

## IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 49(34) 14577–14996 (2025)



### Cover

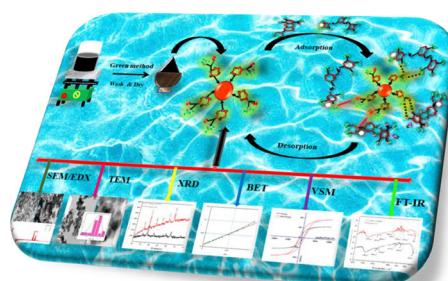
See Zeenat Sheerazi,  
Ishtiyaq Ahmad  
*et al.*, pp. 14590–14604.  
Image reproduced  
by permission  
of Zeenat Sheerazi from  
*New J. Chem.*,  
2025, 49, 14590.  
Acknowledgement:  
The image was created  
with Google Gemini AI.

## PAPERS

14590

### Green synthesis of a nicotinamide-functionalized cobalt ferrite nano-adsorbent for aqueous phase removal of some virulent dyes: evaluation of adsorption isotherms, kinetics, and mechanisms

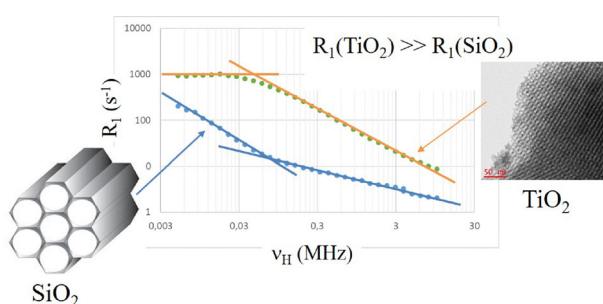
Zeenat Sheerazi,\* Ishtiyaq Ahmad, Saif Ali Chaudhry,  
Aasif Hassan Sheikh and Tabrez Alam Khan



14605

### Water confinement in hierarchical porous silica and titania

Pierrick Gaudin, Yohann Vuillemand, Florian Jonas,  
Sabine Bouquet-Bonnet\* and Jean-Luc Blin\*



# Environmental Science: Atmospheres

GOLD  
OPEN  
ACCESS

## Connecting communities and inspiring new ideas



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

Fundamental questions  
Elemental answers



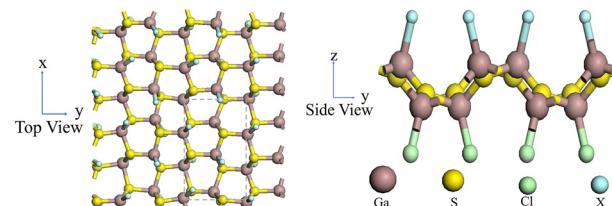
Registered charity number: 207890

## PAPERS

14614

**Janus  $\text{Ga}_4\text{S}_4\text{Cl}_2\text{X}_2$  ( $\text{X} = \text{F}, \text{Br}, \text{I}$ ) monolayers: first-principles investigation of in- and out-of-plane piezoelectric properties**

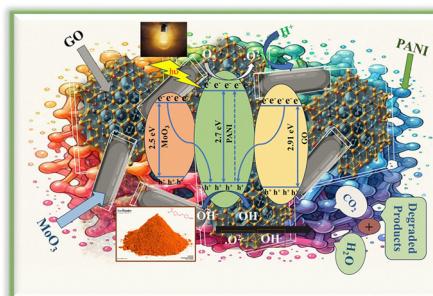
Yi Xie, Xinguo Ma,\* Youyou Guo, Yufeng Wei, Shida Yao, Aolei Xiong, Hui Lv and ZongFu Tang



14623

**Ultrafast charge separation and photostability in PANI/GO/MoO<sub>3</sub> ternary nanocomposites for dual-function solar photocatalysis: enhanced dye degradation and hydrogen evolution under visible light**

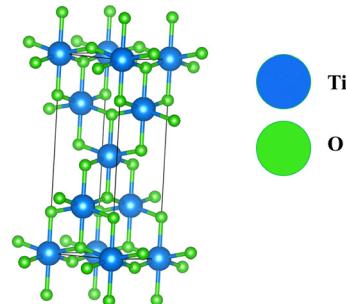
Pritam Hait, Rajeev Mehta and Soumen Basu\*



