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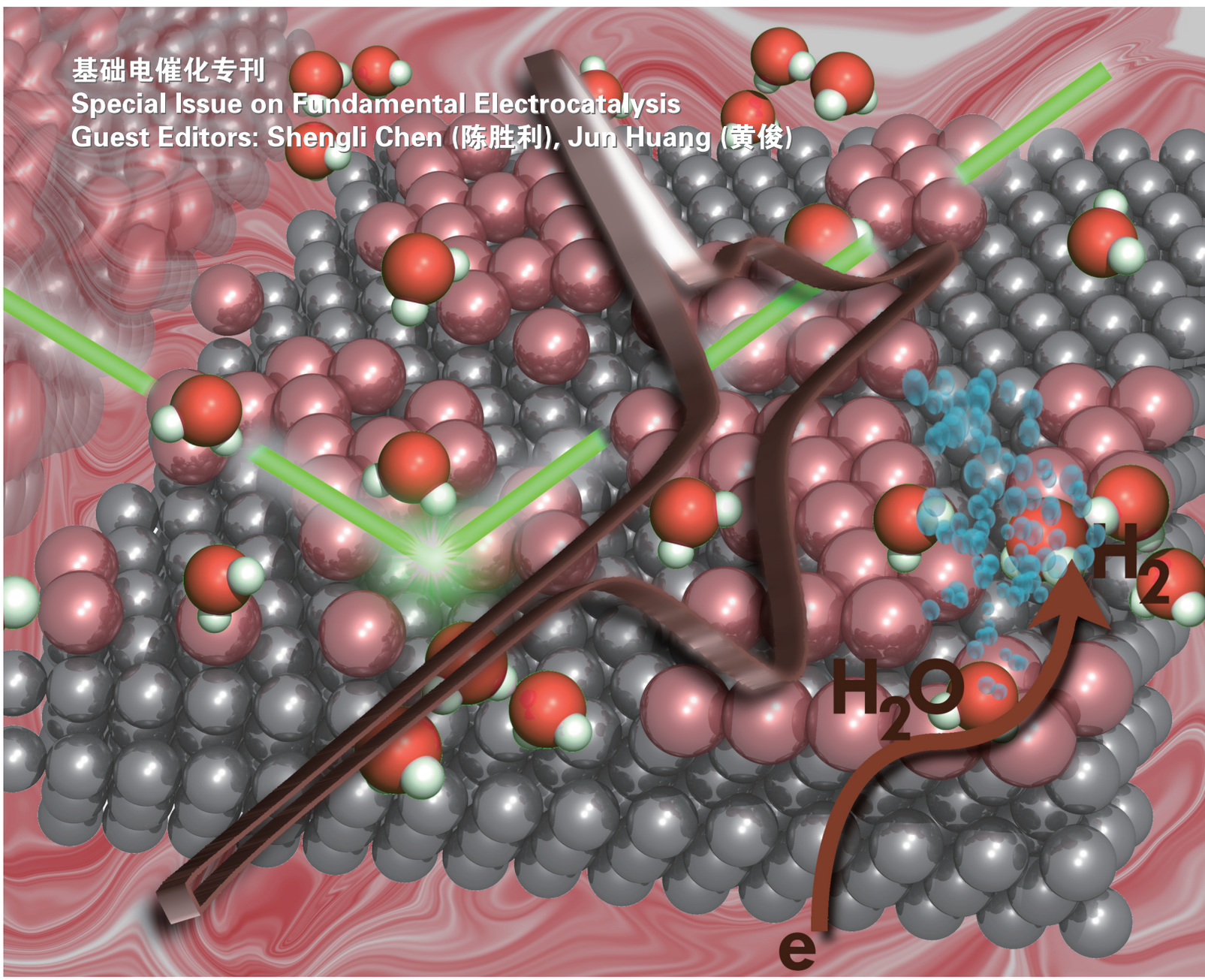

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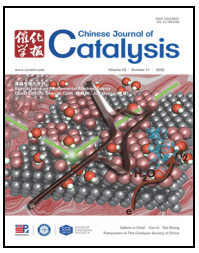


Special Issue on Fundamental Electrocatalysis

Guest Editors: Shengli Chen, Jun Huang

Chinese Journal of Catalysis

Graphical Contents

Editorial

Chin. J. Catal., 2022, 43: 2743–2745 doi: 10.1016/S1872-2067(22)64171-8

Celebrate polysemy of fundamental in electrocatalysis

Shengli Chen, Jun Huang
Wuhan University, China; Institute of Climate and Energy Research, Forschungszentrum Jülich GmbH, Germany

