffee Break**
	Session Chair: Prof. Piotr Piotrowiak
10:30-11:00	**Prof. Frieder JÄKLE (Rutgers)**
11:00-11:30	**Prof. Ding MA (PKU)**
11:30-12:00	**Prof. Elena GALOPPINI (Rutgers)**
12:00 – 13:30	**Lunch Break**

13:30-15:00	**Lab Tour, College of Chemistry and Molecular Engineering (CCME)**
16:00-17:40	**Lab Tour & Round Table Discussion, Beijing Graphene Institute (BGI)**
18:00-21:00	**Dinner**

Sept. 28th, Saturday, Lecture hall (A204), CCME

Time	Lectures

08:30-09:00

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15:30-15:50	**Coffee Break**
	Session Chair: Prof. Hailin PENG
15:50-16:20	**Prof. Deirdre M. O'CARROLL (Rutgers)**
16:20-16:50	**Prof. Junrong ZHENG (PKU)**
16:50-17:20	**Prof. Demyan PROKOPCHUK (Rutgers)**
17:20-17:30	**Closing Remarks – Prof. Huixin He**
17:30-20:00	**Dinner**

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Piotr Piotrowiak * Zheng Gong, Mengdi Liu, Takehiro Kawauchi,
Tomokazu Iyoda, Jianhua Bao, Yaroslav Aulin

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Capture of electrons by a 1 2 branching dendritic network of acceptors (viologen moieties) was investigated with the help of pump-probe spectroscopy. The dependence of the survival of the injected electron on the generation of the dendron could be satisfactorily explained in terms of the site-to-site hopping mechanism for the dendron family in which the pyrene donor is linked to the network via a (-CH_2-)$_4$ bridge. An analogous family with a single -CH_2- bridge at the apex exhibits a more complex behavior and indicates a close competition between electron transfer (ET) and vibrational cooling. Counterintuitively, slowing the injection and charge recombination at the apex increases the yield of electrons injected further into the dendritic network. These observations prompted us to investigate in more detail the vibrational cooling of the monoreduced MV^{+} radical ion in a variety of media, including a supramolecular host molecule. The studies of vibrational cooling took advantage of the ultrafast internal conversion (IC) between the D_1 excited state and the D_0 ground state of monoreduced viologen which occurs within ~240 fs via a conical intersection and allows one to prepare a population of ground state molecules with initial internal temperature in excess of 700 K. The subsequent redistribution of vibrational energy and its dependence on the topology (linear vs branched) of the viologen oligomer was probed by time-resolved spectroscopy and molecular dynamics (MD) simulations. Both the experimental results and modelling point to the importance of ballistic redistribution of energy at the early stages of the cooling process. More broadly, it was concluded that ET processes occurring at the time scale faster than 10-20 ps are likely to deviate, sometimes substantially, from the predictions of the Marcus and Marcus-Jortner theory. These thermal non-equilibrium effects are likely to influence the exciton dissociation yields and charge transport behavior in polymeric materials and devices such as the heterojunction solar cell.

F 5dendron, eletron transfer, tunneling, hot states, vibrational cooling

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1. Z. Gong, J. Bao, K. Nagai, T. Iyoda, T. Kawauchi, P. Piotrowiak, , **-** , **1**, , 4286.
2. M. Liu, T. Kawauchi, T. Iyoda, P. Piotrowiak, , **-** , **4**, , 1847.

Biography

Kd Kd d f is a native of Poland where he obtained MS degree in Chemical Physics (University of Wrocław), which he followed with a PhD in Physical Chemistry (University of Chicago) and a postdoctoral appointment in Radiation Chemistry (Argonne National Laboratory). In 1997 he has moved from the University of New Orleans to Rutgers University-Newark where he is a Professor of Chemistry and serves as the Vice Chancellor for Research and Collaborations. His research interests revolve around fundamental aspects of electron and energy transfer processes in molecules, host-guest assemblies, materials and at interfaces. The work of the group combines ultrafast laser spectroscopy, synthesis and computation. The laboratory facilities include femtosecond laser systems dedicated to transient absorption, fluorescence upconversion, Z-scan and Kerr-gated microscopy mU

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Spiro Metalla-Aromatics

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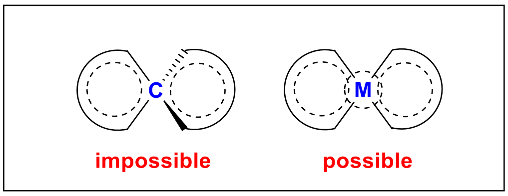
Email: ______________

Spiro compounds with one carbon as the spiro atom are often present in organic chemistry. However, they are impossible to be aromatic. When the spiro atom is replaced by a transition metal, the whole scenario may change completely, because transition metals can make the impossible formation or transformation possible. This presentation will report on the synthesis and characterization of spiro metalla-aromatic compounds, in which a transition metal is the spiro atom, that cross-conjugates two aromatic five-membered metallacycles, featuring either a square planar geometry (M = Pd, Pt, Rh) or a tetrahedral geometry (M = Mn).[1] Our results on metalla-aromatics formed from dilithio reagents and low-valent transition metal complexes demonstrate that organolithium compounds with pi-conjugation can be redox-active.[2-4]



