

# Catalysis Science & Technology

A multidisciplinary journal focussing on all fundamental science and technological aspects of catalysis

[rsc.li/catalysis](http://rsc.li/catalysis)

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

## IN THIS ISSUE

ISSN 2044-4761 CODEN CSTAGD 14(3) 501-778 (2024)



### Cover

See Ruud Kortlever *et al.*, pp. 555–561.  
Image reproduced by permission of Ruud Kortlever from *Catal. Sci. Technol.*, 2024, 14, 555.

## EDITORIAL

512

### Catalysis on the move

Asier Unciti-Broceta\* and Evgeny Rebrov\*

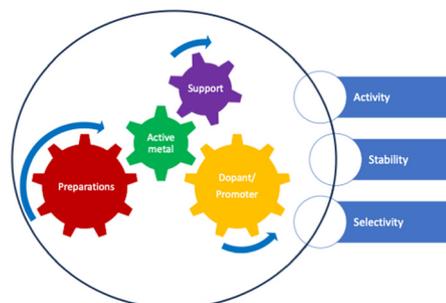


## REVIEWS

515

### The design and optimization of heterogeneous catalysts using computational methods

Shambhawi, Ojus Mohan, Tej S. Choksi and Alexei A. Lapkin\*



# Environmental Science journals

One impactful portfolio for  
every exceptional mind

Harnessing the power of interdisciplinary  
science to preserve our environment



[rsc.li/envsci](https://rsc.li/envsci)

Fundamental questions  
Elemental answers

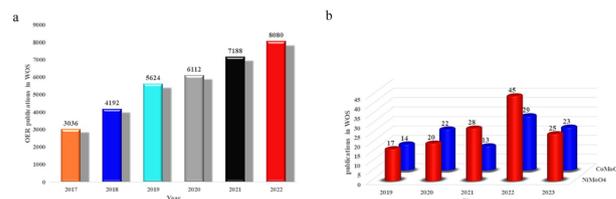


## REVIEWS

533

Application progress of NiMoO<sub>4</sub> electrocatalyst in basic oxygen evolution reaction

Haibin Wang, Zhaobo Wang, Zihang Feng, Jianguan Qiu, Xuefei Lei,\* Biao Wang and Rui Guo\*

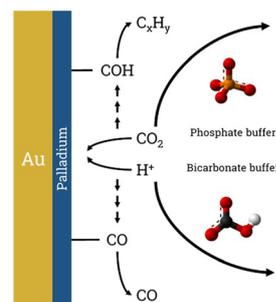


## COMMUNICATIONS

555

The effect of surface conditions on the electrochemical CO<sub>2</sub> reduction performance of bimetallic AuPd electrocatalysts

Daniël van den Berg, Boaz Izelaar, Shilong Fu and Ruud Kortlever\*



562

## Integration of surface polymerization and self-assembly strategies for heterogenization of copper-based catalysts for water oxidation

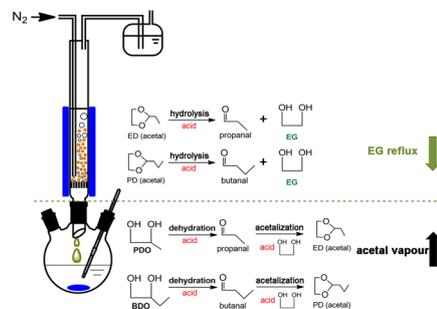
Xin Li, Mengjiao Shao, Xueling Song, Xuesong Jiang, Guisheng Li and Lei Wang\*



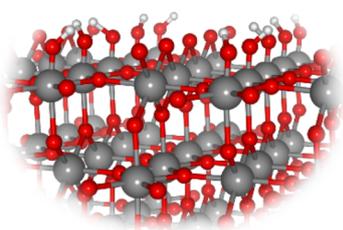
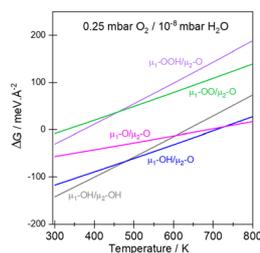
567

## Highly selective conversion of diols into aldehydes for the purification of ethylene glycol with a self-adjusting coupling reactor

