中国科学技术大学
University of Science and Technology of China

ICCK

12TH INTERNATIONAL CONFERENCE ON CHEMICAL KINETICS

HEFEI,CHINA
JUNE 26–29TH,2023

Conference Guide

Preface

Welcome to *the 12th International Conference on Chemical Kinetics* (*ICCK*) held at the University of Science and Technology of China in Hefei, China. We are thrilled to host this esteemed gathering for the first time in China, bringing together researchers, scholars, and industry professionals to share their knowledge, advancements, and challenges in the field of chemical kinetics.

Since its establishment in 1985, the *ICCK* provides an inclusive platform for researchers to exchange their latest findings, ideas, and foster collaborations. Under the theme of "**Smart Modeling: Big Data and Automated Kinetics**", *the 12th ICCK* encompasses a wide range of stimulating topics, including experimental and theoretical methods in chemical kinetics, gas phase and solution-liquid kinetics, catalysis (homogeneous and heterogeneous), ion kinetics, kinetic modeling, uncertainty analysis, real-world applications such as combustion, atmosphere, and space, biocatalysis and enzyme kinetics, computational fluid dynamics, model reduction, and electrochemistry.

We extend our deepest gratitude to all participants whose contributions have led to the success of *the 12th ICCK*. Your collective efforts and dedication will undoubtedly make this conference an enriching and memorable experience. We hope that your time here will be filled with scientific enlightenment, thought-provoking discussions, and opportunities for networking and collaboration. Let us seize this unique occasion to build bridges across nations, cultures, and disciplines, fostering international cooperation in the pursuit of knowledge and innovation.

Once again, welcome to the 12th ICCK in Hefei, China!

Catalogue

Organization

Program Chairs

Name	Affiliation	Nation
Yi Luo	University of Science and Technology of China	China
Feng Zhang	University of Science and Technology of China	China

Standing Committee

Name	Affiliation	Nation
Carl J. Percival	NASA Jet Propulsion Laboratory	USA
Frédérique Battin-Leclerc	CNRS, Université de Lorraine	France
Guillaume Dayma	CNRS, Université de Orléans	France
Guy B. Marin	Ghent University	Belgium
Kenneth Brezinsky	University of Illinois at Chicago	USA
Kevin M. Van Geem	Ghent University	Belgium
Michelle Coote	Australian National University	Australian
Robert Simon Tranter	Argonne National Laboratory	USA
Theodore S. Dibble	SUNY College of Environmental Science and Forestry	USA
William H. Green	Massachusetts Institute of Technology	USA
Xinggui Zhou	East China University of Science and Technology	China

Scientific Advisory Committee

Name	Affiliation	Nation
Alexander M. Mebel	Florida International University	USA
Bin Yang	Tsinghua University	China
Christa Fittschen	University of Lille	France
Fahmi Himo	Stockholm University	Sweden
Guillaume Dayma	CNRS, University of Orléans	France
Jianmin Chen	Fudan University	China
Matthias Olzmann	Karlsruhe Institute of Technology	Germany

Name	Affiliation	Nation
Nicole J. Labbe	University of Colorado Boulder	USA
Nils Hansen	Sandia National Laboratories	USA
Paul Seakins	University of Leeds	UK
Raghu Sivaramakrishnan	Argonne National Laboratory	USA
Weixue Li	University of Science and Technology of China	China
Xinggui Zhou	East China University of Science and Technology	China

Local Organizing Committee

Name	Affiliation	Nation
Feng Zhang	University of Science and Technology of China	China
Huijun Jiang	University of Science and Technology of China	China
Li Bao	University of Science and Technology of China	China
Qiang Fu	University of Science and Technology of China	China
Qun Li	University of Science and Technology of China	China
Xiaoqing Wu	China Jiliang University	China
Xin Li	University of Science and Technology of China	China
Yi Zhang	University of Science and Technology of China	China
Yuanhao Wang	University of Science and Technology of China	China

