

Catalysis Science & Technology

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

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

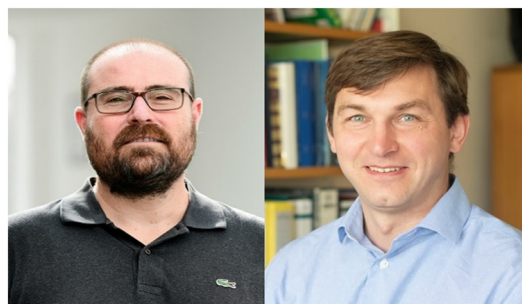
See Ruud Kortlever *et al.*, pp. 555–561.
Image reproduced by permission of Ruud Kortlever from *Catal. Sci. Technol.*, 2024, 14, 555.

EDITORIAL

512

Catalysis on the move

Asier Unciti-Broceta* and Evgeny Rebrov*

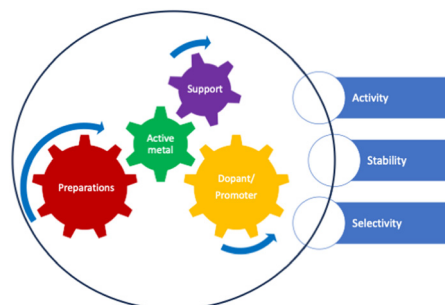


REVIEWS

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

Fundamental questions
Elemental answers

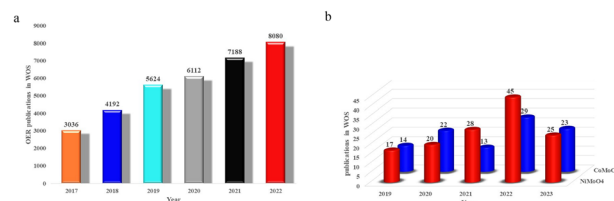


REVIEWS

533

Application progress of NiMoO₄ electrocatalyst in basic oxygen evolution reaction

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

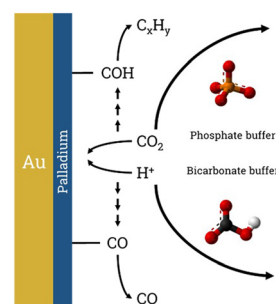


COMMUNICATIONS

555

The effect of surface conditions on the electrochemical CO₂ 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

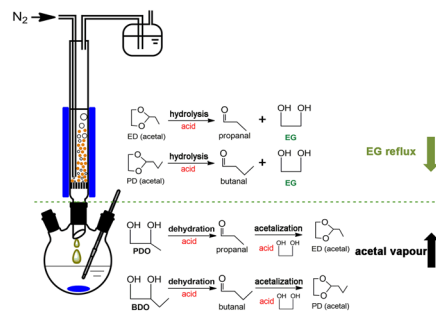
Xin Li, Mengjiao Shao, Xueling Song, Xuesong Jiang, Guisheng Li and Lei Wang*



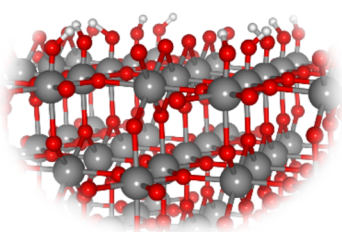
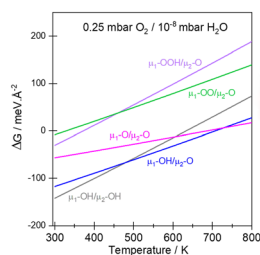
567

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



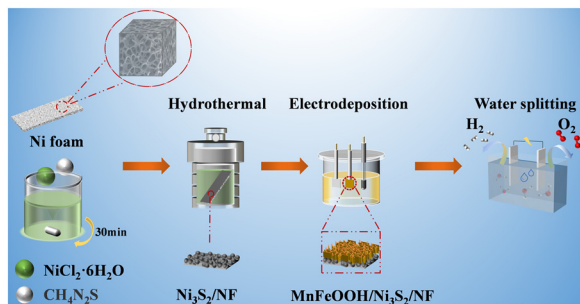
572



Thermal synthesis of electron deficient oxygen species on crystalline IrO₂

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

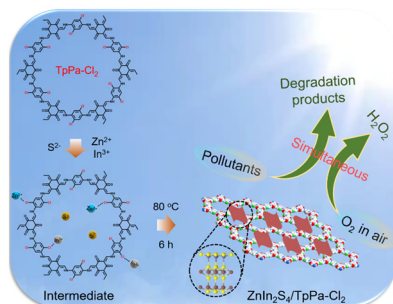
581



Electronic structure modification of ultrathin MnFeOOH and integration with Ni₃S₂ as bifunctional electrocatalysts for improved alkaline water splitting

