



物质科学与技术学院  
School of Physical Science and Technology



WISC

1<sup>2023</sup>  
12.09-10  
Shanghai **WISC**

**ShanghaiTech Workshop on  
Interface Science and Catalysis**

上海科技大学第一届表界面科学与催化论坛

会议手册





## Attendee Guidelines

### 1. Badge Pickup

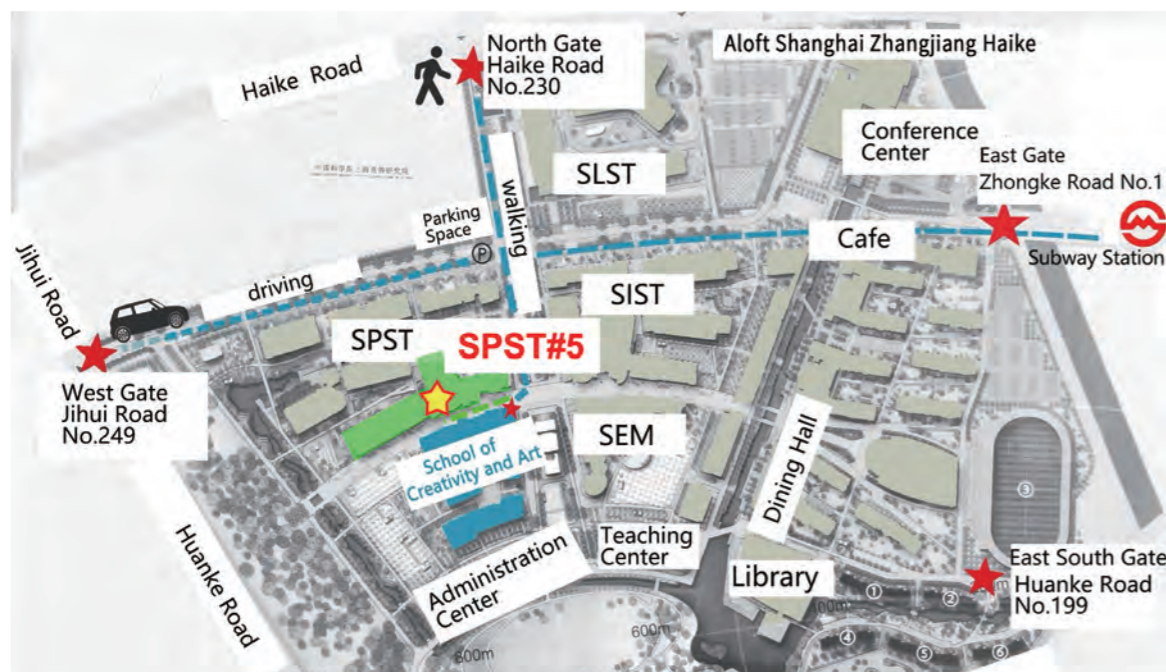
Hours: 12/8/2023 10 am-9 pm, 12/9/2023 7 am-6 pm

Location: Entrance of SPST #5-105 Lecture Hall, ShanghaiTech University

Address: 393 Middle Huaxia Road, Pudong, Shanghai 201210 (Nearest Metro Station: Line 13, Zhongke Road Stop)

### 2. Conference Room

Location: SPST #5-105 Lecture Hall, ShanghaiTech University



### 3. Food & Dining

Dining tickets are provided for all attendees, please refer to the map for the dining location. (<https://map.shanghaitech.edu.cn>)

Hours: Breakfast 6:30 am-8 am, Lunch 12 am-1:30 pm, Dinner 6 pm-9 pm

Note: Dining tickets are not usable for KFC and the 2nd Floor of No.3 Canteen (Magnolia Dining Hall)

## Welcome Message

It is our great honor to have you here for the 1st ShanghaiTech Workshop on Interface Science and Catalysis (WISC-2023), which takes place at ShanghaiTech University on Dec. 9-10, 2023. The workshop is organized by School of Physical Science and Technology and Center for Transformative Science of ShanghaiTech University.

The two-day event will cover the following topics:

Imaging and Spectroscopy of Interfaces

Reactions at Surfaces and Interfaces

Modeling Surfaces/Interfaces

Surface Dynamics and Dynamic Catalysis

We thank you for your participation and for sharing your most-recent work and insights, which would be invaluable to our community's growth and resonate deeply with the workshop's objectives.

Workshop Chair: Zhi Liu

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## Schedule

Saturday, December 9th

| 08:00-08:20 | Registration              |   |   |
|-------------|---------------------------|---|---|
| 08:20-08:30 | Welcome & Opening Remarks |   |   |
| Time        | Speaker                   | Institution                                   | Title   |
| 08:30-09:10 | Christof Wöll             | Karlsruhe Institute of Technology (KIT)       | Characterizing Oxide Particles at Ambient Pressures Using the Surface Ligand IR (SLIR) Approach: Monitoring CeO <sub>2</sub> reduction at CO Pressures of 1 Bar                       |
| 09:10-09:40 | Bin Ren                   | Xiamen University                             | Nanoscale Study of Surface Reactions with Tip-enhanced Raman Spectroscopy   |
| 09:40-10:10 | Ying Jiang                | Peking University                             | Peering into Interfacial Water by qPlus-based Atomic Force Microscopy   |
| 10:10-10:30 | Photo & Coffee Break      |   |   |
| 10:30-11:10 | Charles T. Campbell       | University of Washington                      | Metal Atom Chemical Potential: A Key Descriptor for Predicting Particle Size Effects on Catalyst Performance, and How to Estimate It  |
| 11:10-11:40 | Weixin Huang              | University of Science and Technology of China | Surface Chemistry and Catalysis of Cu <sub>2</sub> O Nanocrystal Model Catalysts  |
| 11:40-12:10 | Mingshu Chen              | Xiamen University                             | Structure and Properties of Ultra-thin TiO <sub>x</sub> and SiO <sub>x</sub> Films on Copper Single Crystal Surfaces  |
| 12:10-14:00 | Lunch Break               |   |   |
| 14:00-14:40 | Markus B. Raschke         | University of Colorado Boulder                | Vibrational Quantum Sensing: A Molecular Ruler to Image Structure, Coupling, and Dynamics on Molecular Length Scales  |
| 14:40-15:10 | Wenjie Shen               | Dalian Institute of Chemical Physics, CAS     | Catalysis at Metal-Oxide Interfaces   |
| 15:10-15:40 | Dong Wang                 | Institute of Chemistry, CAS                   | In-situ Scanning Tunneling Microscopy Investigation of Molecular Electrocatalytic Reactions at the Electrode/Electrolyte Interface  |
| 15:40-16:00 | Coffee Break              |   |   |
| 16:00-16:40 | Alec M. Wodtke            | University of Göttingen                       | High Precision Kinetics of Elementary Surface Reactions: Quantitative Comparison of Experiment and Theory   |
| 16:40-17:10 | Hongfei Wang              | Westlake University                           | Recent Development and New Opportunities in Spectroscopy and Dynamics Studies with Sub-1 cm <sup>-1</sup> High-Resolution Broadband Sum-Frequency Generation Vibrational Spectroscopy |
| 17:10-17:40 | Yong Wang                 | Zhejiang University                           | In Situ ETEM Studies of Nanocatalysts under Reaction Environments   |
| 17:40-18:10 | Junfa Zhu                 | University of Science and Technology of China | Surface Science Studies on Ceria-based Model Catalysts  |
| 18:30       | Banquet                   |   |   |