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General information

Congress Venue

LEBANSHAN HOTELS HEFEI

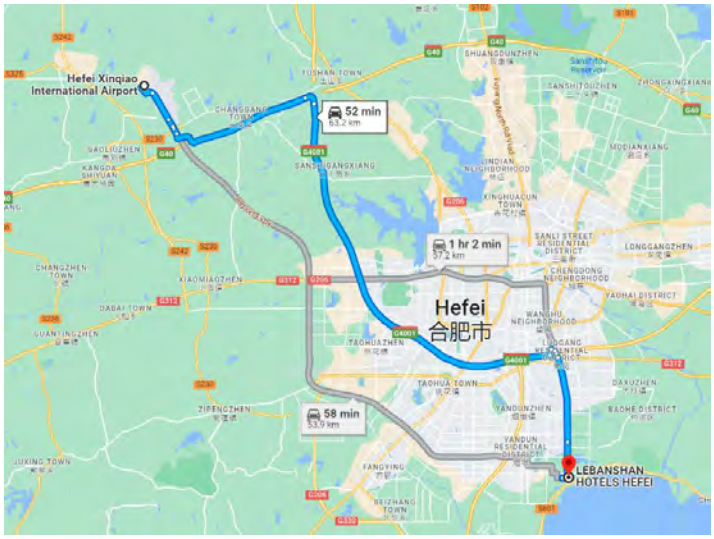
No. 301, Nanning East Road, Hefei

Congress Hotel

The conference is held at Lebanshan Hotels Hefei. Attendees are recommended to book rooms in the conference hotel for convenience. We also provide some useful information about hotels within ~2 km from the conference venue.

Transportation

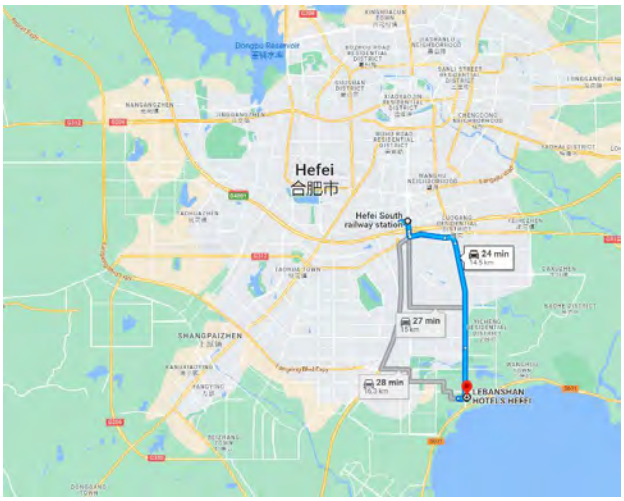
Airplane



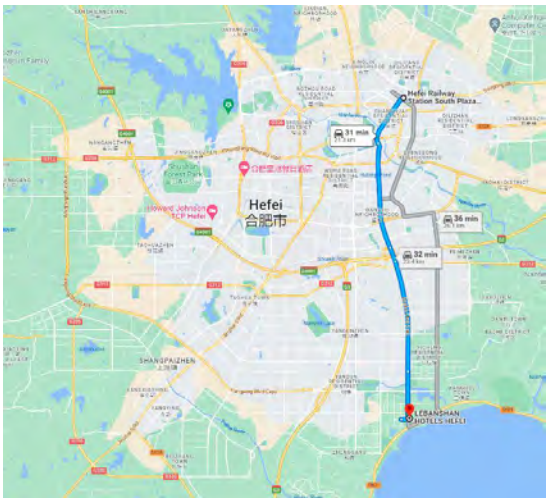
Hefei Xinqiao International Airport

Taxis are available to the congress venue at Hefei Xinqiao International Airport, which is about 60 km away and takes about an hour.

Train



Hefei South Railway Station



Hefei Railway Station

Taxis are available to the congress venue at Hefei South railway station/Hefei South railway station, which is about 15/25 km away and takes about 30/35 minutes.

Taxi

There are taxi spots at the airport and railway station, which are very easy to find.

Congress Website

Conference website: https://conferences.koushare.com/icck2023

Notice

1. The conference is served with meal vouchers, please keep them properly.
2. Please set your phone to silent or vibrate during the conference.
3. The latest check-out time of the hotel is 14:00, please arrange the time reasonably.
4. Please contact the conference team for any matters not mentioned herein.