Jianwei Ji, Shuo Ai,\* Wanguo Yu, Linghui Liu and Chengdu Huang



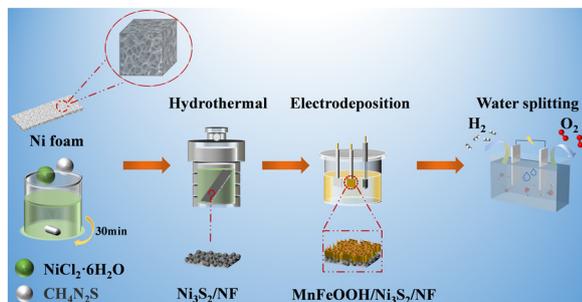
572



### Thermal synthesis of electron deficient oxygen species on crystalline IrO<sub>2</sub>

E. A. Carbonio,\* F. Sulzmann, D. Teschner, J. J. Velasco-Vélez, M. Hävecker, A. Knop Gericke, R. Schlögl and T. Jones\*

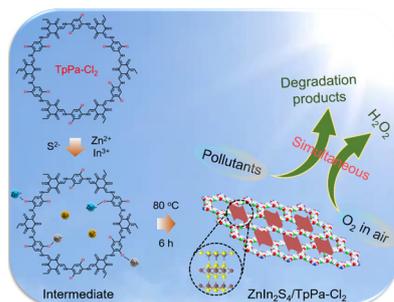
581



### Electronic structure modification of ultrathin MnFeOOH and integration with Ni<sub>3</sub>S<sub>2</sub> as bifunctional electrocatalysts for improved alkaline water splitting

Fu-Min Wang and Si-Fu Tang\*

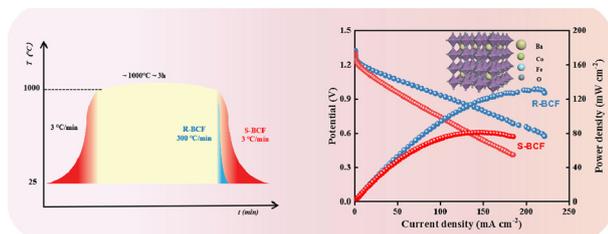
590



### Photocatalytic production of H<sub>2</sub>O<sub>2</sub> from wastewater under visible light by chlorine and ZnIn<sub>2</sub>S<sub>4</sub> co-decorated TpPa-1

Guanglu Xia, Jianhao Qiu,\* Dingliang Dai, Yong Tang, Zhonghao Wu and Jianfeng Yao\*

598



### Compositional engineering of perovskite oxide BaCo<sub>0.5</sub>Fe<sub>0.5</sub>O<sub>3-δ</sub> as an efficient bifunctional electrocatalyst for rechargeable zinc-air batteries

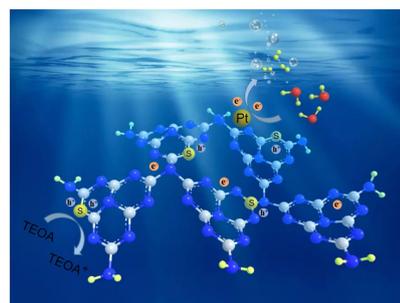
Anqi Xu, Jian Zhou, Tong Liu,\* Jing Wang, Yao Wang, Dong Zhang, Dexuan Huang, Yilin Liu and Xuelei Hu\*



606

### Sulfur-doped g-C<sub>3</sub>N<sub>4</sub> photocatalyst for significantly steered visible light photocatalytic H<sub>2</sub> evolution from water splitting

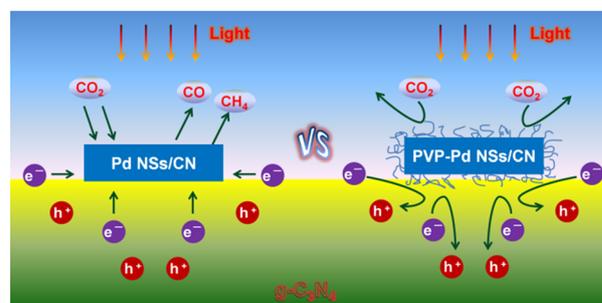
Xiao-Jie Lu, Li Xu, Ikram Ullah, Hong-Bao Li\* and An-Wu Xu\*



615

### Surfactant-free 2D/2D Pd/g-C<sub>3</sub>N<sub>4</sub> for enhanced photocatalytic CO<sub>2</sub> reduction

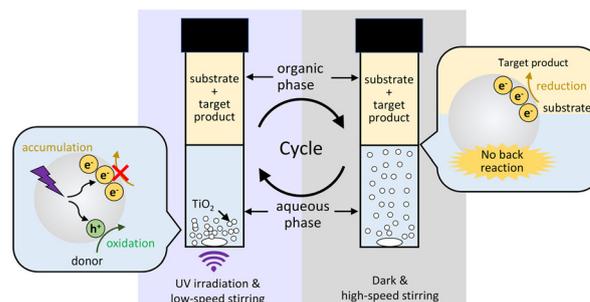
Zhijun Huang,\* Jie Wu, Chunliang Yang, Fengwen Yan\* and Guoqing Yuan