Keywords: aromaticity; metalla-aromatics; spiro-aromatics

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2. (a) Wei, J.; Zhang, W.-X.; Xi, Z. , *1*, 5999. (b) Wei, J.; Zhang, Y.; Zhang, W.-X.; Xi, Z. , *1*, 9986. (c) Wei, J.; Zhang, Y.; Chi, Y.; Liu, L.; Zhang, W.-X.; Xi, Z. , . *05*, 60.
3. (a) Xi, Z. . , *10*, 1342. (b) Wei, J.; Zhang, W.-X.; Xi, Z. . , , 560. ( )
4. For discussions on non-innocent or redox-active ligands, see: (a) Chirik, P. J. . , , 9737. (b) Kaim, W. . , 343. (c) Fairlamb, I. J. S. , *1*, 10415.

Biography

Zhenfeng Xi received his B.Sc. degree from Xiamen University in 1983, M.Sc. degree from Nanjing University, Zhengzhou University and the Henan Institute of Chemistry in 1989, and Ph.D. degree from the Institute for Molecular Sciences (IMS), Japan in 1996. He took an Assistant Professor position at Hokkaido University, Japan in 1997, after he worked as a postdoctoral research fellow with Professor Takahashi. In 1998, he joined the College of Chemistry at Peking University, where he is now a Professor. He received several awards including Yaozeng Huang Organometallic Chemistry Award in 2004, and the CCS-AkzoNobel Chemical Sciences Award in 2014.

Prof. Xi served or is serving for several international journals as editors or advisory board members, including Associate Editor of *Organic Letters* (ACS), *Applied Organometallic Chemistry* (Wiley), Member of the advisory board or the Consulting Board of *Accounts of Chemical Research*, *Synlett/Synthesis*, *Tetrahedron/Tetrahedron Letters*, *Chem. Lett.*, *Asian J. Org. Chem.*, and *Bulletin of the Chemical Society of Japan*. He also serves for several Chinese journals as editors or advisory board members, including Associate Editor of *Chinese Science Bulletin*, and *National Science Review* (NSR).

His current research interest is focused on direct transformation of N_2 into organic compounds.

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Zhongfan Liu*

High quality graphene materials are the footstone of future graphene industry. As experienced in modern carbon fiber industry over last half century, the synthesis will certainly determine the future of graphene materials. Although great efforts have been done on synthesis since the first isolation of graphene in 2004, there still exists a big gap between the theoretical and realistic graphene. For the industry-level applications, one needs to consider the yield and cost issues in addition to purity, layer thickness and uniformity, domain size, lateral size of flakes, and defect density. The graphene synthesis calls for more technological innovations together with fundamental discoveries.

Over last ten years, we have made great efforts on the chemical vapor deposition (CVD) growth of high performance graphene films. We are working along two different directions towards commercial graphene materials. The first direction is the CVD growth of single crystal graphene wafers targeting electronic and optoelectronic purposes. We have realized a pilot level production of 4 inch single crystal graphene wafers using home-made CVD growth system with a capacity of 10,000 wafers/year. Using CuNi(111) alloy catalyst, we have succeeded in the ultrafast epitaxial growth of 6 inch single crystal graphene wafers with a growth rate of 50 times faster than on Cu(111), indicating the possibility of low cost production of high-quality graphene wafers. The second direction is the CVD growth of large scale graphene film using commercial Cu foil. We developed the first roll to roll continuous CVD growth system for this purpose. The production capacity reaches a level of 20,000m^2/year with a domain size of 10-20μm. The cost has been reduced to 200 RMB/m^2. To increase the growth quality, we also developed an A3-size static CVD growth system with a capacity of 10,000m^2/year and an expected domain size of 0.5mm. Superclean graphene is our important contribution to produce high-performance graphene films. During CVD growth, there exists an inevitable contamination of graphene surface arising from amorphous carbon byproduct and not-well developed graphene seeds, which leads to the ordinary “dirty graphene”. We have developed three effective techniques to grow the superclean graphene, including Cu-foam-aided growth, post-growth CO_2 etching, metal-containing precursors and magic lint roller. Such kinds of superclean graphene exhibited the highest carrier mobility, the lowest contact resistance and sheet resistance, and the highest fracture strength. We designed two types of pilot CVD growth systems based on the CO_2 etching technique, A3 size with a capacity of 10,000m^2/year and

300nm x 100mm size with a capacity of 30,000 pieces/year. Moreover, we have made great efforts on directly growing graphene on traditional glass, optical fibers, glass fibers and sapphire wafers. Such kinds of growth products can be directly used for various applications without involving the difficult peeling off and transfer processes. Super graphene glass, graphene-tailored optical fibers and glass fibers using the direct growth technique have become our important research targets in the last few years. The talk will give a brief overview of our last 10 years studies on the industrial level synthesis.