Schedule

Simplified Schedule

Monday, June 26	
13:00 – 21:00	Registration
18:00 – 20:00	Dinner
Tuesday, June 27	
8:30 – 11:40	Plenary speaks (Session 1-1)
11:40 – 14:00	Lunch
14:00 – 15:40	Plenary speaks (Session 1-2)
15:40 – 17:00	Coffee break + Poster presentation
18:00 – 20:00	Conference banquet
Wednesday, June 28	
8:30 – 12:10	Parallel sessions (Session 2-1, 2-2)
12:10 – 14:00	Lunch
14:00 – 18:30	Leisure activity and communication
18:30 – 20:00	Dinner
Thursday, June 29	
8:30 – 12:00	Parallel sessions (Session 3-1-1, 3-2-1, 3-3-1)
12:00 – 14:00	Lunch
14:00 – 17:25	Parallel sessions (Session 3-1-2, 3-2-2, 3-3-2)
17:25 – 17:35	Closing session
18:00 – 20:00	Dinner

* All times are in China Standard Time (GMT+08)

Detailed Schedule

MONDAY, JUNE 26	
13:00-21:00	Registration *(The lobby of LEBANSHAN HOTELS HEFEI)*
18:00-20:00	Dinner *(The Western Restaurant on the first floor of LEBANSHAN HOTELS HEFEI)*
TUESDAY, JUNE 27 *(LEBANSHAN Banquet Hall)*	
8:30-8:40	Opening speech
SESSION 1-1 (Chair: Xin Xu)	
8:40-9:30	**William H. Green** *(Massachusetts Institute of Technology, USA)* Automated Predictive Modeling with Estimates from Large Datasets
9:30-10:20	**Donghui Zhang** *(Dalian Institute of Chemical Physics, CAS, China)* Accurate Potential Energy Surfaces and Quantum Dynamics for Polyatomic Chemical Reactions
10:20-10:50	Group photo; Coffee break
10:50-11:40	**Judit Zádor** *(Sandia National Laboratories, USA)* Automated Elementary Kinetics Calculations in the Gas Phase and on Surfaces
11:40-14:00	Lunch *(The Western Restaurant on the first floor of LEBANSHAN HOTELS HEFEI)*
SESSION 1-2 (Chair: William H. Green)	
14:00-14:50	**Xin Xu** *(Fudan University, China)* Machine Learning Enhanced Reaction Rate Computation for Kinetic Modelling of Heterogeneous Catalysis
14:50-15:40	**Marc-Olivier Coppens** *(University College London, UK)* A NICE Approach to Control the Effective Kinetics of Catalytic Processes
15:40-17:00	Coffee break; Poster presentation
18:00-20:00	Conference banquet *(LEBANSHAN Banquet Hall)*

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Continued

WEDNESDAY, JUNE 28	
8:25-8:30	Announcement
SESSION 2-1 (Chair: Tong Zhu; Carlo Alessandro Cavallotti) *(Hall A of the LEBANSHAN Banquet Hall)*	
8:30-8:55	**Alexander M. Mebel** *(Florida International University, USA)* On the Mechanism of Soot Nucleation
8:55-9:15	**Xiaoqing You** *(Tsinghua University, China)* Effects of Iron Addition on Soot Formation Characteristics
9:15-9:35	**Qian Mao** *(Beijing Institute of Technology, China)* Theoretical Study of Important Reaction Pathways in Polycyclic Aromatic Hydrocarbon Growth and Development of Kinetic Model
9:35-9:55	**Matteo Pelucchi** *(Politecnico di Milano, Italy)* A Comprehensive Chemical Kinetics Framework for Carbon Materials and Turquoise Hydrogen Production from Hydrocarbons Pyrolysis
9:55-10:20	Coffee break
10:20-10:45	**Tong Zhu** *(East China Normal University, China)* Automated Generation of Combustion Reaction Mechanisms
10:45-11:05	**Kai Leonhard** *(RWTH Aachen University, Germany)* ChemTraYzer – A Tool Supporting the Construction of Chemical Models
11:05-11:25	**Liming Cai** *(Tongji University, China)* Fuels of the Future: AI-based Fuel Design Screening Millions of Candidates and Their Highly-automated Chemical Model Development
11:25-11:40	**Chao Xu** *(Northeastern University, USA)* Catalyst Screening for Partial Oxidation of Methane with the Blowers-Masel Approximation
11:40-11:55	**Haoyang (Oscar) Wu** *(Massachusetts Institute of Technology, USA)* QuantumPioneer: Self-Evolving AI Machine for High-Throughput Automated Potential Energy Surface Exploration and Closed-Loop Chemical Reactivity Discovery
12:00-14:00	Lunch *(The Western Restaurant on the first floor of LEBANSHAN HOTELS HEFEI)*
14:00-18:30	Leisure activity and communication
18:30-20:00	Dinner *(The Roman Hall on the second floor of Fillmore Grand Hefei)*