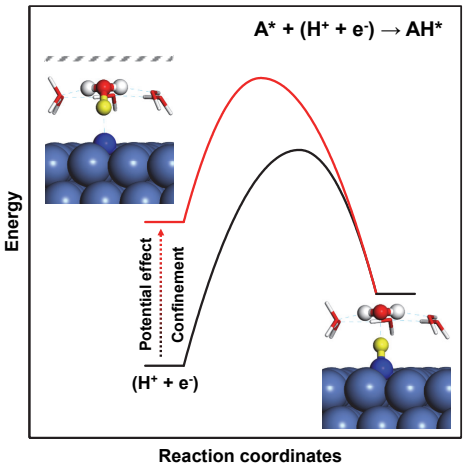
Perspective

Chin. J. Catal., 2022, 43: 2746–2756 doi: 10.1016/S1872-2067(22)64090-7

Theoretical understanding of electrocatalysis beyond thermodynamic analysis

Huan Li, Chenxi Guo, Jun Long, Xiaoyan Fu, Jianping Xiao*
Dalian Institute of Chemical Physics, Chinese Academy of Sciences;
University of Chinese Academy of Sciences;
Zhejiang University;

Potential/confinement effect can play an important role on electrochemical steps by changing the (electro)chemical potential of electron. As a result, potential-dependent energetics and TS structures are essential for a more accurate description of reaction mechanism and activity.

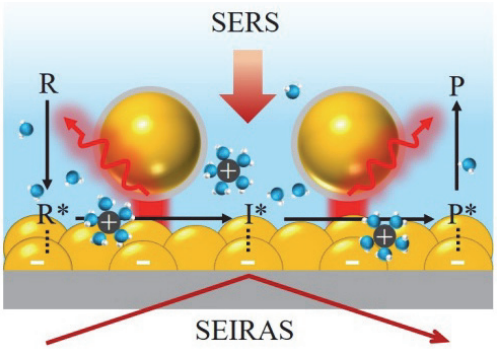


Reviews

Chin. J. Catal., 2022, 43: 2757–2771 doi: 10.1016/S1872-2067(22)64157-3

Surface-enhanced vibrational spectroscopies in electrocatalysis: Fundamentals, challenges, and perspectives

Hai-Sheng Su, Xiaoxia Chang, Bingjun Xu *
Peking University

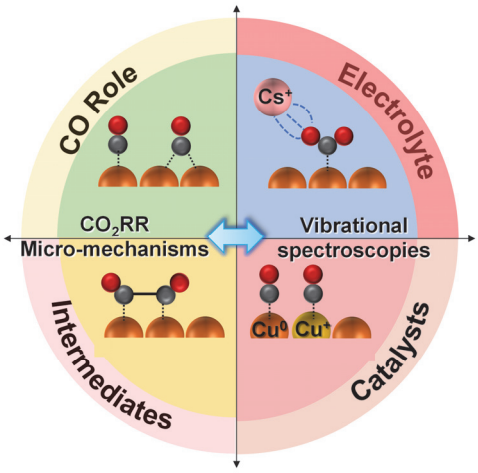


This review emphasizes challenges in applying surface-enhanced Raman spectroscopy (SERS) and surface-enhanced infrared absorption spectroscopy (SEIRAS) and future directions to further unlock their potential in electrocatalytic research.

Chin. J. Catal., 2022, 43: 2772–2791 doi: 10.1016/S1872-2067(22)64095-6

Fundamental aspects in CO_2 electroreduction reaction and solutions from *in situ* vibrational spectroscopies

Hong Li, Kun Jiang, Shou-Zhong Zou *, Wen-Bin Cai *
Fudan University, China; Shanghai Jiao Tong University, China; American University, USA

