

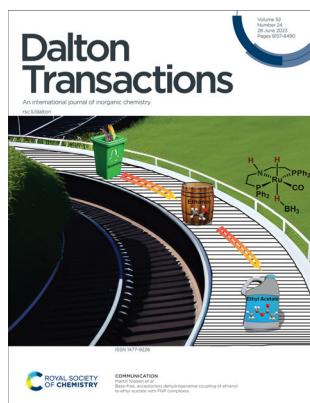
# Dalton Transactions

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## IN THIS ISSUE

ISSN 1477-9226 CODEN DTARAF 52(24) 8157–8490 (2023)



### Cover

See Martin Nielsen et al., pp. 8193–8197.

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### Inside cover

See Rui Wang, Qiaoling Kang, Dongyun Li et al., pp. 8211–8221.

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## EDITORIAL

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### Metallocycles and metallocages

Lin Xu,\* Cally J. E. Haynes\* and James E. M. Lewis\*

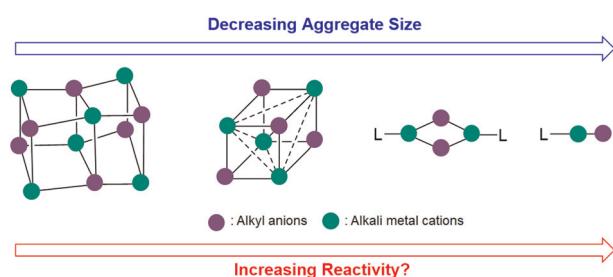


## PERSPECTIVE

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### The quest for organo-alkali metal monomers: unscrambling the structure–reactivity relationship

Nathan Davison\* and Erli Lu\*



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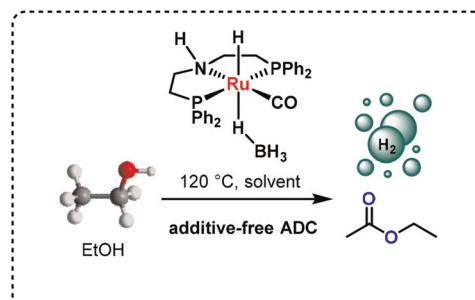
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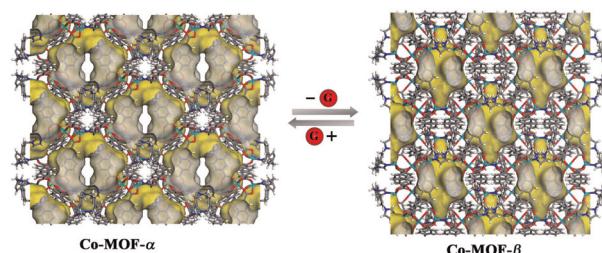


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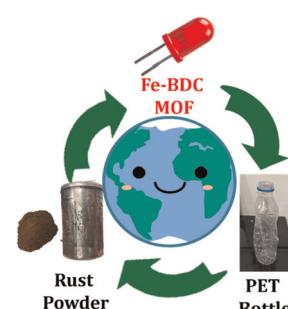
8193

**Base-free, acceptorless dehydrogenative coupling of ethanol to ethyl acetate with PNP complexes**Zhenwei Ni, Rosa Padilla, Rajib Pramanick,  
Mike S. B. Jørgensen and Martin Nielsen\*

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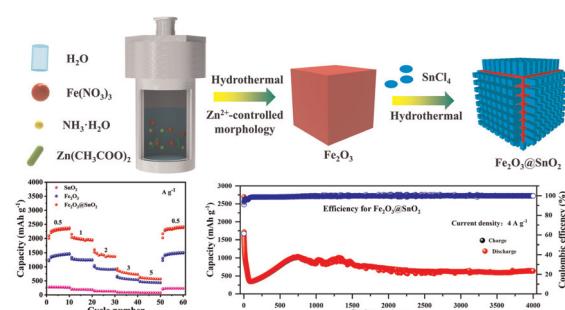
**A 2D flexible cobalt-MOF: reversible solid-state structural transformation, two-step and gate-opening adsorption behaviours, and selective adsorption of C<sub>2</sub>H<sub>2</sub> over CO<sub>2</sub> and CH<sub>4</sub>**Shan-Shan Wang, Yu-Jie Liang, Wei Guo, Yue Yin,  
Xiao-Yu Li, Quan-Qing Xu, Ai-Xin Zhu\* and Bo Huang\*