14638

**Tailoring the structural, elastic, electronic, and optical properties of TiO<sub>2</sub> via carbon doping: a first-principles study**

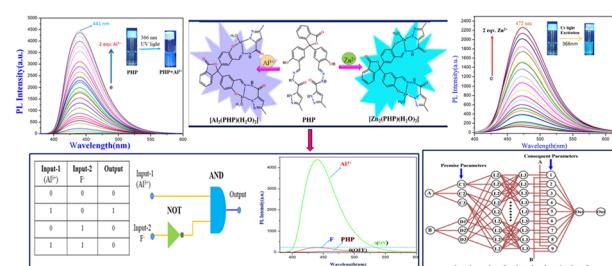
Prakash Kumar Moharana, Debidatta Behera,\* Rituparna Deo, Maya Devi,\* Bidhubhusan Sahu and Sanat Kumar Mukherjee\*



14646

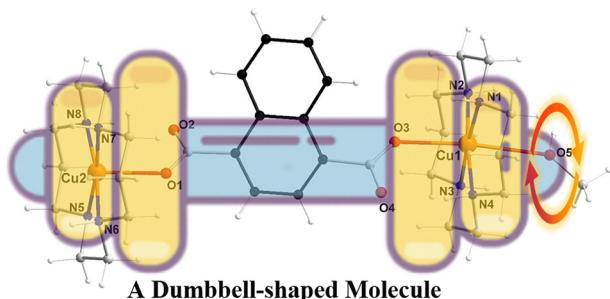
**Fluorescence 'turn-on' dual sensor for the selective detection of Al<sup>3+</sup> and Zn<sup>2+</sup> and the use of AI-based soft computing to predict machine learning outcomes**

Prabhat Kumar Giri, Shashanka Shekhar Samanta, Milan Shyamal, Sourav Mandal, Suraj Barman and Ajay Misra\*



## PAPERS

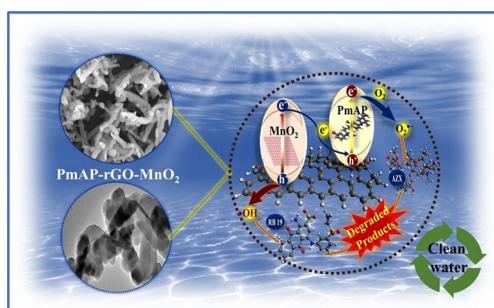
14659



### Boosting the photothermal conversion performance of a dumbbell-shaped molecule with coordinated methanol

Yu-Di Liu, Wenya Jiang, Jianyu Wei, Yuan Wu, Jiaqi Shang, Yimin Wang,\* ShuaiQi Wang\* and Kuan-Guan Liu\*

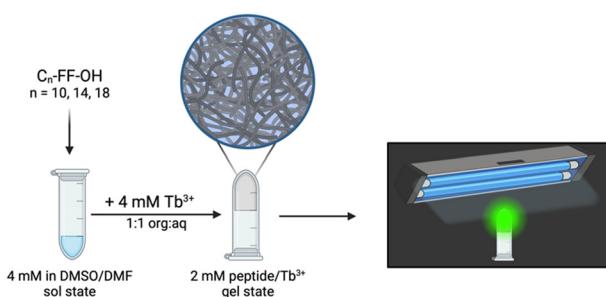
14668



### A visible light-responsive PmAP/rGO/MnO<sub>2</sub> heterojunction: a promising photocatalyst for the degradation of reactive blue 19 and azithromycin