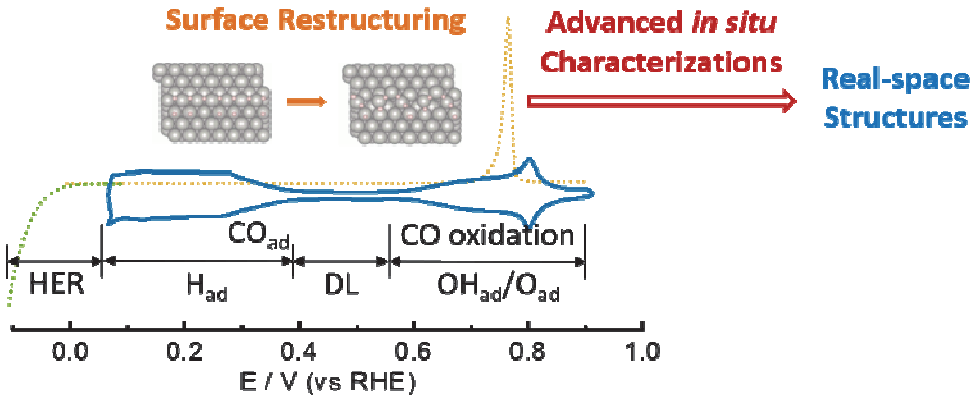


This review summarizes representative results of *in situ* vibrational spectroscopic studies on key fundamental issues in CO_2 electroreduction reaction and gives an outlook for future investigations.

Chin. J. Catal., 2022, 43: 2792–2801 doi: 10.1016/S1872-2067(22)64100-7

Restructuring of well-defined Pt-based electrode surfaces under mild electrochemical conditions

Jie Wei, Wei Chen, Da Zhou, Jun Cai *, Yan-Xia Chen *
University of Science and Technology of China

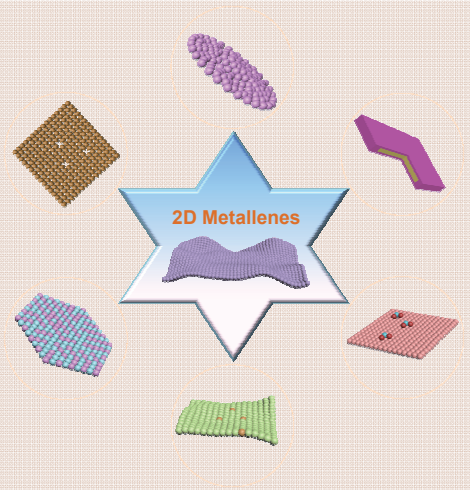


With the advancement of *in situ* characterization techniques, tiny surface restructurings are detected on the well-defined Pt electrode surfaces even under mild electrochemical conditions. Careful examination of *in situ* real-space structures at the electrode-electrolyte interface under benign conditions is emphasized for the accurate deduction of reaction mechanism(s) as well as structure-performance relationship in electrocatalytic systems.

Chin. J. Catal., 2022, 43: 2802–2814 doi: 10.1016/S1872-2067(21)64022-6

Emerging two-dimensional metallenes: Recent advances in structural regulations and electrocatalytic applications

Jiandong Wu, Xiao Zhao *, Xiaoqiang Cui *, Weitao Zheng *
Jilin University



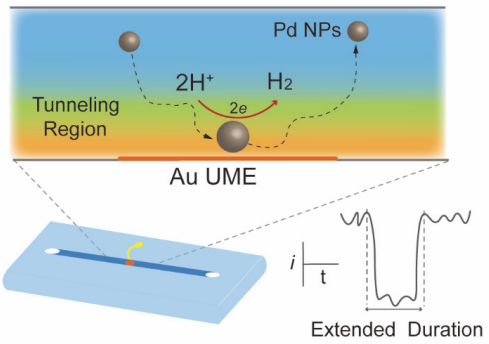
In this review, we present the advances on metallenes in their structurally regulating strategies and promising applications in electrocatalysis.

Communications

Chin. J. Catal., 2022, 43: 2815–2819 doi: 10.1016/S1872-2067(21)64034-2

Enhanced single-nanoparticle collisions for the hydrogen evolution reaction in a confined microchannel

Si-Min Lu, Mengjie Chen, Huilin Wen, Hao-Wei Wang, Ziyi Yu *, Yi-Tao Long *
Nanjing University; Nanjing Tech University