624

### Cyclic time-separated redox reaction using accumulated electrons in titanium(IV) oxide in a two-phase system

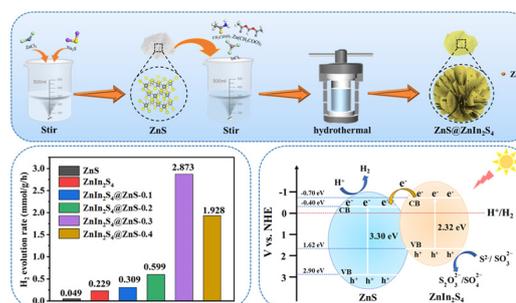
Masato Suenaga and Naoya Murakami\*



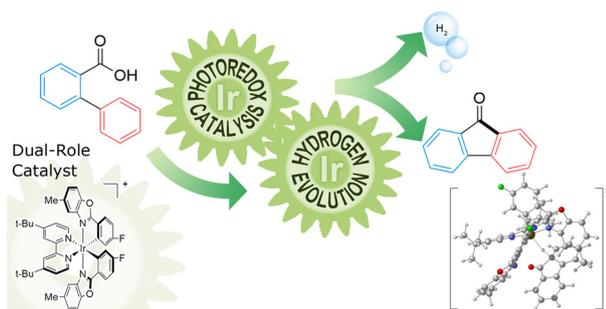
630

### Facile synthesis of ZnIn<sub>2</sub>S<sub>4</sub>@ZnS composites for efficient photocatalytic hydrogen precipitation

Xixi Yuan, Peng Li,\* Siyu Wang, Puyu Liu, Jianwei Zhao,\* Tao Wang and Kun Chang\*



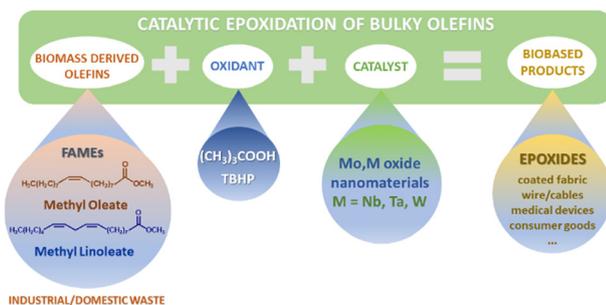
638



### Dual-role catalysis of iridium in photo-irradiation synthesis of 9-fluorenone through intramolecular cyclization *via* hydrogen evolution

Xi Hong, Yi-Wen Zhang, Bing Zhan, Xue-Juan Chen, De-Jun Hu, Zhi-Ming Li\* and Xiu-Feng Hou\*

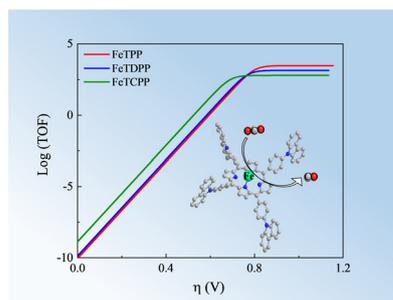
646



### Bulky olefin epoxidation under mild conditions over Mo-based oxide catalysts

Diana M. Gomes, Xingyu Yao, Patrícia Neves,\* Nicola Pinna, Patrícia A. Russo and Anabela A. Valente\*

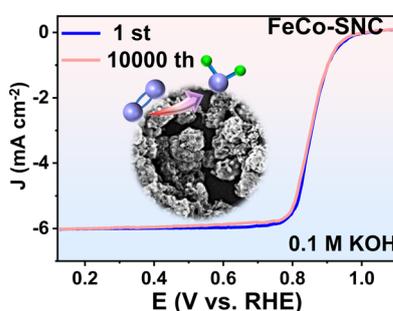
660



### Electrocatalytic reduction of CO<sub>2</sub> to CO by Fe(III) carbazole-porphyrins in homogeneous molecular systems

Hai Sun, Jiahui Wu, Fengkun Tian, Guodong Zhang, Zixiang Xia, Jiabin Rong, Jun-Sheng Qin\* and Heng Rao\*