Priyanka P. Mishra, Nigamananda Das, Bankim C. Tripathy and Ajaya K. Behera\*

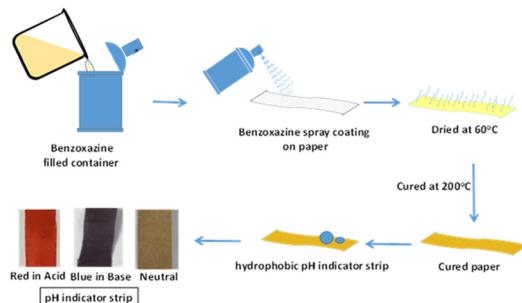
14681



### Lanthanide coordination in *N*-acyl diphenylalanine organohydrogels

Tsuimy Shao, Mozghan Khorasani Motlagh, Meissam Noroozifar and Heinz-Bernhard Kraatz\*

14688



### Development of new polybenzoxazine-coated cellulose strips for extreme acid–base indicator kit applications

Harinei Srinivasan, Hariharan Arumugam\* and Alagar Muthukaruppan

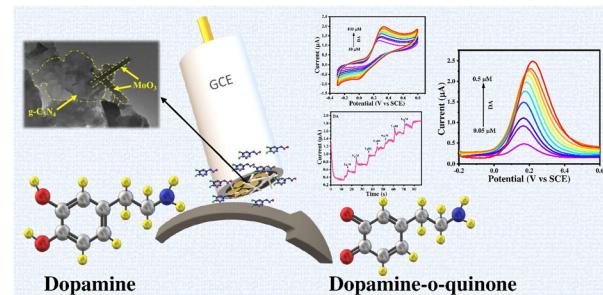


## PAPERS

14697

## Ultrasensitive electrochemical detection of dopamine using an engineered 1D/2D $\text{MoO}_3/\text{g-C}_3\text{N}_4$ nanohybrid

K. Harikrishnan, Bhavani Chukka, Ariful Hoque, Rajendra Patel, Varun Pratap Singh, Umesh Kumar Gaur\* and Manu Sharma\*



14710

## Plasticized composite electrolytes with mesoporous silica nanoparticle-reinforced PVDF-HFP for solid-state lithium–metal batteries

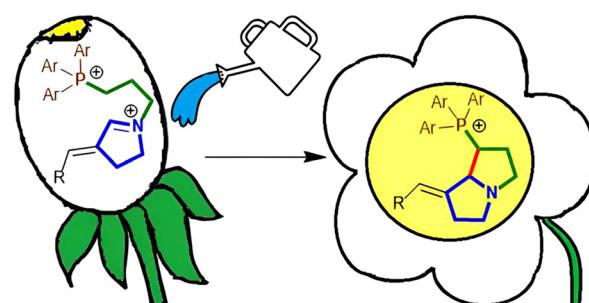
Xi Fu, Qi Wei,\* Wenyu Zheng, Haoyu Bai, Xinyuan Liu, Shuai Hao\* and Wei Lu\*



14718

## Diastereospecific cyclization of 3-arylidene-1-pyrrolinium salts containing an alkyltriarylphosphonium fragment: a path to the synthesis of new pyrrolizidine derivatives

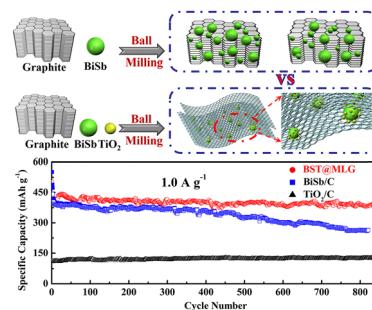
Tanzilya Rizbayeva, Andrey Smolobochkin,\* Almir Gazizov, Olga Babaeva, Anna Lyubina, Anastasiia Sapunova, Alexandra Voloshina, Daria Gerasimova, Alexander Burilov and Michail Pudovik



14728

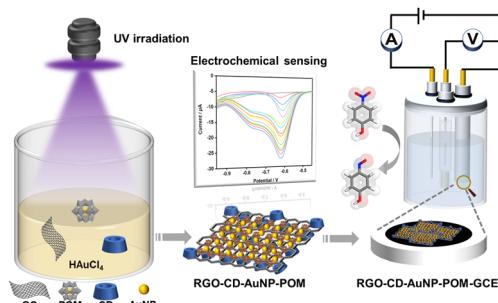
## $\text{TiO}_2$ -Driven graphite exfoliation: a facile approach for designing a high-performance $\text{BiSb}_3/\text{TiO}_2@\text{multilayer graphene}$ anode for potassium-ion batteries