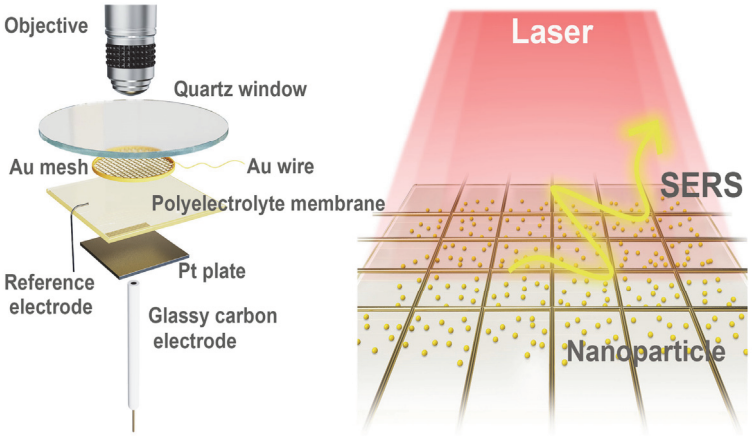


Enhancement of single-nanoparticle collisions for the hydrogen evolution reaction in a confined microchannel, offering a possibility for the application of stochastic collision electrochemistry in energy conversion.

Chin. J. Catal., 2022, 43: 2820–2825 doi: 10.1016/S1872-2067(21)64041-X

***In-situ* electrochemical surface-enhanced Raman spectroscopy in metal/polyelectrolyte interfaces**

Li-Wen Wu, Mo-Li Huang, Yun-Xiao Yang, Yi-Fan Huang *
ShanghaiTech University



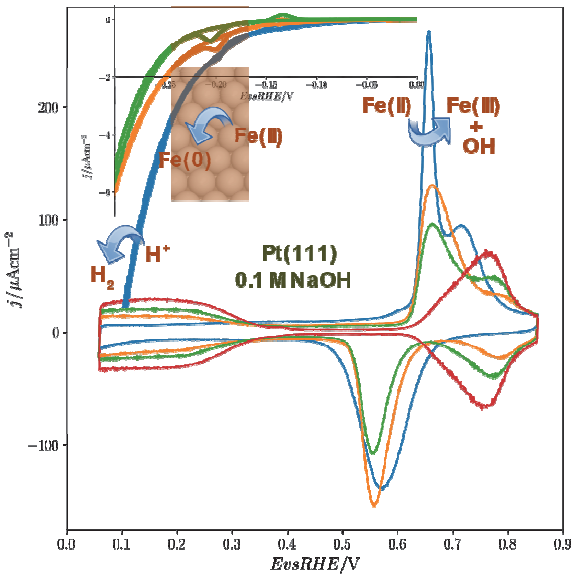
An *in-situ* electrochemical surface-enhanced Raman spectroscopy is developed towards investigating the electrode/polyelectrolyte interfaces in electrocatalysis.

Articles

Chin. J. Catal., 2022, 43: 2826–2836 doi: 10.1016/S1872-2067(22)64141-X

Effect of the interfacial electric field on the HER on Pt(111) modified with iron adatoms in alkaline media

Francisco J. Sarabia, Víctor Climent *, Juan M. Feliu *
Universidad de Alicante, Spain

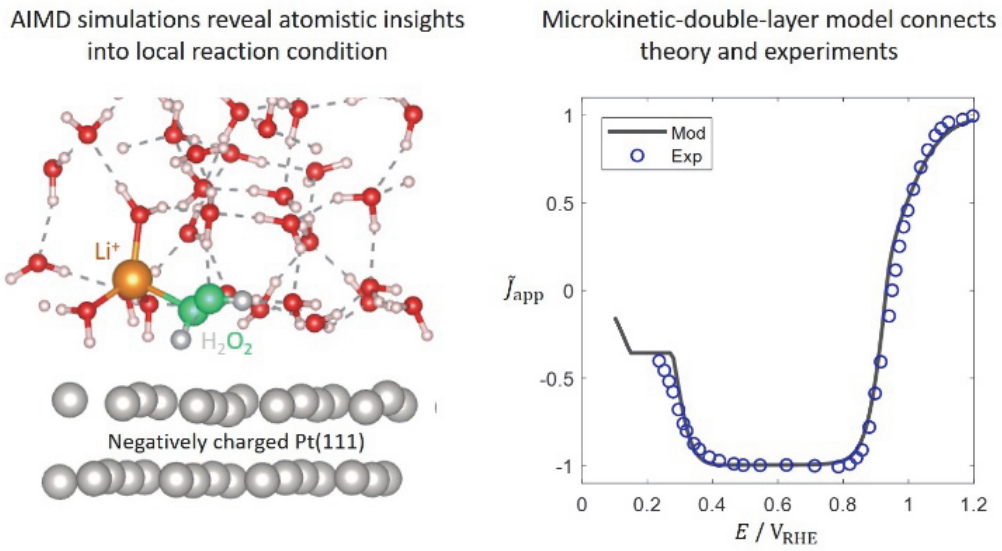


The modification of Pt(111) surfaces with iron adatoms has been studied with cyclic voltammetry and the laser induced temperature jump technique. Changes in the oxidation state of iron are identified with a coulometric analysis. The catalytic effect has been correlated with changes in the magnitude of the electric field.