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Continued

SESSION 2-2 (Chair: Sen Lin, Weixue Li) *(Hall B of the LEBANSHAN Banquet Hall)*	
8:30-8:55	**Weixue Li** *(University of Science and Technology of China, China)* Sabatier Principles of Metal-Support Interaction for Growth of Supported Nanocatalysts
8:55-9:15	**Wenyao Chen** *(East China University of Science and Technology, China)* Mesokinetics as a Tool Bridging the Microscopic-to-Macroscopic Transition to Rationalize Catalyst Design
9:15-9:35	**Zhe-ning Chen** *(Fujian Institute of Research on the Structure of Matter, CAS, China)* Toward Accurate and Efficient Dynamic Computational Strategy for Surface Catalysis
9:35-9:55	**Huijun Jiang** *(University of Science and Technology of China, China)* Effect of Nano-curved Electric Field on Nanoelectrocatalysis
9:55-10:20	Coffee break
10:20-10:45	**Sen Lin** *(Fuzhou University, China)* Single-atom Catalysis: Mechanism and Dynamics
10:45-11:10	**Shilu Chen** *(Beijing Institute of Technology, China)* Quantum Chemical Modeling of Enzymatic Reactions in Extremophiles
11:10-11:30	**Zheng Chen** *(Fudan University, China)* Toward accurate and efficient microkinetic modeling in heterogeneous catalysis
11:30-11:50	**Lu Zhang** *(Fujian Institute of Research on the Structure of Matter, CAS, China)* Understanding the Transcriptional Dynamics and Inhibitors' Acting Mechanisms in Viral RNA Polymerase
11:50-12:10	**Xiang Sheng** *(Tianjin Institute of Industrial Biotechnology, CAS, China)* Mechanism of the Cofactor- and Metal-Free Enzymatic Decarboxylation Facilitated by Local-Oriented Electric Field
12:10-14:00	Lunch *(The Western Restaurant on the first floor of LEBANSHAN HOTELS HEFEI)*
14:00-18:30	Leisure activity and communication
18:30-20:00	Dinner *(The Roman Hall on the second floor of Fillmore Grand Hefei)*

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Continued

THURSDAY, JUNE 29	
8:25-8:30	Announcement
SESSION 3-1-1 (Chair: Yuyang Li, Kai Leonhard) *(Hall A of the LEBANSHAN Banquet Hall)*	
8:30-8:55	**Chaoyang Zhang** *(Institute of Chemical Materials, CAEP, China)* Advantage and Disadvantage of Hydrogen Transfer to the Stability of Energetic Compounds
8:55-9:20	**Xiaoxia Li** *(Institute of Process Engineering, CAS, China)* Making Use of the Kinetic Information from ReaxFF Molecular Dynamics
9:20-9:40	**Dongping Chen** *(Beijing Institute of Technology, China)* Developing the New-generation Forcefield for Solid Propellants
9:40-10:00	**Junjun Wu** *(Chongqing University, China)* Towards Accurate and Efficient Determination of Thermodynamics and Kinetics of Large Complex Reaction System
10:00-10:20	Coffee break
10:20-10:45	**Bin Jiang** *(University of Science and Technology of China, China)* First-principles Surface Reaction Rates by Molecular Dynamics and Neural Network Potentials
10:45-11:05	**Yongle Li** *(Shanghai University, China)* High Accuracy and High Efficiency Rate Coefficients Calculations on High-fidelity PES: Using $Cl(^2P)+HCl \rightarrow HCl + Cl(^2P)$ as an Example
11:05-11:25	**Jun Li** *(Chongqing University, China)* Benchmarking kinetics calculations for combustion elementary steps on full-dimensional accurate potential energy surfaces
11:25-11:45	**Lin Shen** *(Beijing Normal University, China)* Mixed quantum-classical dynamical simulation with long short-term memory networks
11:45-12:00	**Yurui Han** *(University of Science and Technology of China, China)* Ab initio molecular dynamics simulations of the structural evolution of Cu clusters confined in (17,0) carbon nanotubes
12:00-14: 00	Lunch *(The Western Restaurant on the first floor of LEBANSHAN HOTELS HEFEI)*