Jiafeng Zhou,\* Kai Wang, Qingqing Wang, Bo Ding, Chao Dong, Weili Meng and Hao Gong



## PAPERS

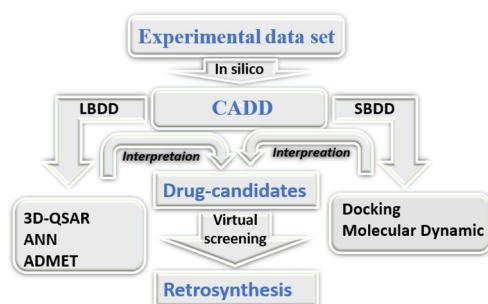
14739



### A green electrochemical sensor for *p*-nitrophenol based on a reduced graphene oxide/β-cyclodextrin/gold nanoparticle/polyoxometalate nanohybrid

Yongyi Xiao, Zuhang Ding, Xu Chai, Qinran Li, Jing Jin,\* Yanjun Yu\* and Jin Zhao\*

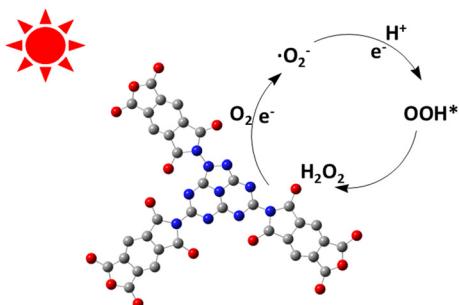
14748



### Integrative computational strategy for anticancer drug discovery: QSAR-ANN modeling, molecular docking, ADMET prediction, molecular dynamics and MM-PBSA simulations, and retrosynthetic analysis

Said El Rhabori,\* Marwa Alaqrabeh, Lhoucine Naanaai, Yassine EL Allouche, Abdellah El Aissouq, Mohammed Bouachrine, Hicham Zaitan, Samir Chtita and Fouad Khalil

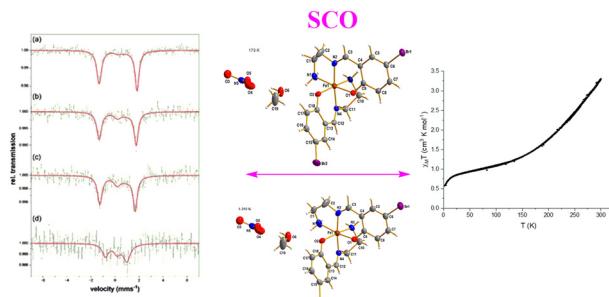
14769



### Polyimide with enhanced $\text{O}_2$ activation for hydrogen peroxide photosynthesis

Feng Lin,\* Chai Jun, Jian Zhang, Shaozheng Zhang, Yulin Wang, Fangsong Guo, Yun Zheng, Yilin Chen, Yufei Zhao and Liang Lv\*

14776



### Broad spin crossover in an iron(III) Schiff base complex with a *cis*- $\text{FeN}_4\text{O}_2$ coordination environment

Dawit Tesfaye, Mamo Gebrezgiabher, Jonas Braun, Juraj Kuchár, Juraj Černák, Atakilt Abebe, Pascal Boulet, Nandakumar Kalarikkal, Tim Hochdörffer, Volker Schünemann, Christopher E. Anson, Madhu Thomas\* and Annie K. Powell\*