## Schedule

Sunday, December 10th

| Time        | Speaker         | Institution                                   | Title  |
|-------------|-----------------|---|--|
| 08:30-09:10 | Philippe Sautet | University of Californias Los Angeles         | Active Site Restructuring, Dynamics and Structure-sensitivity in Heterogeneous Catalysis                                     |
| 09:10-09:40 | Shuhua Li       | Nanjing University                            | Combined Molecular Dynamics and Coordinate Driving Method for Automatically Searching Complicated Reaction Pathways          |
| 09:40-10:10 | Zhi-Pan Liu     | Fudan University                              | LASP Software for Large-Scale Catalysis Simulations  |
| 10:10-10:30 | Coffee Break    |   |  |
| 10:30-11:00 | Jing Ma         | Nanjing University                            | Machine Learning Models for Reactivity and Products Prediction   |
| 11:00-11:30 | Wei-qiao Deng   | Shandong University                           | Digital-Intellectual Design of Catalysts   |
| 11:30-12:00 | Xiao-Dong Wen   | Institute of Coal Chemistry, CAS              | Rational Design of Fe-based Catalysts for Fischer-Tropsch Synthesis from Theoretical Prediction to Experimental Confirmation |
| 12:00-14:00 | Lunch Break     |   |  |
| 14:00-14:30 | Xin Xu          | Fudan University                              | Towards Accurate and Efficient Theoretical Modeling in Heterogeneous Catalysis   |
| 14:30-15:00 | Wei-Xue Li      | University of Science and Technology of China | Principle of Metal-Support Interaction for Rational Design of Stable Catalysts   |
| 15:00-15:30 | Xue-Qing Gong   | Shanghai Jiao Tong University                 | Computational Modeling of Modified CeO <sub>2</sub> Surfaces and Their Catalytic Activities                                  |
| 15:30-16:00 | Junling Lu      | University of Science and Technology of China | Precise Design of Metal-Oxide Interfaces for Selective CO <sub>2</sub> Hydrogenation   |
| 16:00-16:30 | Weitao Liu      | Fudan University                              | Lattice Vibrations at Interfaces Probed by Sum-Frequency Spectroscopy  |
| 16:30-17:00 | Biao Yang       | Soochow University                            | On-Surface Chemical Reaction Methodology   |
| 17:00-17:10 | Closing Remarks |   |  |

## Characterizing Oxide Particles at Ambient Pressures Using the Surface Ligand IR (SLIR) Approach: Monitoring CeO<sub>2</sub> reduction at CO Pressures of 1 Bar

Christof Wöll, Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), Germany



**Christof Wöll**  
Karlsruhe Institute  
of Technology (KIT)  
Germany

Christof Wöll is the director of the Institute of Functional Interfaces at the Karlsruhe Institute of Technology since 2009. After his studies of physics at the University of Göttingen he received his PhD in 1987 from the Max-Planck-Institute of Dynamics and Self-Organization in Göttingen. After a postdoctoral time (1988 to 1989) at the IBM research laboratories, San Jose, USA he accepted a position equivalent to Assistant Professor at the Institute of Applied Physical Chemistry, University of Heidelberg. After his habilitation he took over the chair for Physical Chemistry at the University of Bochum (until 2009). His research interests focus on fundamental processes in Surface Physics and Surface Chemistry, Development and advancement of techniques for the characterization of molecular adsorbates and oxide surfaces, Organic surfaces, Metal-organic frameworks (MOFs).

It is of great importance to gain detailed insight into the complex and often dynamic behavior of catalytically active oxide particles under operando conditions. We demonstrate that the vibrational spectroscopy of small diatomic adsorbates, in particular CO, provide a convenient and direct way to obtain such information for powders under reaction conditions by using information from macroscopic single crystals obtained under ultra-high vacuum (UHV) conditions using Infrared reflection-absorption spectroscopy (IRRAS). Using this approach, also referred to as surface-ligand infrared spectroscopy, or SLIR<sup>[1]</sup>, for cerium oxide surfaces effectively bridges the so-called materials and pressure gaps<sup>[2]</sup>. To this end, in a first step, low temperature CO adsorption (< 80 K) on various well-defined CeO<sub>2</sub> single crystal surfaces is used to determine the distinct vibrational bands specific for a particular crystallographic surface orientation. These vibrations are then assigned to different surface sites using precise ab-initio calculations<sup>[3]</sup>. Here, it is found that employing standard DFT methodology using standard functionals is not sufficient, in case of CeO<sub>2</sub> hybrid functionals (HSE06) have to be used<sup>[4]</sup>. This spectroscopic reference information is then used to analyze

FT-IR data recorded in transmission for powder samples. We show that the spectra obtained for the particles can be related in a straightforward fashion to the single crystal data. In a third step, DRIFTS data recorded at ambient (1 bar) pressures and for temperatures of up to 400 °C. At these high pressures, the DRIFTS data are dominated by CO gas-phase ro-vibrational excitations. In order to observe CO adsorbate vibrations at such high pressures it is necessary to remove these gas-phase P and R branches. We demonstrate that this can be done by subjecting DRIFTS data recorded at high resolution (0.25 cm<sup>-1</sup>) to a novel subtraction scheme. In a next step, the different CO adsorbate vibrational bands were used to monitor surface structural changes of the ceria particles occurring at elevated temperatures. An increase in the concentration of Ce<sup>3+</sup> species as a result of CO-induced reduction could be directly demonstrated even at low (300 K) temperatures. Our results demonstrate important progress towards the non-invasive, non-destructive characterization of real catalysts under operando conditions. First results demonstrate that the same approach can be applied to metal particles (Pt, Pd) supported on the ceria clusters.

Concluding the talk, we will discuss a recent development to use machine-learning (ML) for operando studies in heterogeneous catalysis. Artificial neural networks, trained with single crystal IRRAS data, are utilized to monitor the shapes and reduction states of powder particles in real time.

Our methodology, involving low-temperature CO adsorption under UHV conditions, ab-initio calculations, and high-resolution DRIFTS under operando conditions, not only enhances the understanding of surface structures but also paves the way for novel applications in real-time monitoring using AI-driven techniques. This research marks a significant stride in non-invasive, non-destructive catalyst characterization, offering a glimpse into the future of AI in operando studies for heterogeneous catalysis.