Fu-Min Wang and Si-Fu Tang*

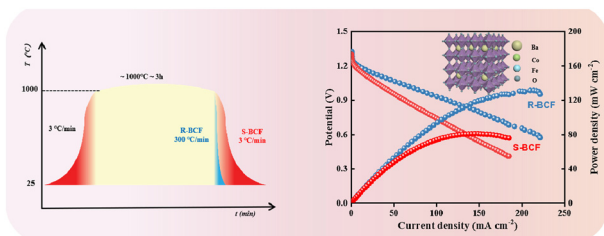
590



Photocatalytic production of H₂O₂ from wastewater under visible light by chlorine and ZnIn₂S₄ co-decorated TpPa-1

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

598



Compositional engineering of perovskite oxide BaCo_{0.5}Fe_{0.5}O_{3-δ} as an efficient bifunctional electrocatalyst for rechargeable zinc-air batteries

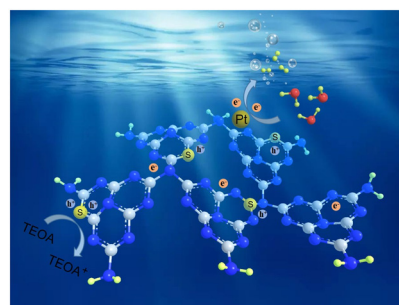
Anqi Xu, Jian Zhou, Tong Liu,* Jing Wang, Yao Wang, Dong Zhang, Dexuan Huang, Yilin Liu and Xuelei Hu*



606

Sulfur-doped g-C₃N₄ photocatalyst for significantly steered visible light photocatalytic H₂ evolution from water splitting

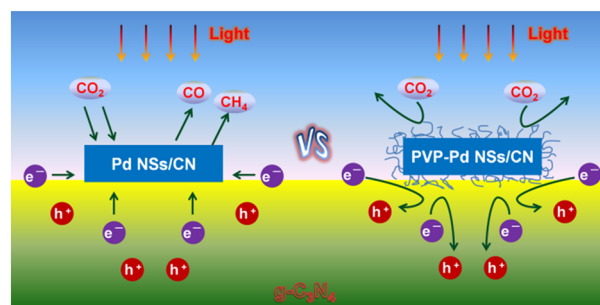
Xiao-Jie Lu, Li Xu, Ikram Ullah, Hong-Bao Li* and An-Wu Xu*



615

Surfactant-free 2D/2D Pd/g-C₃N₄ for enhanced photocatalytic CO₂ reduction

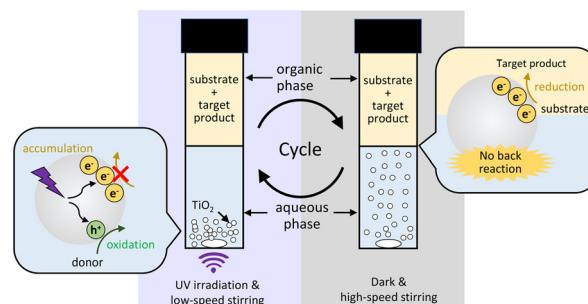
Zhijun Huang,* Jie Wu, Chunliang Yang, Fengwen Yan* and Guoqing Yuan



624

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

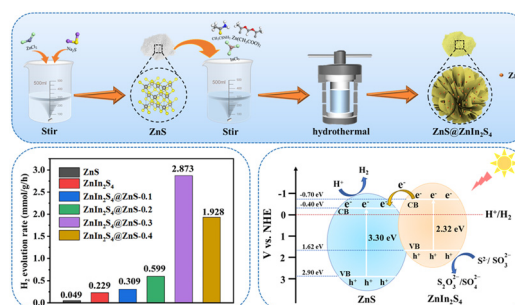
Masato Suenaga and Naoya Murakami*



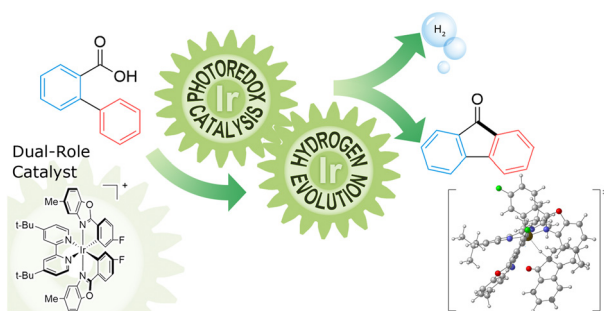
630

Facile synthesis of ZnIn₂S₄@ZnS composites for efficient photocatalytic hydrogen precipitation