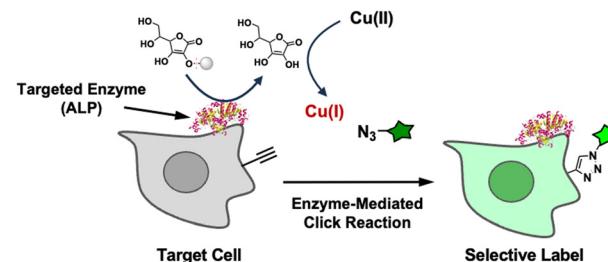


## PAPERS

14782

**Selective cell labeling through enzyme-mediated click reactions**

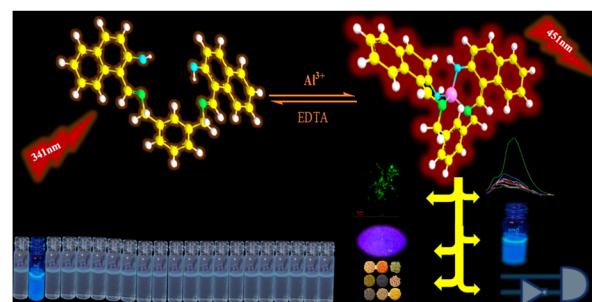
Liang Li, Zhen Li, Yuqi Qian, Guoming Tong,  
Bingfeng Dai\* and Guahan Liu\*



14787

**A reversible and symmetric naphthalene-based ESIPT-active fluorescent chemosensor for Al<sup>3+</sup> ions: real sample applications, molecular logic gates, bioimaging and latent fingerprint visualization**

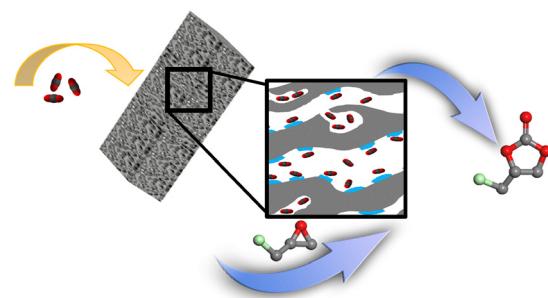
Elizabeth Antony, Narmatha Ganesan,  
Kavanya Srinivasan, S. Prince Makarios Paul,  
Angamuthu Abiram,\* K. Parvatham, Velu Rajesh Kannan  
and Raju Nandakumar\*



14801

**A composite metal–organic framework/carbon aerogel for enhanced CO<sub>2</sub> adsorption and catalytic conversion**

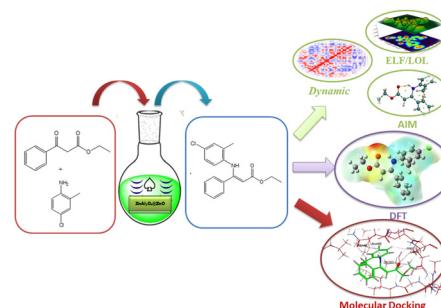
Yi Wu, Yong Chi, Yihong Luo, Xinxin Feng, Penglei Ni,  
Jiawei Zhang, Zhixuan Wu and Zhaojun Chen\*



14810

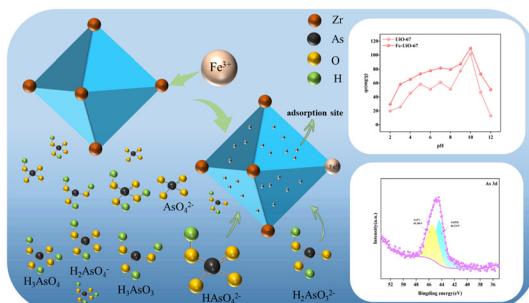
**Molecular docking and computational assessment of spectroscopic analysis of ethyl 3-(4-chloro-2-methylphenylamino)-3-phenylacrylate as a potential antibacterial agent**

Wissam Habibi, Saadia Ouizat, Mohamed Chellegui,\*  
Bushra Shakoor, Marwa Alaqrabeh,  
Mohamed Adel Sayed, Mostafa Khouili,  
Abdessamad Tounsi, Haydar A. Mohammad-Salim and  
Mohamed Anouar Harrad