### References:

- [1] Structure and Chemical Properties of Oxide Nanoparticles Determined by Surface-Ligand IR Spectroscopy. C. Wöll, ACS Catal., 10 (1), 168-176 (2019)
- [2] Bridging the Pressure and Materials Gap in Heterogeneous Catalysis: A Combined UHV, In Situ, and Operando Study Using Infrared Spectroscopy, L. Caulfield, E. Sauter, H. Idriss, Y. Wang, Ch. Wöll, J. Phys. Chem. C, <https://doi.org/10.1021/acs.jpcc.3c03567> (2023)
- [3] Vibrational frequencies of CO bound to all three low-index cerium oxide surfaces: A consistent theoretical description of vacancy-induced changes using density functional theory, P. G. Lustemberg, Ch. Yang, Y. Wang, Ch. Wöll, M. V. Ganduglia-Pirovano, J. Chem.Phys., 159, 034704 (2023)
- [4] Vibrational Frequencies of Cerium Oxide-Bound CO: A Challenge for Conventional DFT Methods, P.G. Lustemberg, Ph. Pleßow, Y. Wang, Ch. Yang, A. Nefedov, F. Studt, Ch. Wöll, M.V. Ganduglia-Pirovano, Physical Review Letters, 125, 256101 (2020)



## Metal Atom Chemical Potential: A Key Descriptor for Predicting Particle Size Effects on Catalyst Performance, and How to Estimate It

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**Charles T. Campbell**  
University of Washington

Prof. Charles T. Campbell is the B. Seymour Rabinovitch Endowed Chair and Professor Emeritus in Chemistry at the University of Washington, where he is also Adjunct Professor of Chemical Engineering and of Physics. He received his BS (1975) and PhD (1979, under JM White) degrees at the University of Texas at Austin in Chemical Engineering and Chemistry, then did postdoctoral research in Germany with Gerhard Ertl (2007 Nobel Prize Winner). He is the author of over 370 publications and two patents on surface chemistry, catalysis, physical chemistry and biosensing, with over 37,000 total citations and an h-index of 100 (Google Scholar). He is an elected Honorary Fellow of the Chinese Chemical Society, Fellow of the ACS, the AVS and the AAAS, and Member of the Washington State Academy of Sciences. He received the Arthur W. Adamson Award of the ACS, the ACS Award for Colloid or Surface Chemistry, the ACS Gabor Somorjai Award for Creative Research in Catalysis, the ACS Catalysis Award for Exceptional Achievements, the Gerhard Ertl Lecture Award, the Robert Burwell Award/Lectureship of the North American Catalysis Society, the Medard W. Welch Award of the AVS, the Gauss Professorship of the Göttingen Academy of Sciences, the Ipatieff Lectureship of Northwestern University and an Alexander von Humboldt Research Award. He serves as Editor-in-Chief of Surface Science Reports, and on the Boards of Catalysis Reviews, Catalysis Letters, Surface Science and Topics in Catalysis. He previously served as Editor-in-Chief of Surface Science for over ten years.

Many important catalysts and electrocatalysts for energy and environmental technologies involve late transition metal nanoparticles dispersed across the surface of some oxide or carbon support. The activity and long-term stability of these materials depend strongly on particle size below 7 nm, and, in this size range, upon the composition and atomic-level structure of the support surface. We have shown that the chemical potential of the metal atoms in such supported catalysts provides a good descriptor of their performance as heterogeneous catalysts that captures many of the effects of particle size, metal-metal alloying and support on catalyst performance. Metal atoms in nanostructures where they have higher metal chemical potential bind small adsorbed catalytic reaction intermediates more strongly. The metal chemical potential also enters directly into the rate equation for catalyst sintering as a negative contribution to the activation energy for sintering. Based upon microcalorimetric measurements of differential heats of metal vapor adsorption, which convert directly into metal chemical potential, we have shown that the metal chemical potential is predictable as a function of metal particle size and the adhesion energy (per unit contact area) of the particle to the support. For oxide supports, this adhesion energy correlates predictably with metal oxophilicity, as we defined based on heats of oxide formation from gaseous metal atoms. For carbon supports, this adhesion energy correlates predictably with metal carbophilicity, as we defined based on DFT estimates of C atom adsorption energies. These correlations provide predictions of metal chemical potential that can enable catalyst design.

Work supported by DOE-OBES under Grant Number DE-FG02-96ER14630.

## Vibrational Quantum Sensing: A Molecular Ruler to Image Structure, Coupling, and Dynamics on Molecular Length Scales

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**Markus B. Raschke**

University of  
Colorado Boulder

Markus Raschke is professor at the Department of Physics at the University of Colorado at Boulder. His research is on the development of novel nano-optical spectroscopy and microscopy techniques with applications to single molecules, quantum materials, and fundamental control of light matter interaction. Based on a long personal interest in field collecting minerals his research also ventured into geology and mineralogy, with projects in Washington, Colorado, and the Sichuan Mountains in Tibet/China. He received his PhD in 2000 from the Max-Planck Institute of Quantum Optics and the Technical University in Munich, Germany. Following appointments at the University of California at Berkeley, and the Max-Born-Institute in Berlin, he became faculty member at the University of Washington, followed by his appointment in Boulder in 2010. He is fellow of the Optical Society of America, the American Physical Society, the American Association for the Advancement of Science, and the Explorers Club.

Properties and functions of molecular materials often emerge from intermolecular interactions and associated nanoscale structure and morphology. However, defects and disorder disturb from energy conversion to carrier transport. Conventional microscopy techniques lack spatial resolution and sensitivity to the low-energy scales of intermolecular interactions and intra-molecular energy relaxation. We address these problems in novel combinations of spatio-spectral and spatio-temporal infrared nano-imaging.

Here, coupling between molecular vibrations leads to collective modes, with distinct spectral features sensitive to intermolecular distance and relative molecular orientation. Resolving this vibrational exciton formation as a molecular ruler in IR nano-spectroscopy, we image competing phases and local disorder in molecular solids – information inaccessible by conventional X-ray or electron-based crystallography.

In the application to the growth of porphyrin model organic electronic nanocrystals we observe the evolution of defects in competing amorphous and crystalline phases with nanometer spatial resolution [1,5]. Similarly, imaging vibrational coupling in polymers [2] and molecular monolayer [3], we image domain formation from the molecular to nano-scale. Further, in another modality through mode selective coupling of vibrational resonances to IR nano-antennas and associated Purcell-enhanced modification of vibrational lifetimes, we resolve intramolecular vibrational interaction and vibrational energy redistribution (IVR) [4]. I will summarize with a perspective for nm-fs resolved precision vibrational nano-spectroscopy for functional imaging in the low-energy landscape of molecular matter.

[1] Muller, et al., PNAS 117, 7030 (2020); [2] Gray, et al., Nano Lett. 21, 5754 (2021); [3] Dönges et al. Nano Lett. 21, 6463 (2021); [4] Wilcken et al. PNAS 120, e2220852120 (2023); [5] Puro, et al. (submitted).

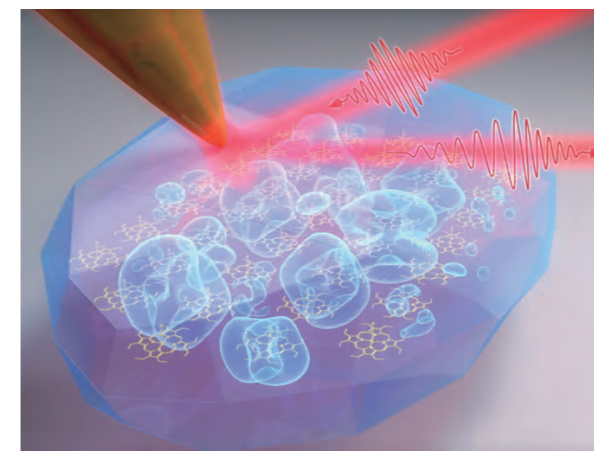


Fig. 1. Infrared nano-imaging of spatial delocalization of the vibrational wavefunction, serving as quantum sensor and molecular ruler of molecular disorder, crystallinity, and intermolecular coupling that control the properties of functional molecular materials at their elementary level.