Biography

Prof. Zhongfan Liu got his PhD in University of Tokyo in 1990. He is now the BOYA Chair Professor of Peking University in chemistry, the Director of Beijing Graphene Institute, and the Vice President of Chinese Chemical Society. His research interest focusses on low dimensional carbon materials, including the CVD growth of graphene and single-walled carbon nanotubes and their unique applications. Prof. Liu has published over 600 peer-reviewed articles and over 130 patents. His recent contributions to graphene areas include, superclean graphene, super graphene glass, graphene optical fiber and photochemical band structure engineering of graphene. The major academic awards he received include, National Natural Science Awards (2008, 2017), Chinese Chemical Society-AkzoNobel Chemical Science Award (2012), Baogang Outstanding Teacher Award (2012), the Lectureship Award of 2016 Colloid and Surface Chemistry Annual Meeting of Chemical Society of Japan, Beijing Municipal Excellent Teacher (2017), and the 2018 ACS Nano Lectureship Award. He was elected as the member of Chinese Academy of Sciences in 2011 and as one of the six outstanding scientists in Ten-Thousand-Talents Program in 2013. Prof. Liu is the Fellow of the Institute of Physics (UK, 2004), the Fellow of Royal Society of Chemistry (UK, 2014) and the Fellow of TWAS(2015).

Borane Lewis Acids: From Molecules to Materials

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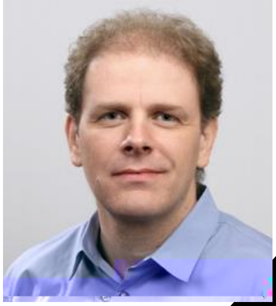
The incorporation of main group elements into conjugated materials is known to result in unusual properties and to enable new functions.[1] The ability of tricoordinate boron to participate in pi-delocalization can have a dramatic effect on the optical properties by selectively lowering the LUMO orbital levels. The electron-deficient character of boron also enables Lewis acid-base interactions, resulting in strong perturbations of the electronic structure. These materials have been studied for applications ranging from biological imaging, lasing, organic photovoltaics, to photochromic materials and molecular switches.

In our recent work, we have explored the effects of boron incorporation into conjugated oligomers, macrocycles, and polymers.[2] We have also demonstrated that base-directed electrophilic aromatic C-H borylation provides an effective means to generate luminescent B-N containing conjugated materials with unusual properties such as self-sensitized singlet oxygen generation.[3] Finally, we have found that "smart" dynamic materials can be achieved by embedding both Lewis acid and base sites into polymer networks.[4]

In this talk I will discuss these discoveries and highlight their impact in applications ranging from luminescent materials, sensors, solar cells to dynamic polymer network materials.

Biography



A d E f [redacted] shed Professor in the Department of Chemistry at the Newark Campus of Rutgers University. He received his Diploma in 1994 and Ph.D. in 1997 from TU München, Germany, under the direction of Prof. Wagner. After a postdoctoral stint with Prof. Manners at the University of Toronto he joined Rutgers University in 2000. His research interests revolve around main group chemistry as applied to materials and catalysis, encompassing projects on organoborane Lewis acids, conjugated hybrid materials, luminescent materials for optoelectronic and sensory applications, stimuli-responsive and supramolecular polymers. He is the recipient of an NSF CAREER award (2004), an Alfred P. Sloan fellowship (2006), a of the Alexander von Humboldt Foundation (2009), the ACS Akron Section Award (2012), the Boron Americas Award (2012) and the Board of Trustees Research Award at Rutgers University (2017). In 2019 he was named a of the American Chemical Society. He has served on the editorial advisory boards of several journals, including Macromolecules, ACS Macro Letters, and Organometallics.

-MoC Catalyst for Water Gas Shift Reaction

Ding Ma

The water gas shift (WGS) reaction ($CO+H_2O=H_2+CO_2$) is an essential process for hydrogen generation/upgrading in various energy-related chemical operations. Normally for a chemical reaction, higher reaction temperature renders higher reaction rate. However, from a thermodynamic point of view, WGS is an equilibrium-limited reaction that is favored at low temperature. In particular, the potential application in fuel cells requires the commercial WGS catalyst to be highly active, stable and energy-efficient. Under these criteria, decreasing the reaction temperature will not only give a considerable rise in the CO equilibrium conversion but will also exhibit potential in reducing the energy consumption, and match the working temperature of on-site hydrogen generation and consumption units. Here by creating Au layered clusters on an α-MoC substrate, we have successfully constructed an interfacial catalyst system for the ultra-low temperature WGS reaction. Water is activated over α-MoC at 303 K, while CO adsorbed on adjacent Au sites is apt to react with surface hydroxyls formed from water splitting, leading to an unprecedented low-temperature WGS activity. **References:**

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2. M. Xu, S. Yao, D. Rao, Y. Niu, N. Liu, M. Peng, P. Zhai, Y. Man, L. Zheng, B. Wang, B. Zhang, D. Ma, M. Wei, *J. Am. Chem. Soc.* 2018, 140, 11241.

Biography

Ding Ma, Professor in *College of Chemistry and Molecular Engineering*, *Peking University*. He read chemistry in Sichuan University (1996), and obtained his Ph.D from the State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics (2001). After his postdoctoral stay in Oxford University and University of Bristol, he started his research career in Dalian Institute of Chemistry as associate professor (2005). He was promoted as a full professor in 2007 and moved to Peking University in 2009. His research interests are heterogeneous catalysis, especially those related with energy issues, including C_1 chemistry (methane and syngas conversion), hydrogen production/transportation, new reaction route for sustainable chemistry and the development of in-situ spectroscopic method that can be operated at working reaction condition to study reaction mechanism. He is Fellow of Royal Society of Chemistry, and Associate Editor for *ACS Catalysis* and *Chinese Journal of Chemistry*. He is also on the Editorial Boards of *Journal of Energy Chemistry*, *Science Bulletin, Joule*, and *Catalysis Science & Technology* etc.