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**Upcycling rust and plastic waste into an Fe MOF for effective energy storage applications: transformation of trash to treasure**Rakesh Deka, Diptangshu Datta Mal and  
Shaikh M. Mobin\*

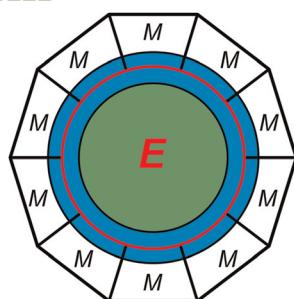
## PAPERS

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**Epitaxial growth of hexahedral Fe<sub>2</sub>O<sub>3</sub>@SnO<sub>2</sub> nano-heterostructure for improved lithium-ion batteries**Xiong Wang, Rui Wang,\* Qiaoling Kang,\* Feng Gao,  
Miaogen Chen, Yang Xu, Hongliang Ge and  
Dongyun Li\*

## PAPERS

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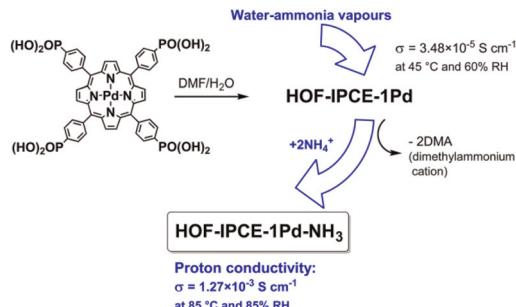
## 8- $N^{\text{eff}}(E)$

Octet rule for polar-covalent multiatomic bonding

### Polarity-extended 8 – $N^{\text{eff}}$ rule for semiconducting main-group compounds with the TiNiSi-type of crystal structure

Riccardo Freccero,\* Yuri Grin and Frank R. Wagner\*

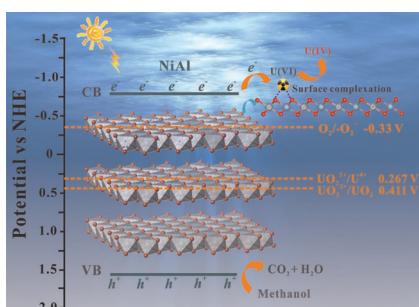
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### An anionic porphyrinylphosphonate-based hydrogen-bonded organic framework: optimization of proton conductivity through the exchange of counterions

Ekaterina A. Zhigileva, Yulia Yu. Enakieva,\* Anna A. Sinelshchikova, Vladimir V. Chernyshev, Ivan N. Senchikhin, Konstantin A. Kovalenko, Irina A. Stenina, Andrey B. Yaroslavtsev, Yulia G. Gorbunova and Aslan Yu. Tsivadze

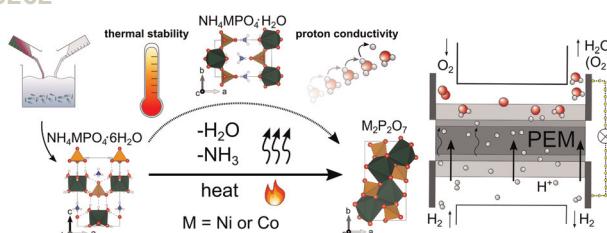
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### Adsorption-photoreduction behaviors and mechanisms of layered double hydroxide loaded on uranium(vi) removal

Qian Ling, Peiling Kuang, Xin Zhong\* and Baowei Hu\*

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### Thermally processed Ni-and Co-struvites as functional materials for proton conductivity

