

Scientific Program

Oct. 20th Thursday

DuoGongNeng Hall of Conference Center

Opening Ceremony Chair: Prof. Jun Nie (The Dean of College of Science)	15:20-15:25	Welcome Address by the President of Beijing University of Chemical and Technology
	15:25-15:30	Opening Address by the Director of Department of Organic Chemistry of National Science Foundation of China
	15:30-15:35	Opening Address by the Dean of Shenzhen Graduate School of Peking University, Prof. Yundong Wu
	15:35-15:40	Opening Address by Prof. Michael B. Hall

Group Photo

The Gate of Conference Center

DuoGongNeng Hall of Conference Center

Keynote Lecture Chair: Weihai Fang	16:00-16:45	Yundong Wu <i>Shenzhen Graduate School of Peking Univ.</i>	New Mechanistic Insights on the Selectivity of Transition-Metal-Catalyzed Organic Reactions: The Role of Computational Chemistry
	16:45-17:30	Zhenfeng Xi <i>Peking Univ.</i>	Synthesis of Metallaaromatics from Dilithio Reagents and Low-Valent Metal Salts

17:30-19:00 **Dinner**

The 1st Floor of GuiZhou Hotel

DuoGongNeng Hall of Conference Center

Invited Lecture Chair: Daniel A. Singleton	19:00-19:30	Djamaladdin G. Musaev <i>Emory Univ.</i>	Computational Insights in Complexity of Chemical Catalysis
	19:30-20:00	Decai Fang <i>Beijing Normal Univ.</i>	Pd Catalytic Reaction Mechanism: Directing Groups, Solvent and Oxidation State
20:00-20:15 Coffee Break			
Invited Lecture Chair: Wenhua Sun	20:15-20:45	ShiLu Chen <i>Beijing Inst. of Technology</i>	How is Methane Formed and Oxidized Reversibly When Catalyzed by Ni-containing Methyl-Coenzyme M Reductase?
	20:45-21:15	Wenhong Yang <i>Inst. of Chem., Chinese Academy of Science</i>	Catalytic Activities of Transition Metal Complexes in Ethylene Oligo/Polymerization

Oct. 21st Friday

DuoGongNeng Hall of Conference Center

Keynote Lecture Chair: Yundong Wu	8:30-9:15	Shigeyoshi Sakaki <i>Kyoto Univ.</i>	Crucial Role of Lewis Acid in Enhancing Reactivity of Organometallic Complex
	9:15-10:00	Fahmi Himo <i>Stockholm Univ.</i>	Quantum Chemical Modeling of Mechanisms and Selectivities in Homogeneous Catalysis
10:00-10:15 Coffee Break			
Invited Lecture Chair: Jeremy Harvey; Zhuofeng Ke	10:15-10:45	Zhi-Xiang Yu <i>Peking Univ.</i>	Mechanism of [5+2+1] Reaction of Ene-Vinylcyclopropanes and Carbon Monoxide
	10:45-11:15	Evert Jan Meijer <i>Univ. of Amsterdam</i>	Modeling Catalytic Reactions in an Aqueous Environment
	11:15-11:45	Yu Lan <i>Chongqing Univ.</i>	Mechanistic Study of Organometallic Reactions Based on Density Functional Theory Calculations
	11:45-12:15	Agustí Lledós <i>Univ. Autònoma de Barcelona</i>	New Radical Pathways in Organometallic Reactions

12:15-13:30 Lunch

The 1st Floor of GuiZhou Hotel

DuoGongNeng Hall of Conference Center

Invited Lecture Chair: Feliu Maseras; Shixuan Du	13:30-14:00	ZhiXiang Wang <i>Univ. of Chinese Academy of Sciences</i>	Computational Developments of Strategies for H ₂ Activation and Hydrogenation: The Prediction Power of Computations
	14:00-14:30	Jeremy N. Harvey <i>KU Leuven</i>	Computational Modelling of the Kinetics of Homogeneous Catalysis: Progress and Challenges
	14:30-15:00	Jing Ma <i>Nanjing Univ.</i>	Noncovalent Bond-mediated Reactions in Solutions
	15:00-15:30	Rong-Zhen Liao <i>Huazhong Univ. of Science and Tech.</i>	Quantum Chemical Modeling of Water Oxidation Catalysis
15:30-15:45 Coffee Break			
Invited Lecture Chair: Agustí Lledós;	15:45-16:15	Paul W. Ayers <i>McMaster Univ.</i>	Conceptual Tools for Noninnocent Ligands
	16:15-16:45	Ganglong Cui <i>Beijing Normal Univ.</i>	DFT Studies on Photo-Induced Reactions Mediated by Ruthenium- and Iridium-Containing Catalysts
	16:45-17:15	Feliu Maseras <i>The Barcelona Inst. of Science and Tech.</i>	How are the electrons transferred in oxidative coupling?