Chromophore Design for Study of Electron Transfer Processes at Metal Oxide Semiconductor Interfaces

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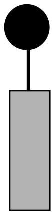
The exchange of charges between photo-excited molecules and a metal oxide semiconductor such as TiO_2 or ZnO is a process of great importance for solar energy conversion research on photovoltaics, artificial photosynthesis, and photocatalysis. Molecular design of chromophore-linker-anchor compounds plays an important role to control, at the molecular level, charge transfer at hybrid organic-inorganic systems and to gain a fundamental understanding of these important interfaces. The talk will address several aspects of molecular design that our group has focused on, including ways to control the energy level alignment between the LUMO and HOMO of organic chromophores and the conduction band of TiO_2 or ZnO surfaces through the presence of permanent dipoles built in the linker unit. The presentation will discuss collaborative research currently funded by the US Department of Energy and the National Science Foundation.



Keywords: organic chromophores; metal oxide semiconductors; nanostructured interfaces

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7. , P.G. Johansson, Y. Zhang, G.J. Meyer , E. Galoppini, **- , . ,** , 7947–7957.

Biography

Elena Galoppini obtained a *Laurea in Chimica* from the Università di Pisa, Italy, a Ph.D. from the University of Chicago in 1994, and conducted postdoctoral research at the University of Texas at Austin prior to joining the faculty at Rutgers University-Newark in 1996, where she is Distinguished Professor since 2017. She is the recipient of a Board of Trustees Award for Excellence in Research and a Kavli Frontiers of Science Alumna (National Academy of Sciences), and Visiting Professor in several countries in Europe and Asia. Her expertise is in organic synthesis aimed at applications for nanostructured semiconductors. The common theme to the highly interdisciplinary research conducted in her synthetic organic group is the controlled functionalization of nanostructured semiconductor surfaces with chromophores and redox-active molecules. Synthetic design and optimization of the organic linkers as well as interfacial host-guest chemistry aim at controlling photo-induced heterogeneous charge transfer processes. These studies are of fundamental importance, but also address some of the most important technological challenges in application fields ranging from solar energy conversion, to electrochromic materials and ultrasensitive nanosensors.

A Phase Separation Perspective for Chromatin Structure Change in Development, Differentiation, Senescence and Certain Diseases

Yiqin Gao*

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2. *Beijing National Lab of Molecular Sciences, Beijing, China*
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4. *Beijing Advanced Innovation Center for Genomics, Peking University, China*

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The high-order chromatin structure plays an important role in gene regulation. The mechanism, especially the sequence dependence for the formation of varied chromatin structures in different cell states remain to be elucidated. In this talk, we try to touch on three questions: (1) What is the sequence dependence and chemical structure basis in the formation of high order chromatin structure, such as compartments? (2) How does the chromatin structure reflect the biological function of different cellular states and tissue-specificity? (3) How does this sequence-dependent chromatin structure formation manifest in different species? We identified CGI (CpG island) forest and prairie genomic domains based on CGI densities, and divided the genome into two sequentially, epigeneia9-55(C)ca1 forded fques5( )-42(do)] TJETq0.00000887

Biography

Yiqin Gao is currently a Professor of Chemistry at the College of Chemistry and Molecular Engineering. He is also an investigator at Beijing National Lab of Molecular Sciences, an investigator at Biomedical Pioneering Innovation Center and Beijing Advanced Innovation Center for Genomics. He received a bachelor degree in Chemistry from Sichuan University, a master degree in Chemistry from Institute of Chemistry, Chinese Academy of Sciences, and a Ph.D from California Institute of Technology. He was a postdoc at Caltech (2001-2002) and Harvard University (2003-2004) before joined Texas A&M University as an assistant professor (2005-2010). He became a professor at Peking University in 2010. He is currently an Editorial Board member of J. Phys. Chem., J. Chem. Phys., Chem. Phys. Lett., ACS Central Sciences, Acta. Phys. Chem., and J. Mater. Chem.

Density Embedding Methods for the Condensed Phase

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Leveraging Subsystem DFT, an open-subsystem formulation of Kohn-Sham Density Functional Theory (KS-DFT) [1], we aim at describing periodic and molecular systems alike, including their electronic and nuclear dynamics. Subsystem DFT enables first principles simulations to approach realistic time- and length-scales, and most importantly sheds light on the dynamical behavior of complex systems. As the accuracy of Subsystem DFT is tied with the use of nonadditive Kinetic Energy Density Functionals (KEDF), we show that employing latest-generation nonlocal KEDF results in KS-DFT accuracy in the simulations at a fraction of the computational cost. Taking subsystem DFT to the time domain allows us to inspect the electron dynamics of condensed-phase systems in real time. In liquids and interfaces, we observe all the relevant regimes proper of non-Markovian open quantum system dynamics, such as electronic energy transfer, and screening [2]. Contrary to interactions between molecular (finite) systems, when molecules interact with metal or semiconductor surfaces [3] the electron dynamics is strongly non-Markovian with dramatic repercussions to the molecule's response to external perturbations.