Stephanos Karafilidis,\* Biswajit Bhattacharya, Ana Guilherme Buzanich, Friedrich Fink, Ines Feldmann, Johan E. ten Elshof, Franziska Emmerling and Tomasz M. Stawski\*

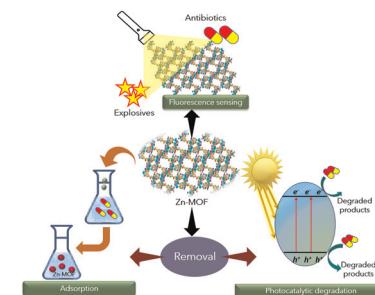


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**Amino decorated adenine based metal–organic framework for multi-faceted applications**

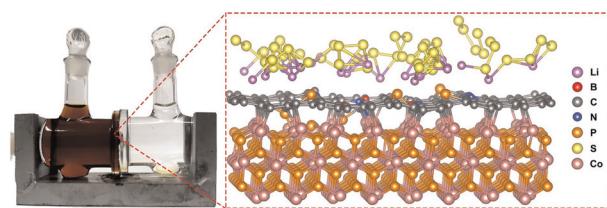
Alehegn Eskemech, Diksha Gambhir, Harpreet Kaur, Anirban Karmakar and Rik Rani Koner\*



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**Synthesis of CoP@B,N,P co-doped porous carbon by a supramolecular gel self-assembly method for lithium–sulfur battery separator modification**

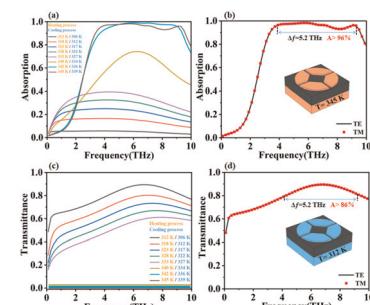
Zhenpu Shi, Yunqi Huang, Juhong Xu, Yudong Pang, Lan Wang, Wanli Zhao, Hongyun Yue, Zongxian Yang, Shuteng Yang\* and Yanhong Yin\*



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**Active thermally tunable and highly sensitive terahertz smart windows based on the combination of a metamaterial and phase change material**

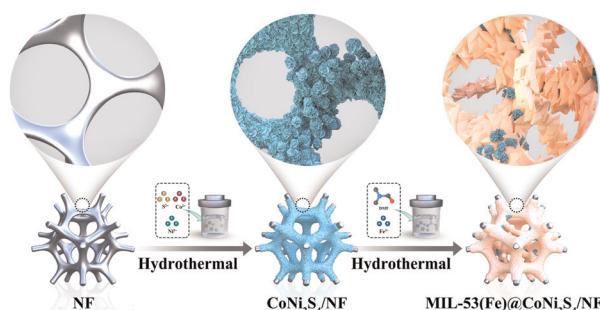
Zhipeng Zheng, Wenchao Zhao, Zao Yi,\* Liang Bian, Hua Yang, Shubo Cheng, Gongfa Li, Liangcai Zeng, Hailiang Li and Peipei Jiang



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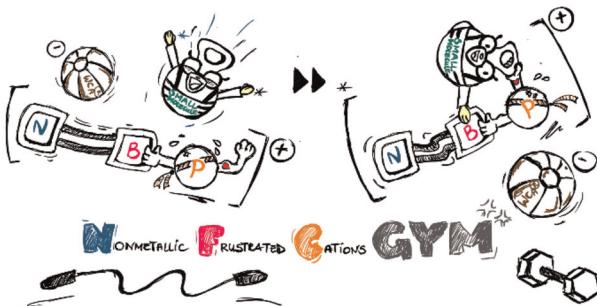
**A hybrid of MIL-53(Fe) rhombus and conductive CoNi<sub>2</sub>S<sub>4</sub> nanosheets as a synergistic electrocatalyst for the oxygen evolution reaction**