17:15-18:30 Dinner

The 1st Floor of GuiZhou Hotel

DuoGongNeng Hall of Conference Center

Invited Lecture Chair: Evert Jan Meijer	18:30-19:00	Siwei Bi <i>Qufu Normal Univ.</i>	Theoretical Rationalization of Kinetic Experimental Phenomena involved in Gold-Catalyzed Cyclization of 2-Alkynyl-N- Propargylanilines
	19:00-19:30	Jiaxi Xu <i>Beijing Univ. of Chem. Tech.</i>	Chemoselectivity in the Copper-Catalyzed Reaction of Diazoacetamide Derivatives
	19:30-20:00	Xinhao Zhang <i>Shenzhen Graduate School of Peking Univ.</i>	A Combined IM-MS/DFT Study on the Role of N-Protected Amino Acid Ligand in Pd-Catalyzed C-H Activation

20:00-21:30 **Poster Section**

DuoGongNeng Hall of Conference Center

Oct. 22nd Saturday

DuoGongNeng Hall of Conference Center

Invited Lecture Chair: Shuhua Li	8:30-9:00	Jun Li <i>Tsinghua Univ.</i>	Single-Atom Catalysis (SAC): Bridging Heterogeneous and Homogenous Catalysis
	9:00-9:30	Jinlan Wang <i>Southeast Univ.</i>	Two-Dimensional Materials for Hydrogen Evolution Reaction
	9:30-10:00	Shixuan Du <i>Inst. of Phys., Chinese Academy of Science</i>	Functionalization of Noble-metal Surfaces for Hydrogen Dissociation
10:00-10:15 Coffee Break			
Invited Lecture Chair: ZhiXiang Wang; Shixuan Du	10:15-10:45	Zhenyang Lin <i>The Hong Kong Univ. of Science and Tech.</i>	Carbon versus Carbon-Boron Coupling Reactions of Primary, Secondary and Tertiary Alkyl Bromides
	10:45-11:15	Raghavan B. Sunoj <i>Indian Inst. of Tech. Bombay</i>	Cooperative Asymmetric Dual Catalysis: Mechanism and Selectivity
	11:15-11:45	Ruiqin Zhang <i>City University Hong Kong</i>	Carbon and Carbon Nitride Quantum Dots for Photoelectrochemical Applications
	11:45-12:15	Xinzheng Yang <i>Inst. of Chem., Chinese Academy of Science</i>	Computational Design of Base Metal Complexes for Catalytic Hydrogenation of Carbon Dioxide

12:15-13:30 Lunch

The 1st Floor of GuiZhou Hotel

DuoGongNeng Hall of Conference Center

Invited Lecture Chair: Zhenyang Lin; Jing Ma	13:30-14:00	Daniel A. Singleton <i>Texas A&M Univ.</i>	Identification and Control of Dynamic Effects on Selectivity
	14:00-14:30	Cunyuan Zhao <i>Sun Yat-Sen Univ.</i>	Theoretical Study on the Hydrolysis Mechanism of Phosphoesters Catalysed by Metal Complexes
	14:30-15:00	Zexing Cao <i>Xiamen Univ.</i>	QM/MM Insight into the Importance of Nonchemical Steps in Enzymatic Catalysis
	15:00-15:30	Shuhua Li <i>Nanjing Univ.</i>	Homolytic Cleavage of B-B Bond via the Cooperative Catalysis of Two Lewis Bases: Computational Design and Experimental Verification
15:30-15:45 Coffee Break			
Keynote Lecture Chair: Jun Li	15:45-16:30	Michael B. Hall <i>Texas A&M Univ.</i>	Intriguing Aspects of Non-innocent Ligands in Transition Metal Complexes
	16:30-17:15	Weihai Fang <i>Beijing Normal Univ.</i>	Mechanism of the Enantioselective Intramolecular Enone [2+2] Photocycloaddition Reaction Explored by the CASPT2//CASSCF calculation

18:00-20:30 Banquet

The 2nd floor of XianHeng Restaurant

Poster Awards and Conference Closing by Prof. Weihai Fang and Prof. Michael Hall