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 *Shenzhen Graduate School of Peking Univ.*	New Mechanistic Insights on the Selectivity of Transition-Metal- Catalyzed Organic Reactions: The Role of Computational Chemistry
	16:45-17:30	Zhenfeng Xi *Peking Univ.*	Synthesis of Metallaaromatics from Dilithio Reagents and Low-Valent Metal Salts

17:30-19:00 **Dinner** The 3rd Floor of ZhaoDai Restaurant

DuoGongNeng Hall of Conference Center

Invited Lecture Chair: Daniel A. Singleton	19:00-19:30	Djamaladdin G. Musaev *Emory Univ.*	Computational Insights in Complexity of Chemical Catalysis
	19:30-20:00	Decai Fang *Beijing Normal Univ.*	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 *Beijing Inst. of Technology*	How is Methane Formed and Oxidized Reversibly When Catalyzed by Ni-containing Methyl-Coenzyme M Reductase?
	20:45-21:15	Wenhong Yang *Inst. of Chem., Chinese Academy of Science*	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 *Kyoto Univ.*	Crucial Role of Lewis Acid in Enhancing Reactivity of Organometallic Complex
	9:15-10:00	Fahmi Himo *Stockholm Univ.*	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 *Peking Univ.*	Mechanism of [5+2+1] Reaction of Ene-Vinylcyclopropanes and Carbon Monoxide
	10:45-11:15	Evert Jan Meijer *Univ. of Amsterdam*	Modeling Catalytic Reactions in an Aqueous Environment
	11:15-11:45	Yu Lan *Chongqing Univ.*	Mechanistic Study of Organometallic Reactions Based on Density Functional Theory Calculations
	11:45-12:15	Agustí Lledós *Univ. Autònoma de Barcelona*	New Radical Pathways in Organometallic Reactions

12:15-13:30 Lunch The 3rd Floor of ZhaoDai Restaurant

DuoGongNeng Hall of Conference Center

Invited Lecture Chair: Feliu Maseras; Shixuan Du	13:30-14:00	ZhiXiang Wang *Univ. of Chinese Academy of Sciences*	Computational Developments of Strategies for H_2 Activation and Hydrogenation: The Prediction Power of Computations
	14:00-14:30	Jeremy N. Harvey *KU Leuven*	Computational Modelling of the Kinetics of Homogeneous Catalysis: Progress and Challenges
	14:30-15:00	Jing Ma *Nanjing Univ.*	Noncovalent Bond-mediated Reactions in Solutions
	15:00-15:30	Rong-Zhen Liao *Huazhong Univ. of Science and Tech.*	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 *McMaster Univ.*	Conceptual Tools for Noninnocent Ligands
	16:15-16:45	Ganglong Cui *Beijing Normal Univ.*	DFT Studies on Photo-Induced Reactions Mediated by Ruthenium- and Iridium-Containing Catalysts
	16:45-17:15	Feliu Maseras *The Barcelona Inst. of Science and Tech.*	How are the electrons transferred in oxidative coupling?

17:15-18:30 Dinner The 3rd Floor of ZhaoDai Restaurant

DuoGongNeng Hall of Conference Center

Invited Lecture Chair: Evert Jan Meijer	18:30-19:00	Siwei Bi *Qufu Normal Univ.*	Theoretical Rationalization of Kinetic Experimental Phenomena involved in Gold-Catalyzed Cyclization of 2-Alkynyl-N- Propargylanilines
	19:00-19:30	Jiaxi Xu *Beijing Univ. of Chem. Tech.*	Chemoselectivity in the Copper-Catalyzed Reaction of Diazoacetamide Derivatives
	19:30-20:00	Xinhao Zhang *Shenzhen Graduate School of Peking Univ.*	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 *Tsinghua Univ.*	Single-Atom Catalysis (SAC): Bridging Heterogeneous and Homogenous Catalysis
	9:00-9:30	Jinlan Wang *Southeast Univ.*	Two-Dimensional Materials for Hydrogen Evolution Reaction
	9:30-10:00	Shixuan Du *Inst. of Phys., Chinese Academy of Science*	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 The *Hong Kong Univ. of Science and Tech.*	Carbon versus Carbon–Boron Coupling Reactions of Primary, Secondary and Tertiary Alkyl Bromides
	10:45-11:15	Raghavan B. Sunoj *Indian Inst. of Tech. Bombay*	Cooperative Asymmetric Dual Catalysis: Mechanism and Selectivity
	11:15-11:45	Ruiqin Zhang *City University Hong Kong*	Carbon and Carbon Nitride Quantum Dots for Photoelectrochemical Applications
	11:45-12:15	Xinzheng Yang *Inst. of Chem., Chinese Academy of Science*	Computational Design of Base Metal Complexes for Catalytic Hydrogenation of Carbon Dioxide

12:15-13:30 Lunch The 3rd Floor of ZhaoDai Restaurant

DuoGongNeng Hall of Conference Center

Invited Lecture Chair: Zhenyang Lin; Jing Ma	13:30-14:00	Daniel A. Singleton *Texas A&M Univ.*	Identification and Control of Dynamic Effects on Selectivity
	14:00-14:30	Cunyuan Zhao *Sun Yat-Sen Univ.*	Theoretical Study on the Hydrolysis Mechanism of Phosphoesters Catalysed by Metal Complexes
	14:30-15:00	Zexing Cao *Xiamen Univ.*	QM/MM Insight into the Importance of Nonchemical Steps in Enzymatic Catalysis
	15:00-15:30	Shuhua Li *Nanjing Univ.*	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 *Texas A&M Univ.*	Intriguing Aspects of Non-innocent Ligands in Transition Metal Complexes
	16:30-17:15	Weihai Fang *Beijing Normal Univ.*	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