SESSION 3-1-2 (Chair: Peng Zhang, Xiaoqing You) *(Hall A of the LEBANSHAN Banquet Hall)*	
14:00-14:25	**Yuyang Li** *(Shanghai Jiao Tong University, China)* Research on Clean Efficient Ammonia Combustion Driven by Chemical Kinetics
14:25-14:45	**Chongwen Zhou** *(Beihang University, China)* A Comprehensive Chemical Kinetic Modeling Study of Ammonia and Ammonia/Hydrogen Combustion
14:45-15:05	**Jian Gao** *(Shenzhen Technology University, China)* Ammonia Combustion via the Partially Pre-Dissociation Strategy: A Review
15:05-15:20	**Maristella Di Teodoro** *(Politecnico di Milano, Italy)* An Investigation of the Gas Phase and Surface Chemical Kinetics Active During the Plasma Assisted Chemical Vapor Deposition of Diamond
15:20-15:40	Coffee break
15:40-16:05	**Peng Zhang** *(City University of Hong Kong, China)* Torsional PES Reconstruction and Metric-Based Assessment for Calculating Partition Functions by the MS-T Methods
16:05-16:25	**Xuefei Xu** *(Tsinghua University, China)* Multi-Structural Torsional Anharmonicity Approximation for Thermodynamics and Kinetics Calculations of Complex Molecules with a Coupled Torsional Potential and Delocalized Torsions Using Redundant
16:25-16:40	**Qian Zhao** *(Xi'an Jiaotong University, China)* $CH_3O\dot{C}H_2 + O_2$: High Level Theory and the Role of Multichannel Kinetics
16:40-16:55	**Luna Pratali Maffei** *(Politecnico di Milano, Italy)* Detailed Theoretical Investigation of the Ring-insertion Pathway Determining the Product Distribution of the $C_6H_5 + O_2$ Reaction
16:55-17:10	**Kevin De Ras** *(Ghent University, Belgium)* Toward Fast Estimation of Kinetics for Unimolecular Decomposition of 1,3-Dioxetane Derivatives
17:25-17:35	Closing ceremony *(Hall A of the LEBANSHAN Banquet Hall)*
18:00-20:00	Dinner *(The Western Restaurant on the first floor of LEBANSHAN HOTELS HEFEI)*

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Continued

SESSION 3-2-1 (Chair: Christa Fittschen, Xiaoguo Zhou) *(Hall B of the LEBANSHAN Banquet Hall)*	
8:30-8:55	**Jianmin Chen** *(Fudan University, China)* Vertical Ozone Formation Mechanism — From ground to mountainside in Mt. Tai
8:55-9:20	**Wenrui Dong** *(Dalian Institute of Chemical Physics, CAS, China)* Kinetics of Criegee Intermediate Relevant Reactions
9:20-9:40	**Shengkai Wang** *(Peking University, China)* Information-Driven Experiment Design for Shock Tube and Laser Absorption Measurements of Fundamental Reaction Rate Constants
9:40-10:00	**Yangang Ren** *(Research centre for eco-environmental sciences, CAS, China)* Kinetic and Mechanism Studies of the Gas-Phase Reaction of O_3 with Diene
10:00-10:20	Coffee break
10:20-10:45	**Christa Fittschen** *(Université Lille, Processus de Combustion et de l'Atmosphère, France)* The Reactivity of Peroxy Radicals
10:45-11:05	**Zhandong Wang** *(University of Science and Technology of China, China)* Quantification of Hydroperoxides in the Low-temperature Oxidation of Alkanes
11:05-11:25	**Xiaofeng Tang** *(Anhui Institute of Optics and Fine Mechanics, CAS, China)* Dimeric Product of Peroxy Radical Self-Reaction Probed with VUV Photoionization Mass Spectrometry
11:25-11:45	**Bo Long** *(Guizhou Minzu University, China)* Quantitative Kinetics of Criegee Intermediates by Using Theoretical Methods
11:45-12:00	**Jia Han** *(University of Science and Technology of China)* A Joint Photoelectron Spectroscopic and Theoretical Study on $[HFIP\text{-}_H{\bullet}H_2O_2]^-$ and $[HFIP\text{-}_H{\bullet}HO_2]^-$ Anion Complexes
12:00-14: 00	Lunch *(The Western Restaurant on the first floor of LEBANSHAN HOTELS HEFEI)*