Chin. J. Catal., 2022, 43: 2837–2849 doi: 10.1016/S1872-2067(22)64138-X

Understanding surface charge effects in electrocatalysis. Part 2: Hydrogen peroxide reactions at platinum

Jun Huang *, Victor Climent, Axel Groß, Juan M. Feliu *
Ulm University, Germany; Universidad de Alicante, Spain; Helmholtz Institute Ulm (HIU), Germany

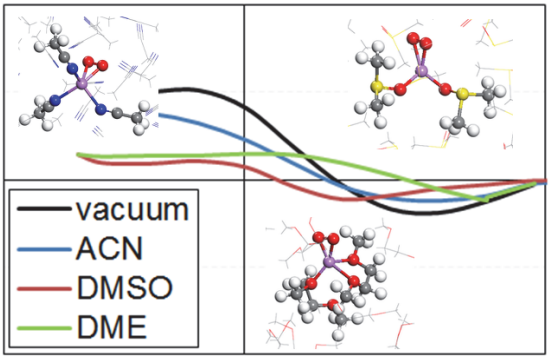


The activation barrier of breaking the oxygen-oxygen bond of the hydrogen peroxide molecule is higher at negatively charged surface, resulting in the abnormal experimental observation that the reduction current is suppressed with decreasing the electrode potential.

Chin. J. Catal., 2022, 43: 2850–2857 doi: 10.1016/S1872-2067(22)64098-1

Solvation structure and dynamics of Li and LiO_2 and their transformation in non-aqueous organic electrolyte solvents from first-principles simulations

Behnaz Rahmani Didar, Axel Groß *
Ulm University, Germany;
Helmholtz Institute Ulm, Germany

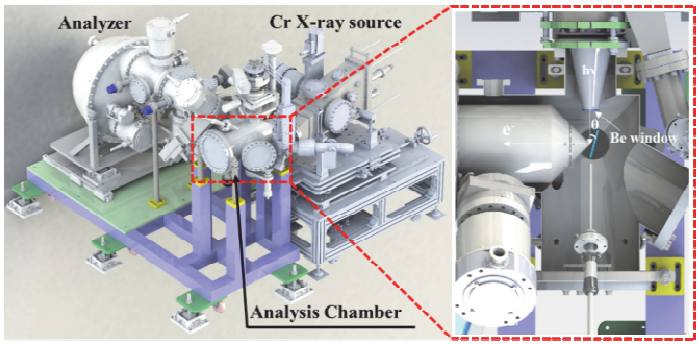


Performing *ab initio* molecular dynamics simulations within the Blue Moon ensemble, it is demonstrated that the oxygen reduction reaction in non-aqueous Li^+ electrolytes occurs spontaneously which is relevant for the understanding of Li-air batteries.

Chin. J. Catal., 2022, 43: 2858–2870 doi: 10.1016/S1872-2067(22)64092-0

Understanding fundamentals of electrochemical reactions with tender X-rays: A new lab-based *operando* X-ray photoelectron spectroscopy method for probing liquid/solid and gas/solid interfaces across a variety of electrochemical systems

Chiyan Liu, Qiao Dong, Yong Han *, Yijing Zang, Hui Zhang, Xiaoming Xie, Yi Yu *, Zhi Liu *
Shanghai Institute of Microsystem and Information Technology, Chinese Academy of Sciences;
ShanghaiTech University; University of Chinese Academy of Sciences

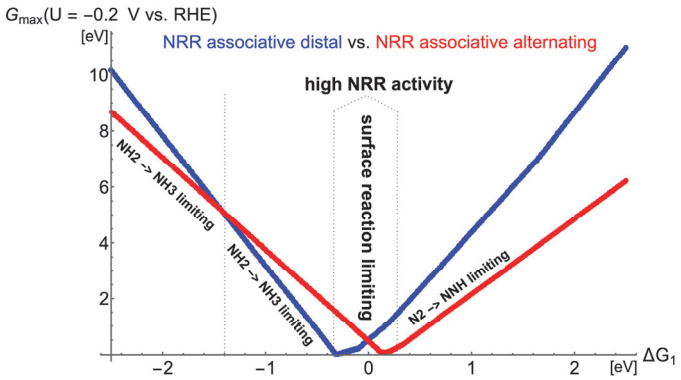


A new lab-based ambient pressure X-ray photoelectron spectroscopy (APXPS) technique was used to probe liquid/solid and gas/solid interfaces in electrochemical systems.