## High Precision Kinetics of Elementary Surface Reactions: Quantitative Comparison of Experiment and Theory

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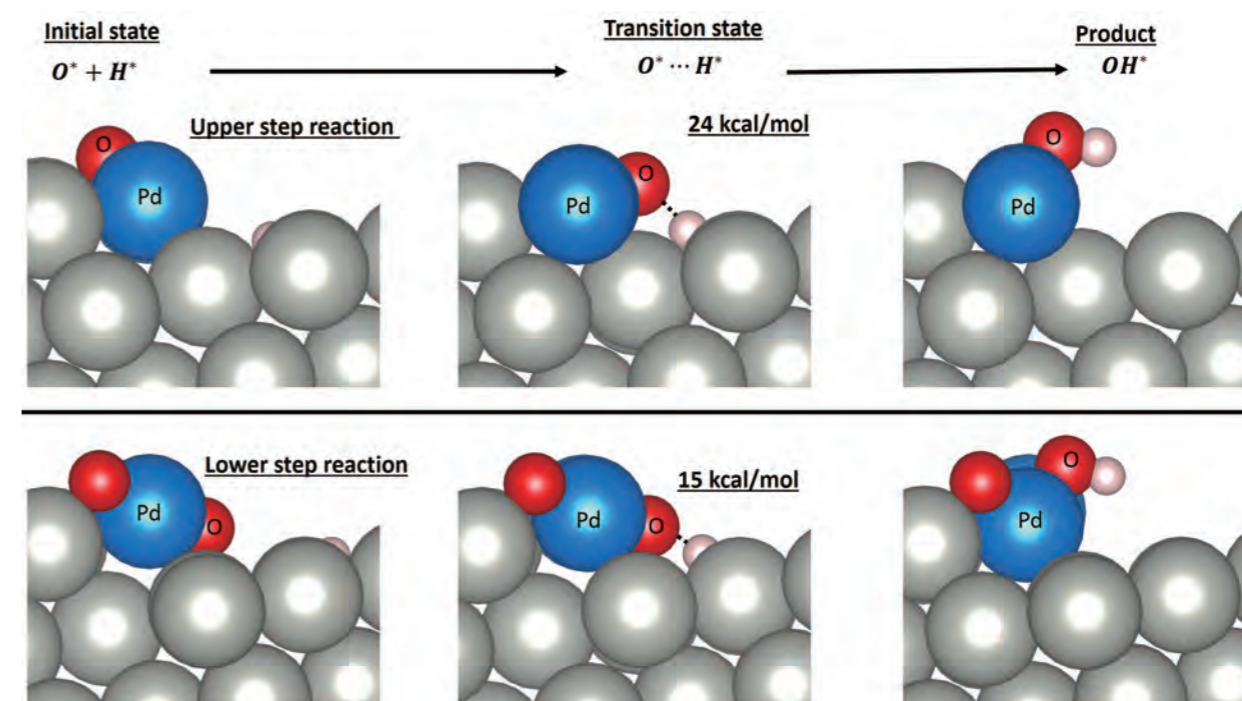


**Alec M. Wodte**  
University of Göttingen

Born 1959 in Salt Lake City, USA. PhD at Univ. California Berkeley, USA (1985), research stays at the MPI for Fluid Dynamics Göttingen, Univ. Kaiserslautern, Catholic University of Nijmegen, the Netherlands, Professor Univ. California, Santa Barbara (1988-2010), Full Professor (since 1996), Director and Scientific Member at the MPI for Biophysical Chemistry (1996-2021), since 2022 Max Planck Institute for Multidisciplinary Sciences. Professor for Physical Chemistry, Univ. Göttingen (since 2010). Numerous prizes and awards, among them the Presidential Young Investigator Award of the National Science Foundation, the Humboldt Research Award (1998) and an Alexander von Humboldt Professorship (2010).

The kinetics of elementary thermal reactions is fundamental to our understanding of heterogeneous catalysis; however, experimental methods for accurately deriving thermal rate constants are unreliable and theoretical methods for predicting rates remain un-validated. Velocity Resolved Kinetics (VRK) is a new method for obtaining highly accurate kinetics data for surface reactions with excellent signal-to-noise. This new data permits quantitative comparisons between experiment and theory for the first time. In this talk I will present two examples of recent work. In a first, VRK is used to observe formic acid decomposition on Palladium, which produces two reactive intermediates. These intermediates decompose to CO<sub>2</sub> and CO with very different rates. Isotopic labeling results in a large kinetic isotope effect that can be used to identify the structures of these intermediates experimentally. The observations can also be understood by comparison to theoretically computed reaction pathways. This allows us to confirm the presence of a previously predicted intermediate in the Water Gas Shift Reaction (WGSR). In the second example, I will show the mechanism

of the hydrogen oxidation reaction can be elucidated by a fruitful interplay between experiment and theory. This work leads to the insight that cooperative adsorbate binding can produce active configurations that behave like molecules embedded in the surface with their own reactive properties. This work also shows that predictions of Transition State Theory (TST) based on DFT-GGA calculations compare well to experiment, when the correct active configurations are chosen.



Reaction pathways for the rate limiting OH\* formation step in the hydrogen oxidation on Pd. Two active sites are required to explain VRK data obtained for:  $10^{-4} \text{ML} < [O^*] < 10^{-1} \text{ML}$ .



## Active Site Restructuring, Dynamics and Structure-sensitivity in Heterogeneous Catalysis



**Philippe Sautet**  
University of California  
Los Angeles

Philippe Sautet has studied at “Ecole Polytechnique” in Paris and defended his doctorate in Theoretical Chemistry at Orsay University (Paris XI) in 1989. He then entered CNRS at the Institute of Research on Catalysis in Lyon, where he developed and lead a group devoted to the applications of theoretical chemistry to heterogeneous catalysis. After being the director of the laboratory of Chemistry at the ENS of Lyon for 8 years, he was director of the “Institut de Chimie de Lyon”, a cluster of chemistry laboratories in Lyon, from 2007 to 2015. Philippe Sautet is now Distinguished Professor at the Chemical and Biomolecular Engineering department and at the Chemistry and Biochemistry department of UCLA., and he was awarded the Levi James Knight, Jr. Chair for Excellence in 2022. He acts as vice chair for graduate studies of the Chemical and Biomolecular Engineering department. He has been associate editor of ACS Catalysis, an international journal published by the American Chemical Society from 2012 to 2021.

His research interests are in the theoretical study at the molecular scale of catalysts and catalyzed reactions. He collaborates with several experimental groups in the field.

He has published over 300 scientific papers. He received several awards including the silver medal of CNRS in 2007, the Paul Pascal Prize of the French Academy of Science in 2008 and the Pierre Süe Grand Prize of the French Chemical Society in 2012. He was elected at the French Academy of Science in 2010. In addition, France distinguished him as “Chevalier de l'Ordre National du Mérite” for his action in research and research organization and as “Chevalier de l'ordre des palmes académiques” for his teaching and action towards students.