## PAPERS

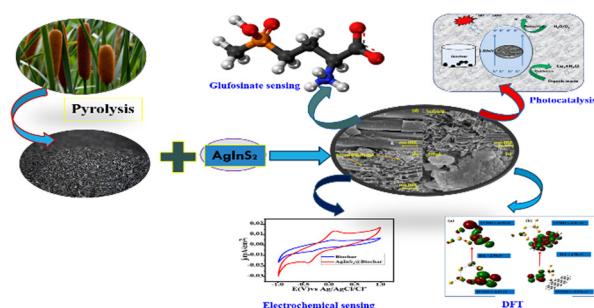
14822



### Efficient capture of arsenic from industrial wastewater by Fe-doped zirconium-based metal-organic frameworks

Mengmeng Geng, Xianjin Qi,\* Junwei Feng, Boyu Du and Meijun Sun

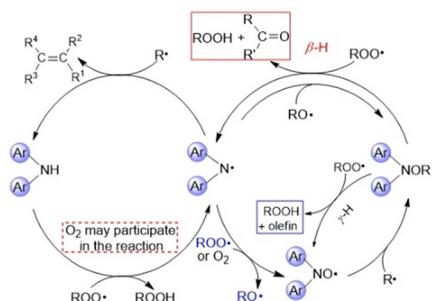
14835



### Hydrothermal synthesis of AgInS<sub>2</sub>@biochar nanocomposites for the photocatalysis and electrochemical sensing of glufosinate herbicides

Firdous Ahmad Ganaie, Irfan Nazir, Aaliya Qureashi, Zia ul Haq, Kaniz Fatima, Arshid Bashir, Altaf Hussain Pandith\* and Mohsin Ahmad Bhat\*

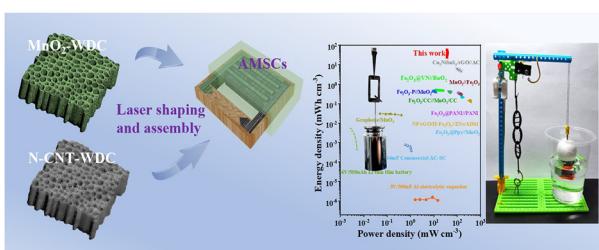
14851



### Theoretical investigations of the catalytic antioxidation mechanism of diarylamine and the coordination effects of Fe(III) and Fe atoms

Junming Wang, Weiguo Xue,\* Zhuozheng Wang, Hao Li, Huiying Lv, Chaoliang Wei, Qingwei Kong, Xiaowei Xu, Kebin Chi, Dejun Shi, Yufeng Liu, Tuanle Li and Yi Luo\*

14866



### Rapid and precise fabrication of a three-dimensional, high-capacity, asymmetric micro-supercapacitor utilizing mortise-and-tenon joint construction

Yubing Sun, Jian Gao,\* Xiaoxiao Du and Xiaodong Zhu\*

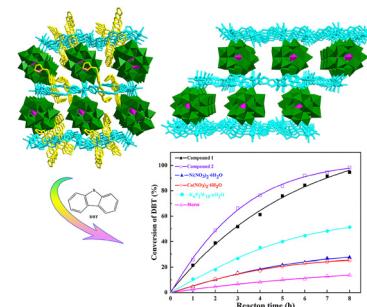


## PAPERS

14874

**Two Dawson-type polyoxometalate-based metal coordination polymers as heterogeneous catalysts for desulfurization**

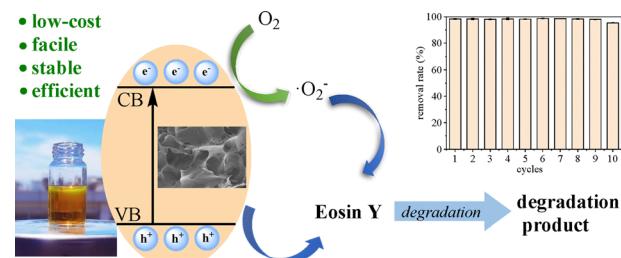
Xiu-Li Hao,\* Chen-Hao Zhang, Chen-Kun Feng, Tian-Ru Su, Mei-mei Zhao and Yan-Zhen Wen



14882

***In situ* preparation of a recyclable hydrogel-based photocatalyst and its application in sunlight-promoted photodegradation of eosin Y**