SESSION 3-2-2 (Chair: Zhandong Wang, Liming Cai) *(Hall B of the LEBANSHAN Banquet Hall)*	
14:00-14:25	**Jianping Xiao** *(Dalian Institute of Chemical Physics, CAS, China)* Steering from Electrochemical Denitrification to Ammonia Synthesis
14:25-14:45	**Tao Yang** *(East China Normal University, China)* Untangling the Molecular Complexity of Interstellar Ices in a Synchrotron-Based Space Simulation Machine
14:45-15:05	**Long Zhao** *(University of Science and Technology of China, China)* VUV photoionization study on the five-carbon-ring involved aromatic propagation
15:05-15:20	**Ziyuan Li** *(University of Science and Technology of China, China)* Electron-Induced Synthesis of Dimethyl Ether in the Liquid−Vapor Interface of Methanol
15:20-15:40	Coffee break
15:40-16:05	**Yi Ouyang** *(Ghent University, Belgium)* Speeding Up Turbulent Reactive Flow Simulation via Deep Artificial Neural Network
16:05-16:25	**Lin Ji** *(Capital Normal University, China)* Coarse-Grained Transition Path Mechanisms Analysis in Methane Combustion System
16:25-16:45	**Yifei Zhu** *(Xi'an Jiaotong University, China)* Smart Modulation of Plasma Reactors with Physics Assisted Machine Learning Methods
16:45-17:05	**Hao Zhao** *(Peking University, China)* Understanding of Real-Fluid Behavior in Supercritical Combustion Theory
17:05-17:25	**Qi Chen** *(Beijing Jiaotong University, China)* Kinetic Investigation of Plasma Catalytic Synthesis of Ammonia
17:25-17:35	Closing ceremony *(Hall A of the LEBANSHAN Banquet Hall)*
18:00-20:00	Dinner *(The Western Restaurant on the first floor of LEBANSHAN HOTELS HEFEI)*

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Continued

SESSION 3-3-1 (hybrid) (Chair: Jianping Xiao, Alexander M. Mebel) *(Jinxiu Hall)*	
8:30-8:55	**Raghu Sivaramakrishnan** *(Argonne National Laboratory, USA)* Modeling Nonthermal Reactions in Combustion
8:55-9:20	**Carlo Alessandro Cavallotti** *(Politecnico di Milano, Italy)* Automation of Rate Constant Evaluation for Barrierless Reactions: Status and Challenges
9:20-9:40	**Guoxing Li** *(Chang'an University, China)* Homogeneous Catalytic Effect of Water on Formic Acid Decomposition: Implication for Kinetic Modeling in Supercritical Water
9:40-10:00	**Hongbo Ning** *(Southwest Jiaotong University, China)* Theoretical Study of the Reaction Kinetics of Methyl Formate + NO_2
10:00-10:20	Coffee break
10:20-10:45	**Xinggui Zhou** *(East China University of Science and Technology, China)* Machanism and Kinetics of Prypylene Epoxidation by H_2 and O_2 on Au-Ti Catalysts
10:45-11:10	**Donghui Quan** *(Zhejiang Laboratory, China)* Origin of PrebioTIc Molecules in the InterStellar Medium (OPTIMISM): Modeling Interstellar Chemistry in AI Era
11:10-11:30	**Matteo Pelucchi** *(Politecnico di Milano, Italy)* Kinetics of Solid Plastic Waste Pyrolysis: Developments and Perspectives for Theoretical Rate Constants and Polymer-Polymer Interactions Investigation
11:30-11:45	**Muhammad Yousuf** *(Institute of Engineering Thermophysics, CAS, China)* Thermodynamic Properties Calculations of Cu-based Species
11:45-12:00	**Yonggang Cheng** *(Ghent University, Belgium)* Microkinetic Analysis of the CO_2 Effect on OCM over a La-Sr/CaO Catalyst
12:00-14: 00	Lunch *(The Western Restaurant on the first floor of LEBANSHAN HOTELS HEFEI)*