Understanding how catalyst active sites dynamically evolve at the atomic scale under reaction conditions is a key challenge and a prerequisite for accurate determination of catalytic mechanisms and predictably developing catalysts. We will show in the lecture that the concept of catalyst restructuring applies similarly to thermo- and electrocatalysis, With methane activation on supported Pt clusters and by an explicit sampling of cluster configurations at the transition state, we will demonstrate that fluxionality and restructuring is required to reach the most active transition state. The capability of the cluster to reconstruct, simultaneously with the C-H dissociation, is a central aspect for catalytic activity. We will combine in-situ time-dependent observation with scanning tunneling microscopy and machine learning-accelerated first-principle atomistic simulations to uncover the mechanism of restructuring for the surface of Pt catalysts under a pressure of carbon monoxide (CO). In parallel, we will unravel the potential- and pH-dependent restructuring of Cu(111) in acidic electrolyte, where Cu adatoms are stabilized on the surface in a (4×4) superstructure and Cu(100) were a paring row reconstruction occurs. Theory applies global optimization techniques accelerated by machine learning potentials at DFT accuracy and grand canonical density functional theory for electrocatalytic modelling. Scanning-tunneling microscopy provides atomic scale real space images of the restructured surface and provide insight on the restructuring mechanism.



## Nanoscale Study of Surface Reactions with Tip-enhanced Raman Spectroscopy



**Bin Ren**

Xiamen University

Tip-enhanced Raman spectroscopy (TERS), which combines scanning probe microscopy and plasmon-enhanced Raman spectroscopy, is capable of simultaneously obtaining the topographical and Raman fingerprint information at nanometer spatial resolution. Such a spatial resolution will allow the identification of the local physicochemical properties of different sites on the nanocatalysts without bothering the averaged effect in ensemble measurements, which makes it possible to disentangle the electronic effect and geometric effect with the change of the size. We visualized the size-specific electronic, geometric and catalytic properties of the different sites located on the individual Pd nanocatalyst by real-space TERS imaging with 3 nm spatial resolution. We further developed electrochemical tip-enhanced Raman spectroscopy (EC-TERS) for in situ monitoring the geometric and electronic evolution of individual active sites of MoS<sub>2</sub> during hydrogen evolution reaction (HER) and revealed the progressive generation of active sites during the electrochemical activation and reaction processes. These discoveries offer new insights into our understanding of the active site and its dynamics during electrocatalytic processes.

## Peering into Interfacial Water by qPlus-based Atomic Force Microscopy



**Ying Jiang**

Peking University

Water/solid interfaces are a central theme across an incredibly broad range of scientific and technological processes. Scanning probe microscopy (SPM) has been extensively applied to probe interfacial water, but there exist two longstanding limitations in the past decades, which makes SPM fall short compared with conventional spectroscopic methods. First, it is very difficult to image H atoms of water molecule directly; Second, it is highly possible to disturb the fragile H-bonding water structure during the imaging process. To this end, we have developed a new imaging method based on qPlus-type atomic force microscopy (AFM), which is sensitive to H and non-invasive to water structure. The key lies in probing the high-order electrostatic force between the quadrupole-like CO-terminated tip and the polar water molecules at large tip-water distances. In this talk, I will showcase the application of this technique to probe water clusters, ion hydrates, 2D ice and even bulk ice surface [1-5]. The possibility of combing qPlus-AFM with quantum sensing technology to perform nanoscale NMR measurement of interfacial water will be also briefly discussed [6-7].

### References:

- [1] Nature Commun. 9, 122 (2018)
- [2] Nature 557, 701 (2018)
- [3] Nature 577, 60 (2020)
- [4] Science 377, 315 (2022)
- [5] Nature Nano. doi: 10.1038/s41565-023-01550-9 (2023)
- [6] Nature Commun. 12, 2457 (2021)
- [7] Nature Physics 18, 1317 (2022)

## Surface Chemistry and Catalysis of Cu<sub>2</sub>O Nanocrystal Model Catalysts



**Weixin Huang**

University of Science and  
Technology of China

Structural complexity and heterogeneity of working catalysts strongly hamper the relevant fundamental studies. Single crystals have been traditionally employed as model catalysts for fundamental studies, but the acquired understandings sometimes encounter the so-called “materials gap” and “pressure gap” when extended to the working catalysts. Uniform catalytic nanocrystals consist of a novel type of model catalyst that can be studied under the same conditions as working catalysts. In this talk, I will report our work using uniform Cu<sub>2</sub>O cubes enclosed with the {100} facets, octahedral enclosed with the {111} facets and rhombic dodecahedra enclosed with the {110} facets to explore structure-activity relations of Cu<sub>2</sub>O catalysis in propylene oxidation with O<sub>2</sub> reactions. Our results demonstrate that uniform oxide nanocrystals can not only serve as model catalysts extending the surface structure-surface chemistry relation acquired from single crystal model catalysts to the surface structure-surface chemistry-catalysis relation but also as candidates for efficient catalysts.

## Structure and Properties of Ultra-thin TiO<sub>x</sub> and SiO<sub>x</sub> Films on Copper Single Crystal Surfaces



**Mingshu Chen**

Xiamen University

The metal-oxide interface plays a crucial role in catalysis, which has been obtained increasing interest in recent years. In this presentation, ultra-thin TiO<sub>x</sub> and SiO<sub>x</sub> films were prepared by evaporating Ti and Si onto Cu(111) and Cu(110) surfaces followed by oxidation and annealing in O<sub>2</sub>. The thickness and structures of the surface thin films were characterized by various surface science techniques. Both TiO<sub>x</sub> and SiO<sub>x</sub> film were grown layer-by-layer and exhibited well-defined two-dimensional network structure on the copper surfaces. X-ray photoelectron spectroscopy (XPS) results confirmed the presence of Cu-O-Ti and Cu-O-Si species and high-resolution electron energy loss spectroscopy (HREELS) showed specific features of the asymmetric stretching modes. Thermal stability experiments illustrated that the well-ordered films were stable under annealing in vacuum. The feature of CO adsorption suggested a CO-Cu<sup>δ+</sup> species induced from the Cu-O-Si linkages. Low energy ion scattering spectroscopy (LEIS) and XPS results demonstrated that some Cu<sub>2</sub>O generated and located over the silica film as exposing the 1 ML SiO<sub>x</sub>/Cu(111) in O<sub>2</sub> at 353 K. A complex surface structure of Cu+(-O-Ti)-O-Cu+/Cu(110) was proposed, in which the topmost surface Cu<sup>+</sup> is highly dispersed, isolated and fixed by the TiO<sub>x</sub> layer. Such a ‘single atom’-like surface site appeared a very narrow CO peak at 2130 cm<sup>-1</sup>, and was more stable upon both CO reduction and vacuum annealing than the Cu<sub>2</sub>O/Cu(110), and also in NO+CO reaction. The studies provides useful information for the design and supplication of single-atom catalysts and understanding the nature of catalytic active centers.