Chin. J. Catal., 2022, 43: 2871–2880 doi: 10.1016/S1872-2067(21)64025-1

Beyond the thermodynamic volcano picture in the nitrogen reduction reaction over transition-metal oxides: Implications for materials screening

Kai S. Exner *
University Duisburg-Essen, Germany; Cluster of Excellence RESOLV, Bochum, Germany;
Center for Nanointegration (CENIDE) Duisburg-Essen, Germany

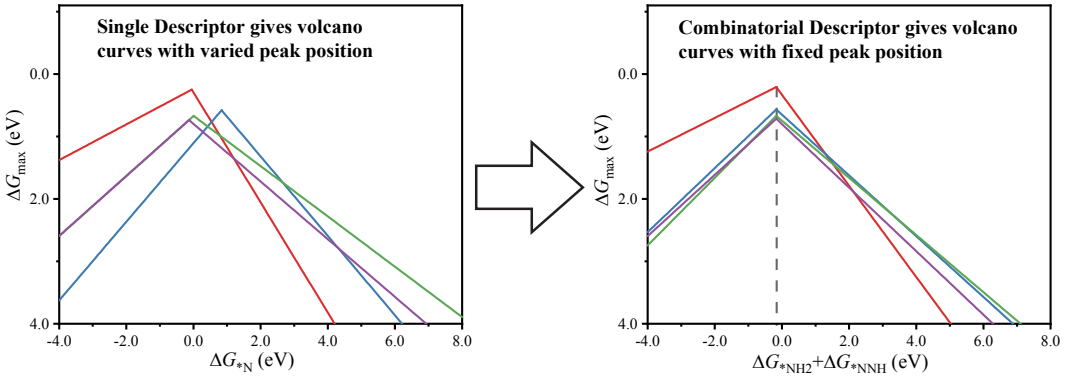


Application of the activity descriptor $G_{max}(\eta)$ allows deriving a kinetic volcano plot to study electrocatalytic nitrogen reduction reaction in a class of materials, thereby moving beyond the thermodynamic volcano picture and the potential-determining step.

Chin. J. Catal., 2022, 43: 2881–2888 doi: 10.1016/S1872-2067(22)64128-7

A combinatorial descriptor for volcano relationships of electrochemical nitrogen reduction reaction

Ziyi Jiang, Youcheng Hu, Jun Huang *, ShengLi Chen *
Wuhan University, China; Ulm University, Germany

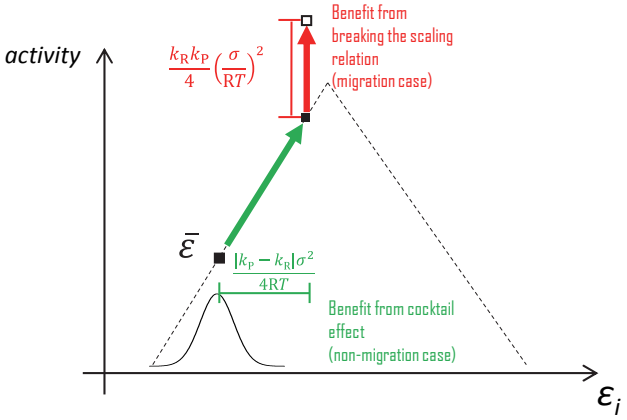


We proposed $\Delta G_{*NH2}+\Delta G_{*NNH}$ as a combinatorial descriptor for scaling relationship of eNRR, which shows better predictive power than single descriptors. Its value corresponding to the volcano peak is fixed as the reaction energy of eNRR (–0.17 eV).