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



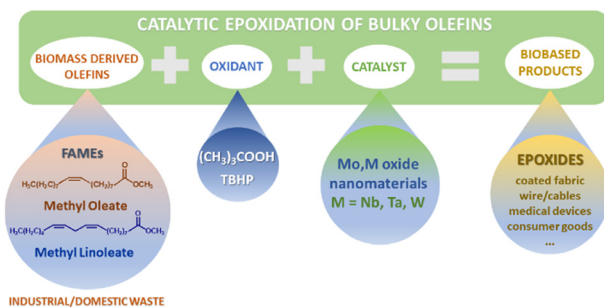
638



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*

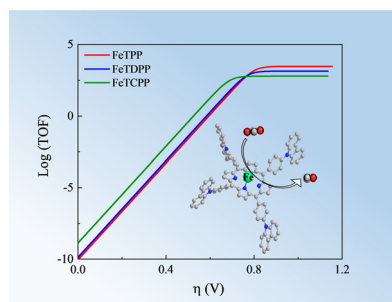
646



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*

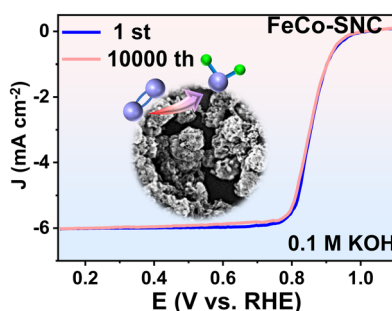
660



Electrocatalytic reduction of CO_2 to CO by Fe(III) carbazole-porphyrins in homogeneous molecular systems

Hai Sun, Jiahui Wu, Fengkun Tian, Guodong Zhang, Zixiang Xia, Jiaxin 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

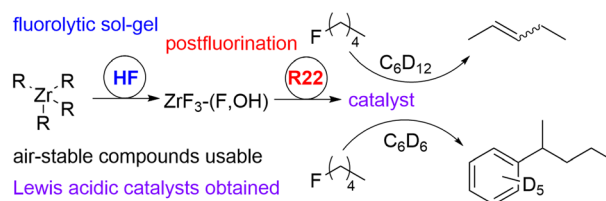
Qiulan Huang, Ruiqin Ren, Jia Li, Muhammad Waqas, Pan Chen, Xiaotian Liu, Dujuan Huang, Zhongyun Yang, Xinglan Peng, Du-Hong Chen,* Youjun Fan* and Wei Chen*



673

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

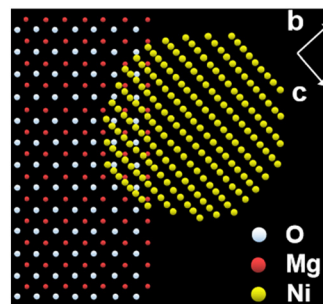
Christian Heinekamp, Sönke Kneiske, Ana Guilherme Buzanich, Mike Ahrens, Thomas Braun* and Franziska Emmerling*



681

Stable Ni nanocrystals on porous single-crystalline MgO particles for enhanced dry reforming activity and durability of CH₄/CO₂

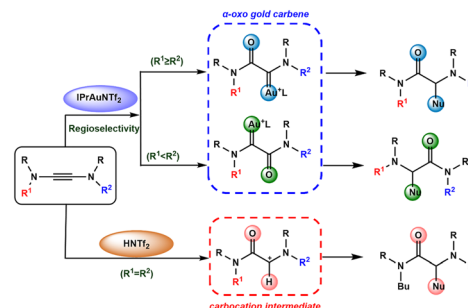
Suning Zhang, Fangyuan Cheng* and Kui Xie*