## Catalysis at Metal-Oxide Interfaces



**Wenjie Shen**

Dalian Institute of  
Chemical Physics, CAS

Metal particles, clusters and isolated atoms, dispersed over reducible oxides, present as the typical forms for catalysis, where the metal-oxide interfaces are commonly viewed as the active sites. Downsizing metal particles to subnanometric clusters and ultimately to single-atoms has been actively pursued to elaborate the structure-reactivity relationships in fundamental studies and to promote the utilization efficiency of metals in practical applications, but the simultaneously changed electronic properties of metal entities alter the catalytic performance profoundly. Here, we show the interplay between geometric and electronic structures of Pt entities play an essential role in heterogeneous catalysis.

Air-calcination redispersed 3 nm Pt particles, over  $\text{TiO}_2$ , to 1 nm monolayers at 773 K and single-atoms at 873 K. When tested for the low-temperature water-gas-shift, the oxidized monomers were much more active than the single-atoms, primary because of the site synergy.  $\text{H}_2$ -reduction of the monolayers at a proper temperature resulted in metallic bilayers, and the catalytic activity enhanced dramatically. The active clusters consisted of a bottom layer of positively-charged Pt atoms bonded on the oxygen vacancies of  $\text{TiO}_2$  and a top layer of metallic Pt atoms. The reaction occurred at the Pt- $\text{TiO}_2$  interfacial perimeter, where CO was adsorbed on the interfacial Pt atoms. While the top-layer metallic Pt atoms coordinated with the interfacial positively-charged Pt atoms and indirectly affected the adsorption of CO.

$\text{H}_2$ -reduction of Pt/ $\text{Fe}_2\text{O}_3$  redispersed 3 nm Pt particles into fully isolated metallic Pt atoms. Starting with a Pt- $\text{Fe}_2\text{O}_3$  heterodimer where a Pt particle sits on a  $\text{Fe}_2\text{O}_3$  particle, the transformation of  $\text{Fe}_2\text{O}_3$  to  $\alpha\text{-Fe}$  under  $\text{H}_2$ , split the Pt particle into Pt atoms that located over a Fe nanoparticle in the form of well-defined Pt-Fe-Pt ensemble. The Pt atoms preferentially hydrogenated the C=O bond that is conjugated to a C=C bond, with simultaneously enhanced activity and selectivity. The left-end Pt atom anchored the C=C bond while the bridging Fe atom activated the C=O bond that was further hydrogenated by H atoms supplied by the right-end Pt atom.

## In-situ Scanning Tunneling Microscopy Investigation of Molecular Electrocatalytic Reactions at the Electrode/Electrolyte Interface



**Dong Wang**

Institute of  
Chemistry, CAS

The electrode/electrolyte interface plays a critical role in the performance of electrochemical energy storage and conversion devices. Understanding the structure and reaction processes at solid/liquid interface is of great importance in surface science and electrochemistry. Metalloporphyrins, a model system of the metal-organic catalysts for different electrocatalytic processes, have attracted considerable attention for the advantages of high efficiency and low cost. Understanding the catalytic role of the active sites in molecular catalysts facilitates the design of high performance metal-organic catalysts. Electrochemical scanning tunnelling microscopy (ECSTM) is a powerful technique for investigating electrocatalytic reaction at solid/liquid interface at the molecular scale. In this presentation, we discuss the application of the high resolution ECSTM to study the interfacial electrochemical reactions by molecular catalysts at molecular level. The time evolution of molecular metalloporphyrins and metallophthalocyanines in several important electrocatalytic processes, such as oxygen reduction reaction, oxygen evolution reaction, can be resolved at the different potential and different electrolyte environment.

## Recent Development and New Opportunities in Spectroscopy and Dynamics Studies with Sub-1 cm<sup>-1</sup> High-Resolution Broadband Sum-Frequency Generation Vibrational Spectroscopy



**Hongfei Wang**  
Westlake University

Since its inception, sub-1 cm<sup>-1</sup> high-resolution broadband sum-frequency generation vibrational spectroscopy (HR-BB-SFG-VS) has provided tremendous new opportunities to unveil detailed spectral, structural and dynamical details of the molecular surfaces and interfaces. However, the high-cost of HR-BB-SFG-VS has limited its implementation and applications except in a couple of laboratories worldwide. Recent development of laser technology has made it possible to construct much compact and much lower cost HR-BB-SFG-VS for the needs of the field. Here we report the development of a new compact sub-1 cm<sup>-1</sup> HR-BB-SFG-VS system at 100 kHz that is sensitive for liquid interface SFG-VS spectra measurements, as well as the new opportunities these new technologies can provide to other nonlinear and multi-dimensional spectroscopy in general.



**Yong Wang**  
Zhejiang University

## In Situ ETEM Studies of Nanocatalysts under Reaction Environments

Over 90% chemical processes involve catalysis. Acquiring the dynamic behavior of catalysts under reaction is the key to understand the catalytic mechanism and then design novel catalysts with high performance. Although indirect information can be obtained through various methods, to directly “see” how the catalyst evolve during reaction at the atomic scale and further reveal the catalytic mechanism remains challenging. To address this issue, we manage to visualize the reaction via environmental TEM with gases into the TEM system and investigate the microstructure evolution of catalyst and its impact on the catalytic performance at the atomic level during real reactions, aiming to provide first-hand data and novel strategy for the design and rational synthesis of catalysts with high performance. In this talk, I will summarize recent progresses in our group, mainly focusing on the dynamic evolution of the active sites of catalysts under reactive environments at the atomic scale [1-11]. In the last, I will give a brief perspective regarding the challenge and opportunity in this field.

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## Surface Science Studies on Ceria-based Model Catalysts



**Junfa Zhu**

University of Science and  
Technology of China

Ceria-supported metal catalysts have obtained intensive attention due to their superior catalytic performance in many important industrial and environmental catalytic applications, such as water-gas shift (WGS) reaction and CO oxidation, etc. In order to unravel the relationship between the catalyst structures and their performances, and the underlying catalytic reaction mechanisms at the atomic-molecular level, we have performed surface science studies of ceria-based metal model catalysts. In this presentation, I will mainly report our recent studies on Cu and Cu-based bimetallic systems on the well-ordered CeO<sub>2</sub>(111) thin films by synchrotron radiation photoemission spectroscopy (SRPES) together with scanning tunneling microscopy (STM), low electron energy diffraction (LEED) and infrared reflection absorption spectroscopy (IRAS). The growth, electronic structure and thermal stability of Cu, Cu-Co and Cu-Ni on CeO<sub>2</sub>(111) have been systematically investigated. Through these model catalyst studies, we aim to gain a fundamental insight into the nature and the extent of copper-ceria interactions as well as the structures of Cu-based bimetallic catalysts, which could help shed some light on the origin of the catalytic performance of CeO<sub>2</sub> supported Cu-based catalysts.