Weidong Liu, Lijun Wang and Yaqiong Gong\*



## PAPERS

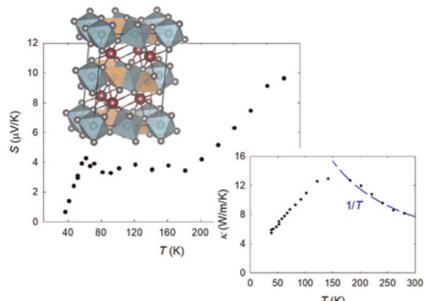
8311



## Application of nonmetallic frustrated cations in the activation of small molecules

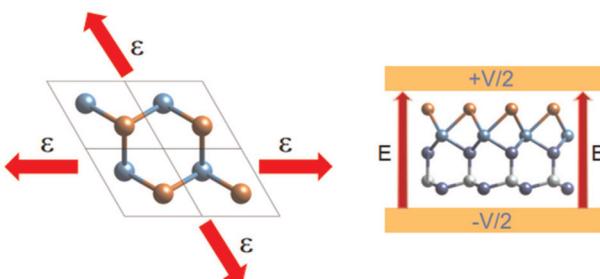
Kinga Kaniewska-Laskowska,\* Marcin Czapla, Jarosław Chojnacki and Rafał Grubba\*

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Structure, electrical and thermal properties of single-crystal  $\text{BaCuGdTe}_3$ 

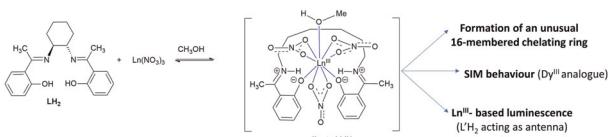
Wilarachchige D. C. B. Gunatilleke, Winnie Wong-Ng, Teian Chang, Yu-Sheng Chen and George S. Nolas\*

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First principles prediction of two-dimensional Janus  $\text{STiXY}_2$  ( $\text{X} = \text{Si, Ge}; \text{Y} = \text{N, P, As}$ ) materials

Zhen Gao, Xin He, Wenzhong Li, Yao He\* and Kai Xiong

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## Interesting chemical and physical features of the products of the reactions between trivalent lanthanoids and a tetradeятate Schiff base derived from cyclohexane-1,2-diamine

I. Mylonas-Margaritis,\* Z. G. Lada, A. A. Kitos, D. Maniaki, K. Skordi, A. J. Tasiopoulos, V. Bekiari, A. Escuer, J. Mayans,\* V. Nastopoulos,\* E. G. Bakalbassis,\* D. Papaioannou\* and S. P. Perlepes\*

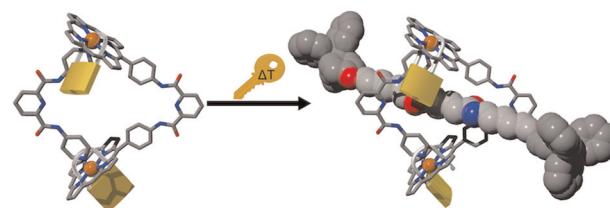


## PAPERS

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**A robust heterodimeric bis-Rh(III)-porphyrin macrocycle for the self-assembly of a kinetically stable [2]-rotaxane**

Naoyuki Hisano,\* Virginia Valderrey, Gemma Aragay and Pablo Ballester\*



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**Synthesis and photothermal performance of non-stoichiometric molybdenum oxide ( $\text{MoO}_{3-x}$ ) prepared by gamma radiation**

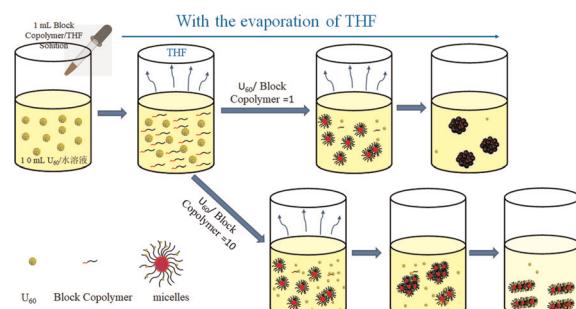
Diane C. A. Lima,\* Aldebarã F. Ferreira, Sôtterferson E. Silva, Severino Alves, Junior, Felipe L. N. Sousa and Walter M. de Azevedo\*