667



### Co, Fe decorated N, S co-doped porous carbon enables high stability for the oxygen reduction reaction

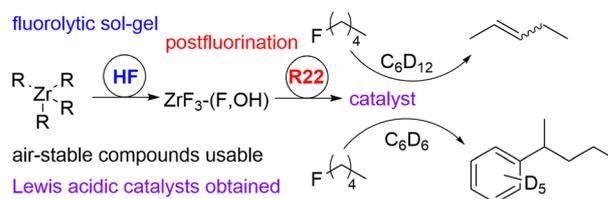
Qiulan Huang, Ruiqin Ren, Jia Li, Muhammad Waqas, Pan Chen, Xiaotian Liu, Dujuan Huang, Zhongyun Yang, Xinglan Peng, Du-Hong Chen,\* Youjun Fan\* and Wei Chen\*



673

## A fluorolytic sol-gel route to access an amorphous Zr fluoride catalyst: a useful tool for C–F bond activation

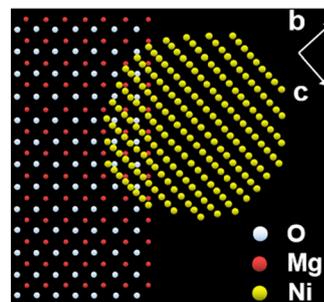
Christian Heinekamp, Sönke Kneiske, Ana Guilherme Buzanich, Mike Ahrens, Thomas Braun\* and Franziska Emmerling\*



681

## Stable Ni nanocrystals on porous single-crystalline MgO particles for enhanced dry reforming activity and durability of CH<sub>4</sub>/CO<sub>2</sub>

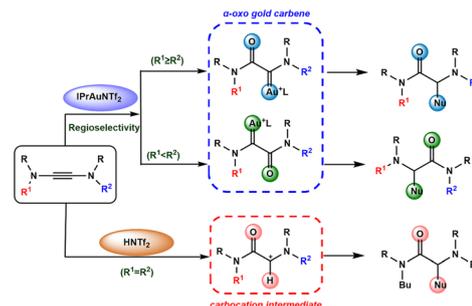
Suning Zhang, Fangyuan Cheng\* and Kui Xie\*



689

## Oxidative functionalization of yndiamides catalyzed by gold(i) or Brønsted acid systems: computational study of mechanism, selectivity patterns, and effects of substituents

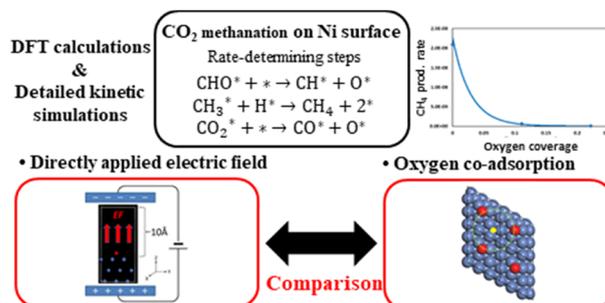
Guowei Yan, Ji Ma, Simeng Qi, Alexander M. Kirillov, Lizi Yang and Ran Fang\*



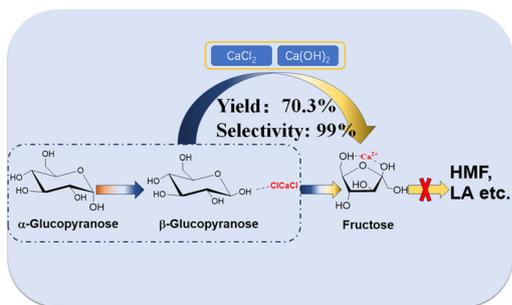
704

## Theoretical study of catalytic activity modifications in CO<sub>2</sub> methanation induced by an electric field in solid-oxide cells

Katsuhiko Wakamatsu,\* Takaaki Yasuda, Masato Aratani and Teppei Ogura\*



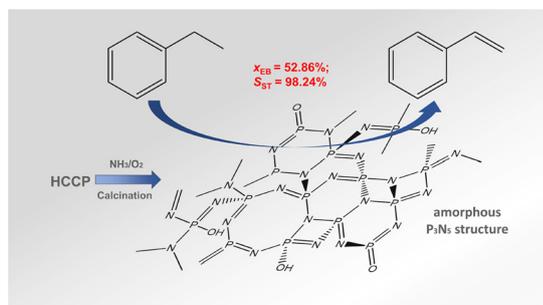
718



### Insight into the alkaline earth metal salt promotion for alkali-catalyzed glucose isomerization

Changqu Lin, Yunlin Shi, Lulu Xu, Zhengyue Wang, Lili Zhao, Hongli Wu,\* Fei Cao and Ping Wei