Chin. J. Catal., 2022, 43: 2889–2897 doi: 10.1016/S1872-2067(22)64161-5

Locating the cocktail and scaling-relation breaking effects of high-entropy alloy catalysts on the electrocatalytic volcano plot

Junxiang Chen *, Yaxin Ji
Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences;
Fujian Normal University

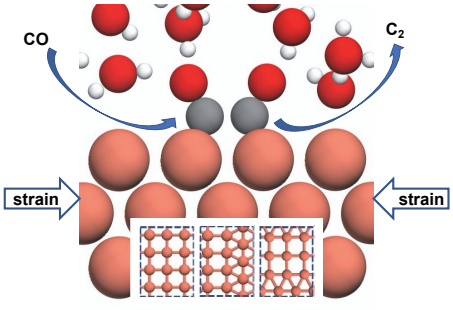


Schematic representation of the benefits of the cocktail effect and the scaling-relation-breaking effect for electrocatalytic activity on high entropy alloys. k_P and k_R are the scaling factors. ε and σ^2 are the mean value and variance of the adsorption energy.

Chin. J. Catal., 2022, 43: 2898–2905 doi: 10.1016/S1872-2067(21)64044-5

Tunable activity of electrocatalytic CO dimerization on strained Cu surfaces: Insights from *ab initio* molecular dynamics simulations

Hong Liu, Jian Liu, Bo Yang*
ShanghaiTech University;
Shanghai Institute of Microsystem and Information Technology,
Chinese Academy of Sciences

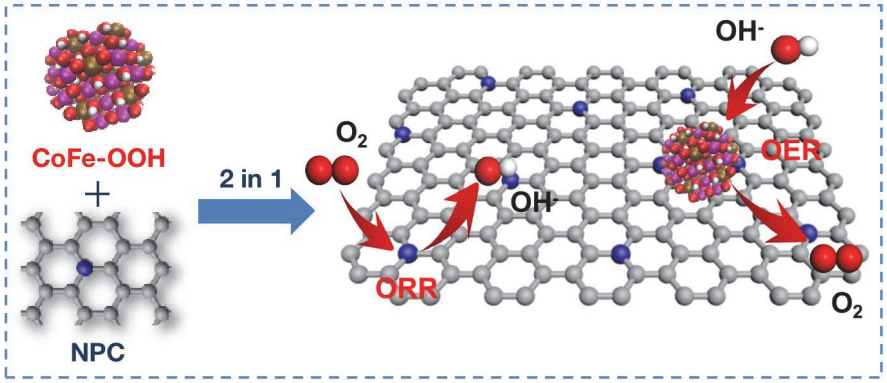


Ab initio molecular dynamics simulation associated with free energy sampling technology were performed to study the energetics of the electrocatalytic CO dimerization on strained Cu(100) with an explicit aqueous solvent model.

Chin. J. Catal., 2022, 43: 2906–2912 doi: 10.1016/S1872-2067(21)63979-7

Two-in-one strategy to construct bifunctional oxygen electrocatalysts for rechargeable Zn-air battery

Huibing Liu, Rixin Xie, Ziqiang Niu, Qiaohuan Jia, Liu Yang *, Shitao Wang, Dapeng Cao *
Beijing University of Chemical Technology

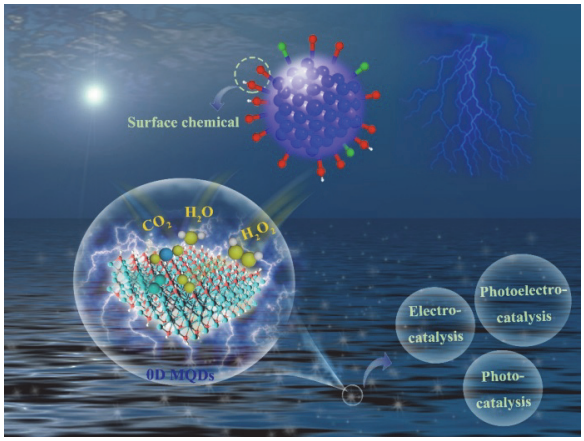


The simple 2-in-1 strategy to design the metal oxyhydroxide supported on N-doped porous carbons as ORR and OER bifunctional electrocatalysts for rechargeable Zn-air battery.

Chin. J. Catal., 2022, 43: 2913–2935 doi: 10.1016/S1872-2067(22)64167-6 **[Review]**

Surface chemistry of MXene quantum dots: Virus mechanism-inspired mini-lab for catalysis

Yuhua Liu, Wei Zhang *, Weitao Zheng *
Jilin University



This review focuses on the surface chemistry of 0D MQDs, proposes the surface functional groups of MQDs as virus mechanism-inspired mini-lab, followed with exploration of their different roles in catalysis *via* surface modification, including electrocatalysis, photocatalysis, photoelectrocatalysis.

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