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**Hydrogen bonding and phase separation cooperatively guide the self-assembly of  $\text{U}_{60}$  and the polymer to fabricate multiscale nanostructures**

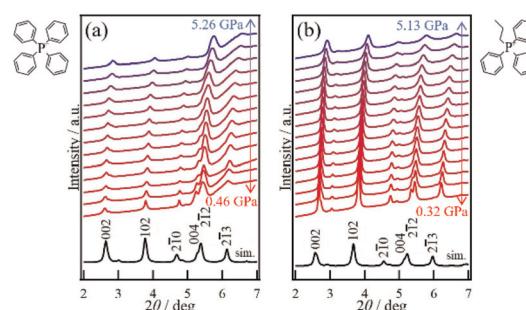
Jie Hu,\* Yingxuan Mei, Huifen Wu, Yan Zhao, Dongping Wu, Nan Ye, Peng Yi, Yu Yang and Minmeng Liao



8368

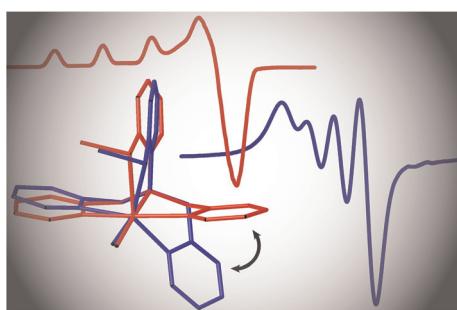
**$^{57}\text{Fe}$  Mössbauer spectroscopy and high-pressure structural analysis for the mechanism of pressure-induced unique magnetic behaviour in (cation)  $[\text{Fe}^{\text{II}}\text{Fe}^{\text{III}}(\text{dto})_3]$  (cation =  $\text{Ph}_4\text{P}$  and  ${}^n\text{PrPh}_3\text{P}$ ; dto = 1,2-dithiooxalato)**

Ryosuke Taniai, Tsubasa Endo, Takuya Kanetomo,\* Atsushi Okazawa, Hirokazu Kadobayashi, Saori I. Kawaguchi and Masaya Enomoto\*



## PAPERS

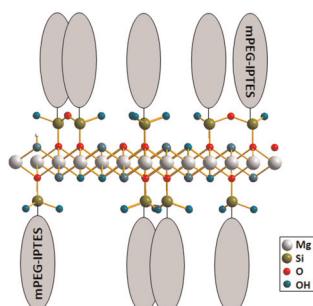
8376



## Conformational dynamicity in a copper(II) coordination complex

Paul J. Griffin, Matthew J. Dake, Alesandro D. Remolina and Lisa Olshansky\*

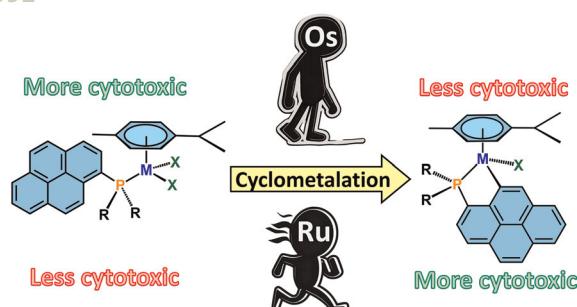
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## *In situ* preparation of compounds using silanized mPEG inspired by talc-like structures

Liva Dzene,\* Anne-Sophie Schuller, Frédéryck Tidas, Séverinne Rigolet, Jocelyne Brendlé and Christelle Delaite