Keywords: DFT; TDDFT; Embedding

References:

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Biography

Michele Pavanello obtained his MSc in Theoretical Chemistry from the University of Pisa in 2004 under the supervision of Prof Benedetta Mennucci working on the Polarizable Continuum Model (PCM) for describing molecule-solvent interactions. He then worked on high-accuracy variational calculations of small molecules, such as H_3^+, in the laboratory of Prof Ludwik Adamowicz at the University of Arizona. After a postdoc at Leiden University in the Netherlands funded by a Marie Curie Fellowship, Pavanello joined the faculty at Rutgers University-Newark in 2012. Since then, the Pavanello Research Group (PRG) has established itself as a leader in the development of multiscale modeling methods, such as density embedding methods, for the theoretical description of molecular and condensed phase systems in and out of equilibrium.

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** Email: jinzhang@pku.edu.cn*

Single-walled carbon nanotubes (SWNTs) had received broad attention in the past decades due to its dramatic physical and chemical properties. As synthesis determined the future, in this talk, I will focus on the chirality controlled growth of horizontal carbon nanotubes array with designed catalysts: 1) By using open-end SWNTs as ‘seeds/catalysts’, SWNTs could be grown and cloned from the parent segments via an open-end growth mechanism. These findings provide a new approach for growing SWNTs with controlled chirality; 2) Using symmetry matching strategy, a structure-family (2m, m) horizontally aligned SWNTs were successfully obtained on uniform carbide (WC and Mo2C) solid catalysts. It is based on a consideration of nanotube/catalyst interfacial thermodynamics determined by symmetry, and the kinetic growth rates set by the number of kinks; 3) For the application of SWNTs in electronic device, a new family of semiconducting SWNTs, (n, n-1) carbon nanotubes with different diameters can be grown using near-equilibrium nucleation growth mode. This new strategy adds a new degree of freedom for selective growth of SWNTs and opens up a new route for growth of SWNTs families beyond catalysts design.

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2. Jin Zhang et. al., Nature, 543(2017), 234-238.
3. Jin Zhang et. al., Chem, 5(2019), 1-12.

d b c

Ed Uc b received his PhD from Lanzhou University and Peking University in 1997. After a two-years postdoctoral fellowship at the University of Leeds, UK, he returned to Peking University where he was appointed Associate Professor (2000) and promoted to Full Professor in 2006. In 2013, he was appointed as Changjiang professor. He also is the Fellow of RSC. His research focuses on the controlled synthesis and spectroscopic characterization of carbon nanomaterials. He was a recipient of the Second Prize of National Natural Science and the National Natural Science Funds for Distinguished Young Scholar. He has published over 260 peer-reviewed journal articles.

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Huixin He*

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Microwave heating assisted chemistries have been well-known for high speed synthesis. Even though the observed rate enhancements have been mainly ascribed to thermal/kinetic effects, i.e., a consequence of high local temperatures which can be achieved rapidly, these unique effects could also enable the fabrication of designed/desired products with high selectivity, which are difficult to be realized with traditional convection heating assisted chemistries. In the first part of this presentation, I would share with you our recent efforts in exploiting microwave chemistry, including dry microwave chemistry, for rapid fabrication of for rapid fabrication of solvent processible graphene nanoplatelets with roughly controlled oxidation levels, lateral sizes, holey structures in their basal planes, and geometric structures (zigzag vs. armchair) along their edges.[1-3] Their unique structures and the associated application in energy conversion/storage, such as metal-free heterogenous catalysts by themselves, or as unique highly conductive supports for the development of single atom based catalysts will be discussed. The challenge of microwave chemistry, especially dry microwave chemistry in non-uniform heating profile distribution, which would influence not only productivity, selectivity, of course, the purity of the product, will be shortly discussed. Finally, I would also share with you our recent exploration in using electrochemical controlled scanning probe microscopy in fundamental understanding of the charging/discharging behavior of current popular battery materials.

Keywords: microwave; graphene; catalysts, battery

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Chi-Yuan Yang, Yang Lu, Jie-Yu Wang, Jian Pei*

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In the past several decades, conducting polymers have achieved remarkable progress and have been widely applied as the active materials for optoelectronics. So far, p-type conducting polymers exhibit high conductivities over 1000 S cm^{-1} and thermoelectric performance comparable to that of inorganic materials; however, only a few n-type conducting polymers showed conductivities over 1 S cm^{-1} after doping. The low conductivity of n-type conducting polymers is considered as the major barrier for further enhancing their thermoelectric performances. In our group, we tried to enhance the conductivity of n-type polymer thermoelectric materials, including n-doping efficiency in n-type polymers, factors influencing charge carrier mobilities after doping, and the stability of n-type conducting polymers. Using several representative examples, we developed the strategies of decreasing the LUMO level, improving the miscibility, reinforcing the doping efficacy to enhance the n-doping efficiency, and the strategies of the backbone planarization, alkyl chain engineering, morphology and microstructure tuning, device fabrication optimization to enhance the charge carrier transport. These strategies have proven to be effective in enhancing the conductivity of n-type polymer thermoelectric materials. Recent development and strategies to enhance the conductivity of n-type conjugated polymers demonstrated the efficiency in the rational material design and the device engineering guidelines for the future high-performance polymer thermoelectric materials research and development.