## Combined Molecular Dynamics and Coordinate Driving Method for Automatically Searching Complicated Reaction Pathways



**Shuhua Li**

Nanjing University

Theoretical prediction for mechanistic details of complicated reactions has been a challenging subject due to the presence of numerous reaction pathways. In this talk, I will present our recent development on automated methods for exploring chemical reaction networks. The approach we proposed is called as combined molecular dynamics and coordinate driving (MD/CD) method, in which MD simulations are used to explore the conformational space of minimal structures, and the modified CD method is employed to construct reaction pathways for representative conformers.<sup>1</sup> It provides a cost-effective computational strategy for a wide range of organic reactions. With selective integrated tempering sampling-based MD simulations and quantum mechanics/molecular mechanics calculations, the MD/CD method enables reaction networks for reactions in the condensed phase to be explored.<sup>2</sup> Recently, we have extended and generalized the MD/CD method by utilizing the well-parameterized GFN family of methods for MD simulations.<sup>3</sup> This extension allows us to explore reaction networks in quite complicated reactions, including transition-metal-catalyzed reactions, single-electron-transfer (SET) involved processes, and so on. The MD/CD method presented here is anticipated to serve as an efficient tool for the automated exploration of reaction networks, facilitating the design of new reactions and catalysts.

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## LASP Software for Large-Scale Catalysis Simulations



**Zhi-Pan Liu**  
Fudan University

This lecture introduces our recent progress in LASP (Large-scale Atomic Simulation with neural network Potential) software ([www.lasphub.com](http://www.lasphub.com)) and its application in catalysis. In 2018 we designed a “Global-to-Global” approach for material discovery by combining our SSW (stochastic surface walking) global optimization method with neural network (NN) techniques, which led to the SSW-NN method and the global neural network (G-NN) potential method. The SSW-NN method is the key functionality of LASP software and has been utilized widely in solving different challenging problems. LASP 3.6 now utilizes the many-body function corrected global neural network potential (G-MBNN) framework, which shows a great advantage in improving the large-range interaction and reaction activity prediction. I will also introduce two recent LASP applications from our group, namely Ag-catalyzed ethene epoxidation and Fischer-Tropsch synthesis, to demonstrate the automated global data set generation, the improved NN training procedure, and the application in resolving stable structures and reaction mechanism. As a general tool for chemistry simulation, the SSW-NN method implemented in LASP software provides an efficient and predictive platform for obtaining material properties.

## Machine Learning Models for Reactivity and Products Prediction



**Jing Ma**  
Nanjing University

Electronic structure methods and molecular simulation techniques have been applied to understand and rationalize the reactivity and products in various reactions. Recently, machine learning techniques accelerate the exploration of huge chemical space of chemical reactions. In this talk, I will give some examples of the study on chemical reactions. (1) Conversion from nitrogen to ammonia is crucial to the industrial production of fertilizers and other fundamental chemicals. To predict the capture of nitrogen and possible reaction pathways and barriers of the nitrogen reduction reaction (NRR) in metal-zeolites, we setup a dataset. Both graph convolutional neural network (GCNN) model with the multilevel attention mechanism and feature learning methods have been used to give good prediction performance of reaction energies and could also be transferred to 2D materials and the non-metal systems.<sup>[1]</sup> (2) Carbon dioxide (CO<sub>2</sub>) capture, utilization, and storage technologies are optimal options for reducing global warming and producing various high-value chemicals and fuels. We investigate the selective adsorption and separation of CO<sub>2</sub>/N<sub>2</sub>/H<sub>2</sub>O on metal-zeolites. The energy change for reaction intermediate and product probability of CO<sub>2</sub>RR to methanol, methane and formaldehyde on metal-zeolites were predicted. ML models also work well for MOFs, 2D materials, and molecular complexes.<sup>[2]</sup>

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## Digital-Intellectual Design of Catalysts



**Weiqiao Deng**  
Shandong University

Traditional design strategy for new materials with targeted properties is trial-and-error method, which is time- and cost-consuming. In recent decades, computational materials design has been gaining rapid development including materials genome and machine learning. Recently, we proposed a digital-intellectual materials design method, in which digitization is embodied in big data and intelligence here means not only the wisdom of artificial intelligence (AI) but also human expertise. It requires the seamless integration of data, AI and especially human expertise. This new way of materials design can be divided into three processes: development of a property prediction method, high-throughput material screening and retro synthesis of designed material. Here, we would introduce several cases of digital-intellectual design in the fields of catalytic materials, which have been achieved in our group recently. We developed a van der Waals force field for describing the adsorption of gas in porous materials and used it to design and synthesize series of Metal COFs materials which can capture carbon dioxide and convert it to valuable chemicals at room temperature and atmospheric pressure. Moreover, we developed a two-dimensional descriptor for oxygen evolution reaction and used it to screen and design covalent organic frameworks electrocatalysts. To promote the control of the COVID-19 pandemic, we built a machine learning model that can accurately classify COVID-19 patients and healthy subjects based on the fractional exhaled nitric oxide (FeNO) value and human body characteristics. Then a portable intelligent device to detect FeNO was designed with nickel single-atom material. With the rapid development of computational materials science, we believe that the computation materials design especially digital-intellectual materials design may accelerate the materials discovery process.

## Rational Design of Fe-based Catalysts for Fischer-Tropsch Synthesis from Theoretical Prediction to Experimental Confirmation



**Xiao-Dong Wen**  
Institute of Coal  
Chemistry, CAS

Fischer-Tropsch process converts syngas (CO and H<sub>2</sub> which can be derived from nature gas, coal and biomass, etc.) into clean liquid fuels and high valuable chemicals. In China, the so-called Coal To Liquid (CTL) via Fischer-Tropsch synthesis (FTS) is not only to achieve the clean/efficient usage of coal, but also to alleviate China's excessive dependence on oil imports with important strategic significance to national security. We have been performing systematical studies on FTS for more than 30 years across from the fundamental research to R&D to industrial practice. The FTS in two 160,000 tons/year demo plants has passed the long-term operation and technical verification (more than 7 years), and achieved a remarkable successful application of the world's largest single-set of Coal-to-Oil industrial plant in Shenhua Ningmei with a production capacity of 4 million tons/year

In the talk, the corresponding fundamental researches on FTS will be focused. The rational design of Fe-based catalysts for FTS will be presented via combining experimental and theoretical insights. In details, starting with theoretical studies, the quantum mechanics approach is extensively used to study the active phases of Fe-based catalyst for FTS (across from detailed benchmarks on method to prediction on morphology/surface to design new generation Fe-based industrial catalysts), as well as FT reaction mechanism. The purpose of theoretical study is to provide theoretical insights for experimental designs, and to further guide the development of new generation FTS catalysts. Finally, the new generation Fe-based catalysts are designed rationally from theoretical prediction to experiment confirmation. In the meantime, the new challenge on designing Fe-based catalysts will be discussed.

## Towards Accurate and Efficient Theoretical Modeling in Heterogeneous Catalysis



**Xin Xu**

Fudan University

Catalysis is extremely important. It produces fuels and chemicals, provides sustainable energy, and reduces pollution and waste.

Modern catalysis research combines theoretical and experimental work. Many different catalysts and conditions can be screened computationally. This allows researchers to narrow down options before performing experiments, significantly speeding up discovery and optimization processes.

Density functional theory (DFT) is the most widely used computational method for modeling catalysis. It provides molecular-level insights into reaction mechanisms, active site natures, transition state requirements, and more. However, DFT methods approximate electron correlation effects. Accurately modeling transition state energies and reaction energies remains difficult for catalyzed reactions on the surfaces. We proposed a new class of doubly hybrid density functionals, namely xDHs, that are promising for accurate surface energetics.