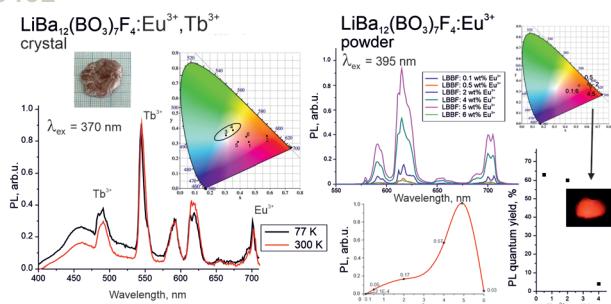
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## Cytotoxicity of osmium(II) and cycloosmated half-sandwich complexes from 1-pyrenyl-containing phosphane ligands

Dana Josa, David Aguilà, Pere Fontova, Vanessa Soto-Cerrato, Piedad Herrera-Ramírez, Laia Rafols, Arnald Grabulosa\* and Patrick Gamez\*

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## $\text{LiBa}_{12}(\text{BO}_3)_7\text{F}_4$ (LBBF) crystals doped with $\text{Eu}^{3+}$ , $\text{Tb}^{3+}$ , $\text{Ce}^{3+}$ : structure and luminescence properties

Tatyana B. Bekker,\* Alexey A. Ryadun, Alexey V. Davydov and Sergey V. Rashchenko

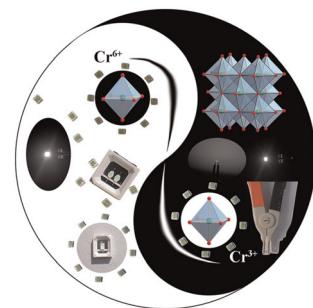


## PAPERS

8414

**A broadband near-infrared  $\text{Cr}^{3+}$ -doped phosphor applied to near-infrared light-emitting diodes: enhanced luminescence and thermal stability by annealing**

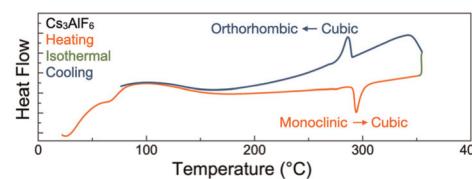
Tao Tan, Ran Pang,\* Shangwei Wang, Haiyan Wu, Jiutian Wang, Su Zhang, Chengyu Li\* and Hongjie Zhang



8425

**Polymorphism in  $\text{A}_3\text{MF}_6$  ( $\text{A} = \text{Rb, Cs}$ ;  $\text{M} = \text{Al, Ga}$ ) grown using mixed halide fluxes**

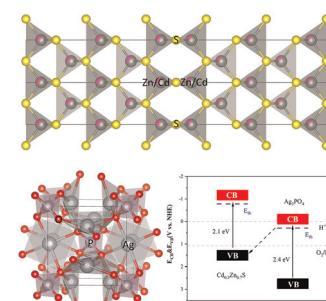
Gregory Morrison, Lakshani W. Masachchi, Hunter B. Tisdale, Tieyan Chang, Virginia G. Jones, K. Pilar Zamorano, Logan S. Breton, Mark D. Smith, Yu-Sheng Chen and Hans-Conrad zur Loye\*



8434

**Defective  $\text{Cd}_{0.3}\text{Zn}_{0.7}\text{S}$  twin crystal/ $\text{Ag}_3\text{PO}_4$  Z-scheme heterojunctions toward optimized visible-light-driven photocatalytic hydrogen evolution**

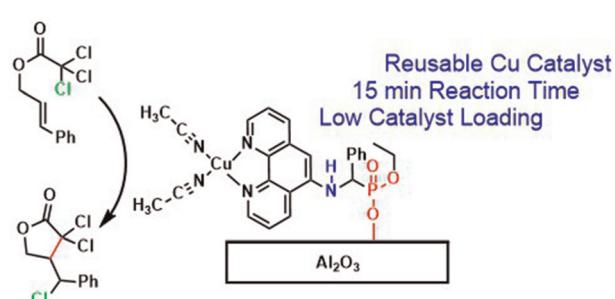
Jie Chen, Haitao Yu,\* Ying Xie,\* Zhenzi Li and Wei Zhou\*