Keywords: conjugated polymer; conductivity; thermoelectric

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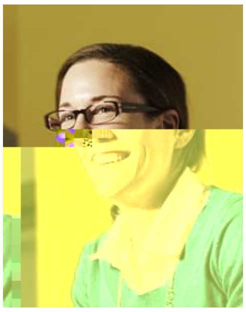
Biography

Ed K dstudied chemistry from 1985 to 1995 and obtained his Ph. D. in organic chemistry at Peking University, China. From 1995 to 1997, he worked in National University of Singapore in the field of organic reactions in aqueous media. From 1997 to 2001, he joined in the Institute of Materials Research and Engineering and worked in the synthesis, characterization, and device fabrication of organic semiconducting materials. During this period, he spent around two years in the group of Prof. Alan J. Heeger in the University of California at Santa Barbara.

In 2001, he joined in Peking University as an associate professor, and was promoted to full professor in 2005. In 2004, he received the National Natural Science Funds for Distinguished Young Scholar of China and in 2011 he became Yangtze River Scholar. He is currently the vice dean of the College of Chemistry and Molecular Engineering, Peking University. His research focuses on organic electronics (organic field-effect transistors and organic solar cells). His research group is particularly interested in the development of new conjugated unit for organic semiconducting materials and studying how alkyl chains and the aggregation behaviors affect the device performance.

Biography



Stacey Brenner-Moyer completed her Sc.B. in chemistry at Brown University. She earned her Ph.D. from Stanford University, under the tutelage of Prof. Paul Wender. Afterwards, she was a post-doctoral research associate in the laboratory of Prof. Steven Ley at the University of Cambridge in England. Prof. Brenner-Moyer began her independent career at the City University of New York (CUNY), where she was the recipient of the prestigious National Science Foundation CAREER Award in 2012. In 2014, she joined the faculty at Rutgers University-Newark as an associate professor.

Cellular Synthesis of Topological Proteins

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Chemical topology has emerged as a unique dimension for protein engineering. Nature has demonstrated the power of protein topology engineering in a small yet elegant set of proteins with nontrivial topology (such as cyclotides and lasso peptides possessing exceptional bioactivity and stability). However, artificial topological proteins remain scarce. In this talk, I will discuss our recent efforts in the field of protein topology engineering from the development of genetically encoded protein chemical tools to the cellular synthesis of topological/mechano-proteins and further to their biological significance and potential applications. Through strategies such as the "assembly-reaction" synergy and the active-template method, we have prepared various topological proteins including cyclic proteins, star proteins, θ proteins, protein catenanes, lasso proteins, protein heterocatenanes and polycatenanes. Their unique topologies have been proven by combined techniques such as controlled digestion experiments, NMR spectrometry, and protein crystallography. Among them, proteins with mechanical bonds ("mechanoproteins") are of particular interest owing to their potential functional benefits such as structure stabilization, quaternary structure control, synergistic multivalency effect and dynamic mechanical sliding/switching properties. Specifically, protein catenanes containing folded structural domains have been found to exhibit enhanced stability toward proteolytic digestion, heat/chemical denaturation, and freeze-thawing treatments, which are highly desired features for enzymes in industry and protein therapeutics. These results suggest that topology is indeed a unique dimension for protein engineering.

Keywords: Topology; Protein Engineering; Catenane; Mechanical Bond

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Biography

Wen-Bin Zhang is currently an Assistant Professor at the College of Chemistry and Molecular Engineering of Peking University. He received his BS from Peking University in 2004 and his PhD in Polymer Science from the University of Akron in 2010. He continued there as a postdoc for one year, before moving to Caltech for a second postdoc. His research in the past decade has been the pursuit of precision in macromolecular science at both molecular and supramolecular level. His goal is to integrate the design principles and building blocks of both synthetic and biological polymers for the development of precision macromolecules with unique functions for health-related applications. He received the “1000 Talent Award (Youth)” in 2013 and the “Distinguished Lectureship Award” from the Chemical Society of Japan in 2017. He also serves as the editorial board of rising stars for the journal *Chinese Journal of Chemistry* (since 2017), the executive board member for the journal *Polymer* (since 2019), and the committee member for the Division of Supramolecular Chemistry, Chinese Chemical Society (since 2018).

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The unique structure and properties of two-dimensional (2D) crystals have a large impact on fundamental research as well as applications in electronics, photonics, optoelectronics and energy sciences. Here our recent studies on the controlled synthesis of high-mobility 2D crystals such as graphene and layered bismuth oxychalcogenides (BOX, Bi_2O_2X: X = S, Se, Te), as well as their functional devices will be discussed. We achieved batch-fabrication of ultraclean graphene films and membranes towards their killer applications. In addition, novel air-stable ultrahigh-mobility semiconducting 2D BOX can be readily synthesized via chemical vapor deposition and fabricated into high-performance field-effect transistors and NIR photodetectors, in which pronounced quantum oscillations were also observed. Our studies suggest that high-quality 2D crystals hold great promise for future applications.