SESSION 3-3-2 (Hybrid) (Chair: Kevin Van Geem, Bin Yang) *(Jinxiu Hall)*	
14:00-14:25	**Guillaume Dayma** *(Université d'Orléans, France)* On the Impact of the O-Atom on the Ignition of a 5-Membered Ring: A Comparative Study Between Cyclopentane and Tetrahydrofuran
14:25-14:50	**Emilio Martínez Núñez** *(University of Santiago de Compostela, Spain)* Automated Reaction Mechanism Discovery and (Semi) Automated Kinetics
14:50-15:15	**Paul Seakins** *(University of Leeds, UK)* The OH + Methyformate Reaction – Site Selective Chemistry and the Fate of the Radical Products
15:15-15:40	**Nils Hansen** *(Sandia National Laboratories, USA)* Hydrocarbon Radical-Radical Reactions: Well-Skipping
15:40-16:05	**Richard H. West** *(Northeastern University, USA)* Automating the Generation of Kinetic Models for Halogenated Hydrocarbons
16:05-16:25	**Tibor Nagy** *(Research Centre for Natural Sciences, Hungary)* A Novel Active Parameter Selection Strategy for the Efficient Optimization of Combustion Mechanisms
16:25-16:45	**Mirosław Szukiewicz** *(Rzeszów University of Technology, Poland)* Linear and Non-linear Mechanism of Catalytic Hydrogenation of Propene
16:45-17:05	**István Gyula Zsély** *(ELTE Eötvös Loránd University, Hungary)* Recent Advancements in the Reaction Kinetics Branch of the ReSpecTh Information System
17:05-17:20	**Jeroen Aerssens** *(Ghent University, Belgium)* Kinetic Modelling of Chloroethane Pyrolysis: A Computational Case Study for Chlorinated Hydrocarbons
17:25-17:35	Closing ceremony *(Hall A of the LEBANSHAN Banquet Hall)*
18:00-20:00	Dinner *(The Western Restaurant on the first floor of LEBANSHAN HOTELS HEFEI)*

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Poster

No.	Name	Title
1	Aijing Guo	Mechanistic Investigation of the Kinetic Resolution of α-methyl-Substituted Phenylacetaldehyde by Norcoclaurine Synthase
2	Cheng Xie	Theoretical rate coefficients for tert-butyl hydroperoxide decomposition
3	Chengcheng Liu	Bayesian Inference of Combustion Kinetics Models via Neural Network Accelerated Hamiltonian Monte Carlo
4	Chenyue Tao	Chemical Kinetic Model Study on Ammonia and Ammonia/Hydrogen Combustion
5	Cuihong Zhang	Kinetics Measurements of $C_2H_5O_2$ with Cl and CH_3O_2 by Cavity Ring down Spectroscopy
6	Fuqiang Chen	Reaction Mechanism, Regioselectivity and Substrate Specificity of Achmatowicz Rearrangement Catalyzed by Chloroperoxidase
7	Hang Xiao	Neural-Network-Based Molecular Dynamics Study on the Initial Pyrolysis Mechanism of Spiro-Norbornanes
8	Haodong Chen	Synchrotron Photoionization Mass Spectrometry Study of Plasma-Assisted Low-Temperature Oxidation of N-Alkanes
9	Haofeng Sun	Hierarchical Palladium Catalyst for Highly Oxidation in Acidic Media Active and Stable Water
10	Jiabin Huang	Calculation of photodetachment cross sections and photoelectron angular distributions of negative ions using density functional theory
11	Jingchen Xie	Dissociation Dynamics of Anionic Carbon Monoxide in Dark States
12	Lingfeng Li	Kinetic Modeling and Mechanistic Analysis of Hydrogenolysis of Bisphenol a Based Polycarbonate over NiO Supported on Mg(Al)O
13	Ling-Ya Peng	Theoretical Studies on Photohotocatalytic Reduction of CO_2 by an Iridium Catalyst: Mechanism and Selectivity
14	Mengqi Wu	Reaction kinetics of CN + toluene and its implication on the production of aromatic nitriles in the Taurus molecular cloud and Titan's atmosphere
15	Mengyuan Fan	The Dynamics of the Dissociation Electron Attachment to CO_2 Clusters