8442

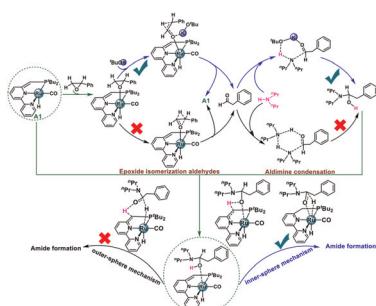
**Surface immobilized Cu-1,10-phenanthroline complexes with  $\alpha$ -aminophosphonate groups in the 5-position as heterogenous catalysts for efficient atom-transfer radical cyclizations**

Sarah E. Maier, Osman Bunjaku, Elif Kaya, Michael Dyballa, Wolfgang Frey and Deven P. Estes\*



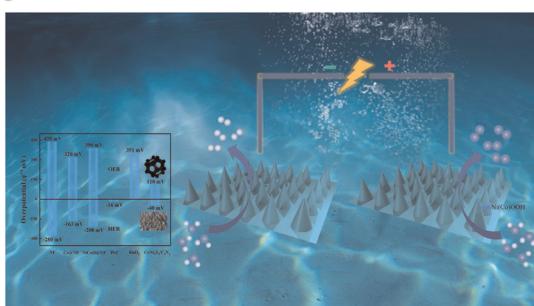
## PAPERS

8449


**Mechanistic insights into amide formation from aryl epoxides and amines catalyzed by ruthenium pincer complexes: a DFT study**

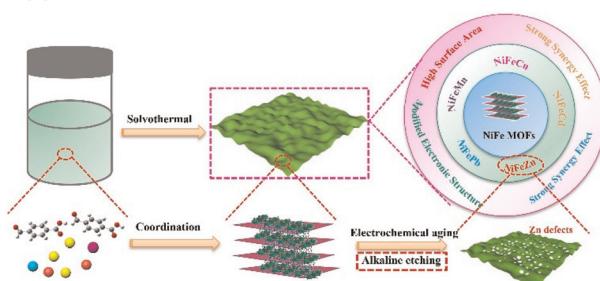
Jing Wen, Zhewei Li, Yanhui Tang, Min Pu\* and Ming Lei\*

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**Tentacle-like core–shell  $\text{CoNi}_2\text{S}_4/\text{C}_3\text{N}_4$  bifunctional electrocatalysts for efficient overall alkaline water splitting**

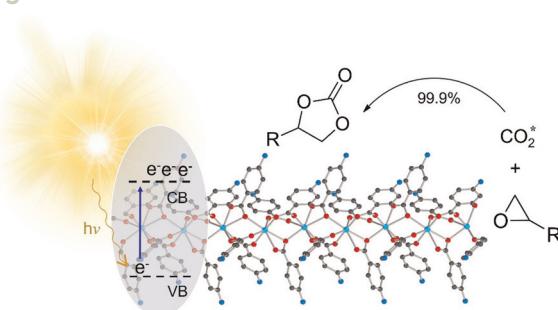
Qingfei Li, Nan Li,\* Mianmian Wu, Guifang Sun, Wenjing Shen, Minghao Shi and Jiangquan Ma\*

8466


**Engineering defective trimetallic metal–organic framework nanosheets for advanced water oxidation electrocatalysis**

Hui Xu, Cheng Wang, Guangyu He\* and Haiqun Chen\*

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**Lanthanide(III) (Er/Ho) coordination polymers for a photocatalytic  $\text{CO}_2$  cycloaddition reaction**

Reem H. Alzard, Lamia A. Siddig, Abdalla S. Abdelhamid, Alejandro Perez Paz, Ha L. Nguyen, K. Sethupathi, P. K. Sreejith and Ahmed Alzamly\*



## CORRECTION

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**Correction: An insight into the optical properties of a sub nanosize glutathione stabilized gold cluster**

Lakshmi V. Nair, Resmi V. Nair and Ramapurath S. Jayasree\*