Keywords: 2D materials; CVD; high mobility; oxychalcogenide; graphene

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Biography

C[redacted] professor at Peking University, China. He received his B.S. in chemistry from Jilin University in 2000, and a PhD in physical chemistry from Peking University in 2005. He pursued postdoctoral studies at Stanford University during 2005–2009. His current research interests focus on high-mobility 2D materials and nanodevices. He has issued 20 patents and published more than 180 papers including 20 Science & Nature's sister papers and >60 JACS/Nano Lett./Adv. Mater./PRL papers. He was awarded the National Science Fund for Outstanding Young Scholar of China (2015), the Chief Scientist of 973 Program Youth Project, the second prize of National Natural Science Award of China (2017), SMALL Young Innovator Award (2017), the MRS Singapore ICON-2DMAT Young Scientist Award (2017), Young Scientist Award in the Ministry of Education of China (2018), and “Ten thousand plan”-National high level talents special support plan (2018).

Information-Directed Self-Assembly of Nucleic Acid Nanostructures and Devices

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Deoxyribonucleic acid (DNA) has emerged as an excellent molecular building block for creating nano-sized objects. Its unique features, such as having predictable spatial arrangements and programmable Watson-Crick base pairing interactions, facilitate the information-directed self-assembly of precisely defined nanostructures and nano-

Biography

Fei Zhang newly joined the Chemistry Department at the Rutgers University-Newark as an Assistant Professor in 2019. She received her B.S. in Chemistry and Molecular Engineering from Peking University in 2010 and her Ph.D. in Chemistry and Biochemistry from Arizona State University in 2015. After graduation, Dr. Zhang started as an assistant research scientist, and was promoted to research professor in 2016. She just started her new lab at the Rutgers University in September. Her primary research has focused on designing nucleic-acid nanostructures with increasing complexity and precision, constructing dynamic DNA devices with programmable behaviors, and ultimately rebuilding synthetic biochemical molecular systems that approach the complexity and sophistication that nature exhibits.

Amino Acid-Derived Biomimetic Polymers for Sustainability and Protein Therapeutics

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Proteins are structural and functional biomacromolecules composed of α-amino acids (AAs). Owing to their intrinsic biocompatibility, multifunctionalities, and chirality, AAs are ideal building blocks to construct not only synthetic polypeptides, but also many other types of biodegradable ecopolymers such as polyesters, polyamides, and polythioesters. Such polymers can find broad applications in materials sciences and biomedicines. The *overarching goal* of the Lu lab at Peking University is to *develop tools for the controlled synthesis of novel amino acid-derived biomimetic polymers for sustainability and protein modification*. To do this, we integrate and harness the power of organic/polymeric synthesis, molecular design, protein engineering, nanotechnology, and advanced biotechnologies. On this theme, we have been rigorously pursuing three focused directions: 1. Design and synthesis of degradable and/or recyclable functional polymers based on amino acids. 2. In-situ functionalization of synthetic polypeptides for facile protein-polypeptide conjugation (PEPylation). 3. In vivo structure-activity relationship (SAR) analysis and therapeutic applications of PEPylated proteins.

Keywords: Amino acid; PEPylation; Polythioester

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Biography

C G is an assistant professor in the College of Chemistry and Molecular Engineering, Peking University (PKU). He obtained his B.Sc. in chemistry from PKU in 2006 and PH.D. in Materials Science from the University of Illinois at Urbana-Champaign in 2011. He worked as a Damon Runyon Cancer Research Foundation postdoctoral fellow at The Scripps Research Institute (La Jolla) before he started his independent research in PKU in 2014. His research focuses on the development of methodologies for the controlled synthesis and medical applications of poly(α-amino acid)s, sustainable polymers, and protein-polymer hybrids. He is a recipient of ACS AkzoNobel Award for Outstanding Graduate Research in Polymer Chemistry (2013), Youth Thousand Talent Program (2015), Excellent Young Investigator Grant of NSFC (2017), and Chinese Chemical Society Prize for Young Scientists (2017).

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In thin-film organic optoelectronic devices, manipulation of light below the diffraction limit in a two-dimensional plane is important for efficient light utilization within the semiconductor active layer. Two dimensional plasmonic surfaces are promising materials for this purpose because of their thinness and their ability to localize the electric field of light at their surface. In this talk, our work on improving light trapping and light extraction in organic semiconductor thin films using plasmonic surfaces will be presented. Optical phenomena, such as absorption induced scattering, out-of-plane waveguiding and morphology-dependent surface plasmon outcoupling, are identified due to exciton-plasmon coupling between the organic semiconductor and the metasurface. Interactions between localized and propagating surface plasmon polaritons and the excitonic transitions of a variety of organic and organometallic materials will be discussed and ways in which these interactions may be optimized for particular thin-film optoelectronic applications will be presented.