689

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

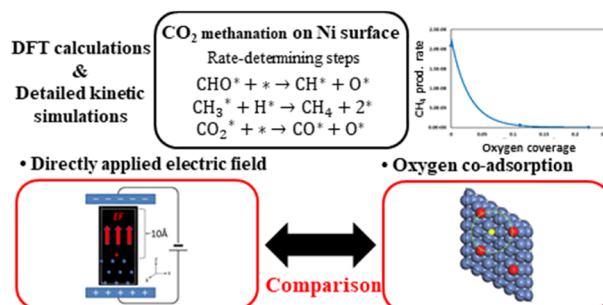
Guowei Yan, Ji Ma, Simeng Qi, Alexander M. Kirillov, Lizi Yang and Ran Fang*



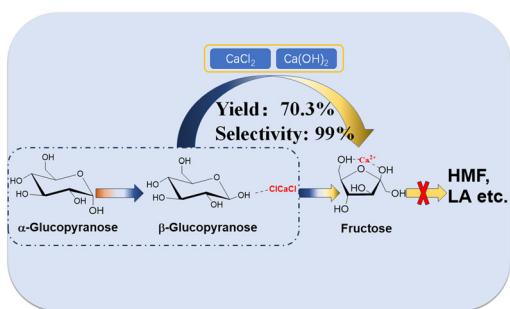
704

Theoretical study of catalytic activity modifications in CO₂ methanation induced by an electric field in solid-oxide cells

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



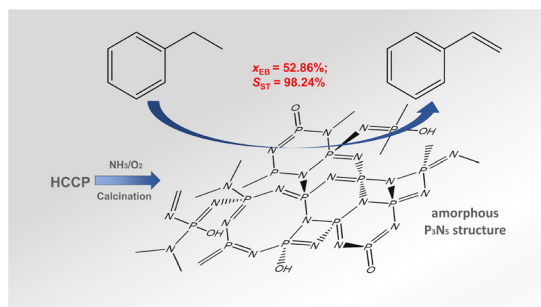
718



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

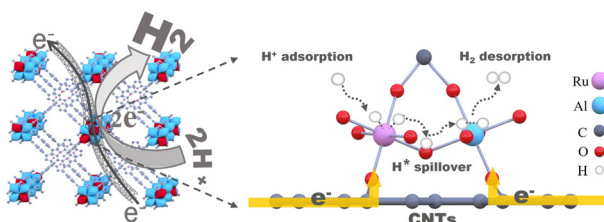
728



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*

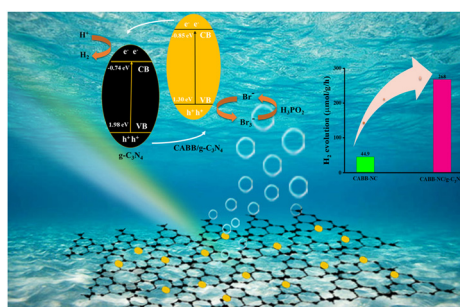
735



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 $Cs_2AgBiBr_6$ -NC/g- C_3N_4 nanocomposites

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

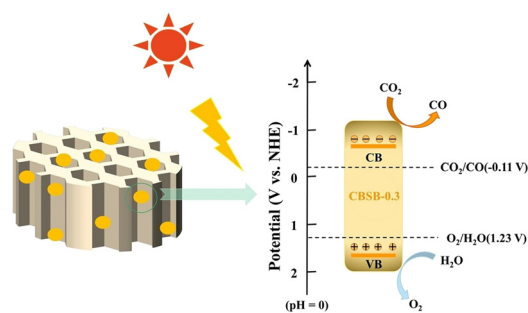


PAPERS

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 CO_2 reduction

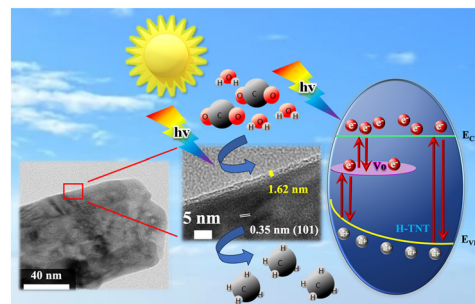
Miaomiao Gao, Xiaolei Liu,* Liwen Yin, Jinghang Chen, Zeyan Wang, Zhaoke Zheng, Yuanyuan Liu, Hefeng Cheng, Ying Dai, Baibiao Huang, Zehui Zhang* and Peng Wang*



767

Engineered CO_2 conversion performance of nanostructured 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*