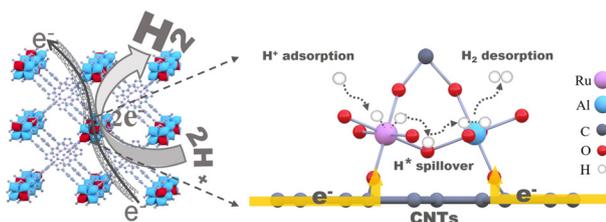
728



### Amorphous phosphorus oxynitride as a robust catalyst for steam-free direct dehydrogenation of ethylbenzene to styrene: effect of calcination temperature

Lukai Luo, Yuan Ma, Yuwei Liu, Baining Lin, Chaojun Guo, Jun Gong, Yating Xie and Yonghua Zhou\*

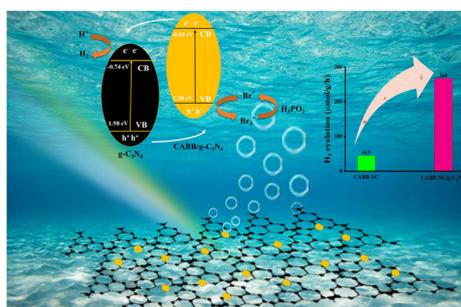
735



### Steering the electronic communication between Al/Ru bimetallic clusters in metal-organic framework composites for accelerating hydrogen evolution kinetics

Xueting Song, Haifeng Yang, Chenghua Zhang,\* Guizhi Zhang, Hong Wu, Youzhou He, Min Fu, Xingyan Liu,\* Siqi Li and Siping Wei\*

746



### Enhanced photocatalytic hydrogen evolution through suppressed electron-hole recombination in $\text{Cs}_2\text{AgBiBr}_6\text{-NC/g-C}_3\text{N}_4$ nanocomposites

C. Vidhya, B. Meera, Revathy B. Nair and Sajith Kurian\*

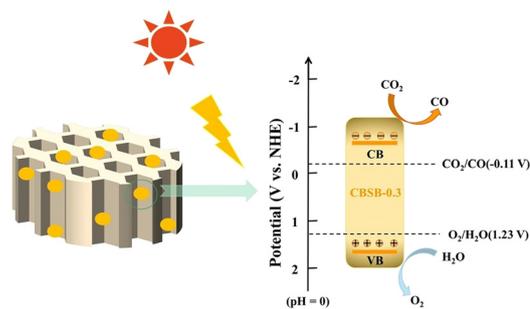


## PAPERS

758

### Synthesis of small size lead-free $\text{Cs}_3\text{Bi}_{2x}\text{Sb}_{2-2x}\text{Br}_9$ solid-solutions using a spatially confined growth method for efficient photocatalytic $\text{CO}_2$ reduction

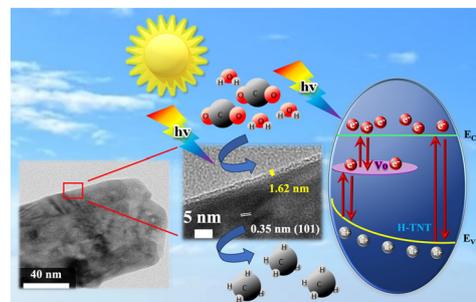
Miaomiao Gao, Xiaolei Liu,\* Liwen Yin, Jinghang Chen, Zeyan Wang, Zhaoke Zheng, Yuanyuan Liu, Hefeng Cheng, Ying Dai, Baibiao Huang, Zehui Zhang\* and Peng Wang\*



767

### Engineered $\text{CO}_2$ conversion performance of nanostructured $\text{TiO}_2$ photocatalysts via electrochemical hydrogenation

Jacky Chen-Chin Lee, Hossam A. E. Omr, Po-Wei Lai and Hyeonseok Lee\*



## CORRECTION

775

### Correction: Adipic acid formation from cyclohexanediol using platinum and vanadium catalysts: elucidating the role of homogeneous vanadium species

Owen Rogers, Samuel Patisson, Rebecca V. Engel, Robert L. Jenkins, Keith Whiston, Stuart H. Taylor and Graham J. Hutchings\*