Microkinetics provides the central gateway to go from DFT energetics at the microscopic level to macroscopic observables in heterogeneous catalysis. While microkinetics based on kinetic Monte Carlo simulations are computationally too expensive for complex systems, standard mean-field approximation is unreliable in many cases. We proposed the XPK model, which enables an efficient and accurate microkinetic modeling for heterogeneous catalysis.

Challenges remain in modeling complex catalytic systems but meeting them will open new theoretical capabilities.

## Principle of Metal-Support Interaction for Rational Design of Stable Catalysts



**Wei-Xue Li**

University of Science and  
Technology of China

The activity, selectivity, and stability of supported nanocatalysts is crucial to meeting environmental and energy challenges and necessitates fundamental theory to relieve trial-and-error experimentation and accelerate lab-to-fab translation. Among others, metal-support interaction is thought as one of the fundamental concepts and vital to the overall performance of supported nanocatalysts. In particular, strong metal-support interaction received long standing attention since it was proposed in 1969, though the description was phenomenal and qualitative. Here we report a Sabatier principle of metal-support interaction (MSI) for stabilizing metal nanocatalysts against sintering based on the kinetic simulations of 323 metal-support pairs based on MSI scaling relations extracted from 1252 energetics data (Science 374 (2021) 1360-1365). For the first time, MSI and criterion for strong MSI are quantified and established, respectively. Too strong of an interaction is shown to trigger Ostwald ripening whereas too weak of an interaction stimulates particle migration and coalescence. The identified optimum MSI enables high-throughput screening of supports to stabilize the nanocatalysts (~3nm) to reach the Tammann temperature on single functional supports. For high temperature reactions, cluster catalysts and those with poor chemical stabilities, bifunctional supports is proposed to break the scaling relationships. This theory is substantiated by first-principles neural network molecular dynamics simulations and available experiments.

## Computational Modeling of Modified CeO<sub>2</sub> Surfaces and Their Catalytic Activities



**Xue-Qing Gong**

Shanghai Jiao Tong  
University

Cerium dioxide (CeO<sub>2</sub>) is one of the most important rare earth metal oxides and has found applications in wide range of areas. Usually, CeO<sub>2</sub> catalysts can be modified through adsorption or doping with other species. However, the detailed understanding of the structures of such CeO<sub>2</sub> surfaces and their catalytic activities is still limited. In particular, it is still unclear how the unique electronic properties of Ce can be involved in such modifications. In several recent studies, we used density functional theory calculations corrected for on-site Coulomb interactions (DFT+U) to study several important modified CeO<sub>2</sub> surfaces, including those with surface hydroxyls, doped metals, and adsorbed metal oxide clusters. Their structural features were carefully examined as well as their electronic properties. Moreover, the catalytic reactions, such as CO oxidation, methanol dehydrogenation, N-SCR, were investigated to illustrate the modification effects. It was generally found that, together with the characteristic highly localized Ce 4f orbitals/electrons, these modification schemes can tune the activities of the surface O and provide extra active sites for the various reactions.

## Precise Design of Metal-Oxide Interfaces for Selective CO<sub>2</sub> Hydrogenation



**Junling Lu**

University of Science and  
Technology of China

Selective hydrogenation of CO<sub>2</sub> to value-added chemicals, e.g., methanol, using green hydrogen retrieved from renewable resources is a promising approach for reducing CO<sub>2</sub> emissions and improving carbon resource utilization. Precisely engineering metal-oxide interfaces in nanoscale has been regarded as an efficient way to promote the methanol formation. In this presentation, I will talk about our three recent studies about precise design of metal-oxide interfaces using atomic layer deposition for selective CO<sub>2</sub> hydrogenation: (i) Highly dispersed ZnO on Cu for the understanding the nature of active sites in the Cu-ZnO catalyst systems by combining high-pressure in situ X-ray adsorption spectroscopy measurements of ZnO/Cu inverse catalysts and theory <sup>[1]</sup>; (ii) Atomically thick Ga<sub>2</sub>O<sub>3</sub> coating of Pd nanoparticles, which initiates low-temperature reactive metal-support interactions (RMSIs) to form Ga-rich PdGa alloy phases. Therein, the enriched PdGa-Ga<sub>2</sub>O<sub>3</sub> interfaces remarkably boosted the formation of methanol <sup>[2]</sup>; (iii) InO<sub>x</sub> coating of PdCu bimetallic nanoparticles to construct intimate InO<sub>x</sub>/Cu and InO<sub>x</sub>/PdIn dual interfaces which allow breaking the conversion-selectivity trade-off in selective CO<sub>2</sub> hydrogenation <sup>[3]</sup>.

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## Lattice Vibrations at Interfaces Probed by Sum-Frequency Spectroscopy



**Weitao Liu**

Fudan University

The charged oxide aqueous interfaces are ubiquitous in the Earth crust, and involved in a huge variety of phenomena. Sum-frequency vibrational spectroscopy can access the interface in situ and have revealed crucial information about the interfacial water structures, however much remains unclear about the oxide surfaces. Here we utilized an oxide thin film with enhanced local field strength at the buried oxide water interface to enable in situ and direct probing of charged surface groups. The fused silica/water interface was chosen as a model system. The protonation and de-protonation processes were readily observed, providing new structural information of charged surface groups.

## On-Surface Chemical Reaction Methodology



**Biao Yang**

Soochow University

Over the past decade, on-surface reaction has become a fascinating concept in surface chemistry. With the advanced surface characterization techniques (e.g., scanning tunneling microscopy, STM, noncontact atomic force microscopy, nc-AFM, and X-ray photoelectron spectroscopy, XPS), on-surface reactions provide promising strategies for the synthesis of functional materials such as single-layer 2D covalent networks or functional conjugated molecular nanostructures, offering promising avenues for advanced materials preparation. Common prototype molecular reactions have dominated the catalytic effect of metal surfaces, while a significant challenge lies in the limited range of applicable reaction types on surfaces. Overcoming this limitation demands the exploration of expansive reaction systems and the development of new strategies. This presentation addresses these challenges by introducing diverse strategies for on-surface synthesis, emphasizing mono-component molecular reactions involving gas and water mediation, and bi-component molecular reactions, particularly condensation reactions. By offering insights into methodologies for expanding viable surface reactions, we seek to facilitate practical implementations, advancing the synthesis of functional materials with broad applications.







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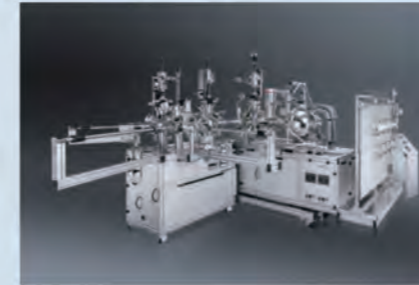
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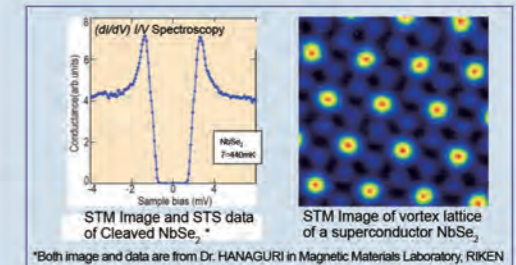
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