Keywords: organic semiconductors; plasmonics; thin films

Biography

d J" [redacted]e Professor of Materials Science & Engineering and Chemistry at Rutgers University where she leads a research group working in the areas of nanophotonics and organic optoelectronics. She obtained her B.E. (Elec. Eng., 2002) and PhD (Microelectronics, 2008) at University College Cork and the Tyndall National Institute, Ireland. Prior to joining Rutgers in 2011, she conducted postdoctoral research in plasmonics at California Institute of Technology in the US and at the University of Strasbourg and CNRS in France. She has received numerous awards for her research including a National Science Foundation CAREER Award (2016), an American Chemical Society Young Investigator Award in Polymer Material Science and Engineering (2017) and a Science Foundation Ireland Future Research Leaders Award (2018). She has published more than 50 peer-reviewed journal publications in the areas of nanophotonics, organic optoelectronic materials, plasmonics and nanotechnology.

Electron/Hole Transformations Between Two Atomic Layers

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Electron/hole transformations on interfaces determine fundamental properties of opto-electro-chemical devices, but remain a grand challenge to experimentally investigate and theoretically describe. Herein combining ultrafast VIS/NIR/MIR frequency-mixed microspectroscopy and state-of-the-art two-dimensional atomic device fabrications, we are able to directly monitor the phase transitions of charged quasiparticles in real time on the ultimate interfaces – between two atomic layers. On type II semiconductor/semiconductor interfaces between two transition metal dichalcogenide (TMDC) monolayers, interfacial charge transfers occur within 50fs and interlayer hot excitons (unbound interlayer e/h pairs) are the necessary intermediate of the process for both energy and momentum conservations [1]. On semiconductor/conductor (graphene) interfaces, interlayer charge transfers result in an unexpected transformation of conducting free carriers into insulating interlayer excitons between the conducting graphene and the semiconducting TMDC. The formation of interlayer excitons significantly improves the charge separation efficiency between the two atomic layers for more than twenty times [2].

Keywords: Interface charge transfer; TMDC; Femtosecond spectroscopy

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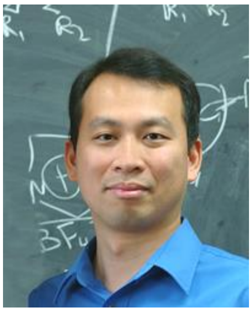
Biography

Zhihao Yu is an associate professor of College of Chemistry and Molecular Engineering, Peking University. He received his B.S. degree in Tsinghua University, Beijing, China in 2005, and his Ph.D. degree in the Institute of Physics, Chinese Academy of Sciences in 2010. He worked as a postdoctoral fellow in Chemistry Department of Rutgers University until 2012. He joined ECE department of Virginia Tech and worked as a research associate in 2012-2015. Later he worked at Chemistry Department of Rice University as a research associate in 2015-2016, and joined Peking University by the end of 2016.



Junrong Zheng is a professor of College of Chemistry and Molecular Engineering, Peking University. He is a recipient of the 2011 Air Force Young Investigator Award by the USA Air Force Office of Scientific Research. He also received the Norman Hackerman Welch Young Investigator Award in the year of 2008 when he started his independent research at Rice University. Dr. Zheng worked as a Postdoctoral Fellow in the same lab at Stanford University for one year after receiving his Ph.D. in physical chemistry in 2007. He received master's degrees in polymer physics and polymer chemistry from Rensselaer Polytechnic Institute and Peking University, respectively. He also earned a bachelor' s degree in Chemistry from Peking University.

Molecular Catalysts for Chemical Energy Conversion: Using Nature as a Template for Ligand Design

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Utilizing energy while minimizing negative environmental impact is a grand challenge that would benefit humankind for generations to come. One strategy to meet this goal is by designing new and improved catalysts that can reversibly facilitate the conversion of chemical energy ($H_2 \leftrightarrow H^+/e^-$, $CO_2 \leftrightarrow CO \leftrightarrow CH_3OH$, $NH_3 \leftrightarrow N_2$, etc.) into electrochemical energy. In order for such technology to be implemented on a large scale, abundant elements and materials must be utilized. We take inspiration from Nature to design new homogeneous (molecular) compounds using abundant transition metals that react with small molecule substrates relevant to chemical energy conversion. By carefully choosing the metal, ligand, and oxidation state, we can engender unique reactivity at the metal and ligand to design efficient electrocatalysts that enable these important chemical transformations.

Keywords: electrocatalysis; renewable energy; metal complexes

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Biography

Demyan Prokopchuk was born in Saskatoon, Canada. In 2009, he received his BSc in Chemistry (High Honors) and Computer Science (Minor) from the University of Saskatchewan. In 2015, he completed his PhD at the University of Toronto under the supervision of Prof. Robert Morris, funded by provincial (OGS) and federal (NSERC) scholarships. During this time, he also spent five months at ETH Zürich in the laboratory of Prof. Hansjörg Grützmacher. From 2015-2017, Demyan was a postdoctoral fellow at Pacific Northwest National Laboratory in the Center for Molecular Electrocatalysis, co-supervised by Dr. Morris Bullock and Dr. Michael Mock. After a CFREF postdoctoral fellowship (2017-2018) at the University of Calgary with Prof. Warren Piers, Demyan began his independent career in the Department of Chemistry at Rutgers-Newark in 2019

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