No.	Name	Title
16	Michael Stuhr	UV Photolysis of Oxalyl Chloride: Decomposition of the Clco Radical and Quantum Yield of the Cl_2 Elimination Channel
17	Mingming Zhang	Low-Temperature Chemistry in Plasma-Driven Ammonia Oxidative Pyrolysis
18	Mo Yang	Unraveling the Impacts of Anharmonicity, Recrossing and Tunneling on Hydrogen Abstraction Kinetics of Cyclopentanol and Cyclopentane by Hydroperoxyl Radical
19	Muhammad Bilal	Laser-Based Diagnosis of Flames with Machine Learning
20	Nan Liu	Kinetic Roles of Electronically Excited States Species of Plasma Assisted N-Pentane Oxidation in a Nanosecond-Pulsed Discharge
21	Pengcheng Liu	Infrared Photodissociation Spectroscopic Study of $Sc_2O_2(CO_2)n$ + (n = 1 – 4) Cluster Cations
22	Qiao Wang	An Experimental and Modeling Study on the Co-Oxidation of Ammonia and Dimethyl Ether: Exploring the Future of Low-Carbon Combustion
23	Qifeng Hou	Exploring the chemistry behind low temperature auto-ignition of isopropyl nitrate in an RCM: an experimental and kinetic modeling study
24	Qifeng Hou	Bayesian analysis for RRKM/Master equation based kinetic predictions: A case study of ethyl with oxygen
25	Qilong Fang	A Comparative Study on Flow Reactor Pyrolysis and Laminar Flame Propagation of Flame Synthesis Precursors: Tetraethoxysilane and Its Oxygenated Hydrocarbon Counterpart
26	Qingbo Zhu	Experimental and Kinetic Model Studies on the Pyrolysis of Hydroxylamine Nitrate Ionic Liquid and Hydroxylamine
27	Qinrou Li	Quantum Chemical Study on the Enantioselective Sulfoxidation Catalyzed by Vanadium-Dependent Bromoperoxidase
28	Rui-Ning Li	Theoretical Study on Catalytic Mechanism of Diiron Cofactor in Metalloenzyme SznF
29	Shiping Wang	Theoretical investigation on the reaction mechanism of CO_2 hydrogenation by the artificial enzyme LmrR
30	Siyu Chen	Effect of Multi-structure on Kinetics of Peroxy Radical Hydrogen Migration Reaction of Diethoxymethane (DEM)

No.	Name	Title
31	Wang Li	VUV Photoionization Study of the Gas Formation of Indene-A Molecular Building Block of Nonplanar PAHs
32	Wanxiong Liao	An Experimental and Kinetic Investigation on the Two-Stage Ignition Behavior of NH_3/H_2 Mixtures in an RCM
33	Wei Shen	Systematic Construction of Combustion Reaction Models for Large Hydrocarbon Fuels Based on a Two-Step Reaction Scheme
34	Wenjie Wang	Sulfur-Induced Dynamic Reconstruction of Iron-Nitrogen Species for Highly Active Neutral Oxygen Reduction Reactions
35	Wenqi Chen	Accelerating Variable Reaction Coordinate Transition State Theory (VRC-TST) Calculations Using Gaussian Process Regression (GPR)-based Surrogate Potential Energy Surface
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* The numbers of the on-site posters are consistent with the order of this table

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