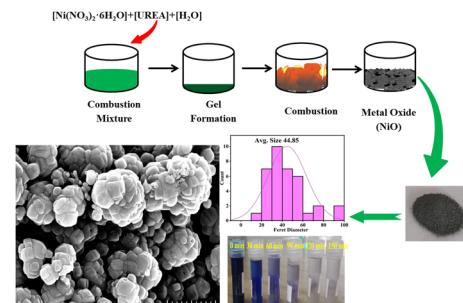
Xiaoxia Liu, Sa Yang, Yanli Cheng, Donglei Wei,\* Hou Chen,\* Liangjiu Bai, Wenxiang Wang, Huawei Yang, Lixia Yang and Kun Yin



14892

**Novel dual metal ion-doped NiO ( $\text{Ni}_{0.9}\text{Cu}_{0.1-x}\text{Zn}_x\text{O}$ ) nanoparticles developed by a solution combustion method for harmful contaminant removal from wastewater**

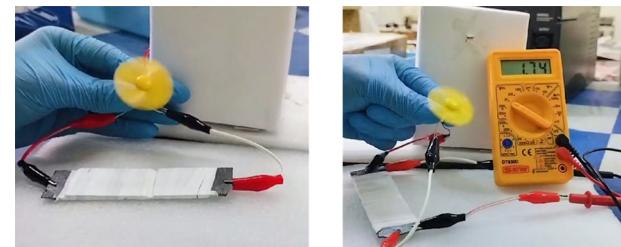
Ashwani Kumar,\* Manpreet Kaur, Nitu, Shruti, S. K. Tripathi, Talat Ali and Mohd. Shkir



14910

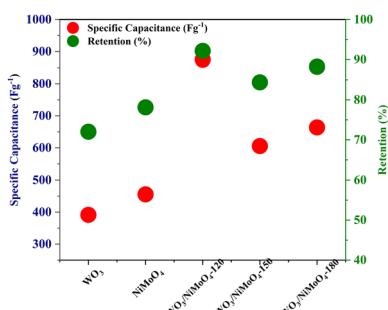
**Phase conversion effect on cobalt phosphate for asymmetric supercapacitor applications**

S. Mohammed Elias, R. Yuvakkumar,\* G. Ravi,\* A. Deepak and R. Shankar



## PAPERS

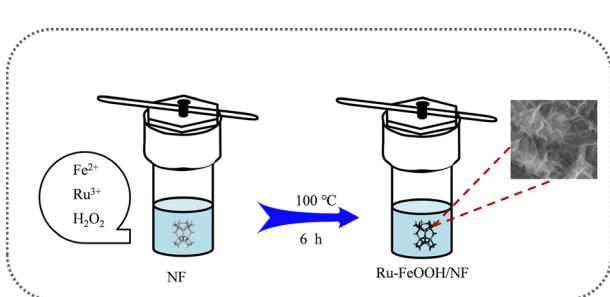
14927



### Insight into the synergetic effect of $\text{WO}_3$ -supported $\text{NiMoO}_4$ nanocomposite application in high-performance electrochemical supercapacitor

Raguram Karunagaran, Rajesh Rajendiran, Ezhilan Jayabal, Chakraborty Antara and Venkatesan Rengarajan\*

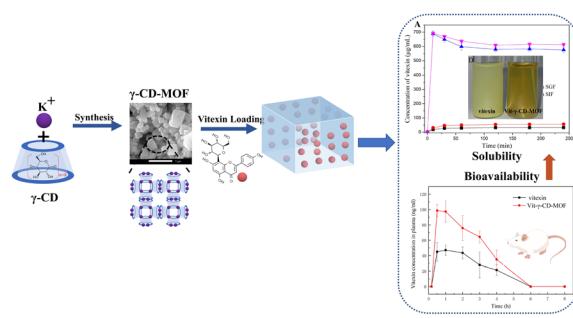
14944



### Ru-doped FeOOH nanosheets as a robust bifunctional electrocatalyst for overall water splitting

Congli Qin, Yanhong Lu, Guangxian Liu, Di Zhao, Hongyan Liu, Fangxu Yang and Aixin Fan\*

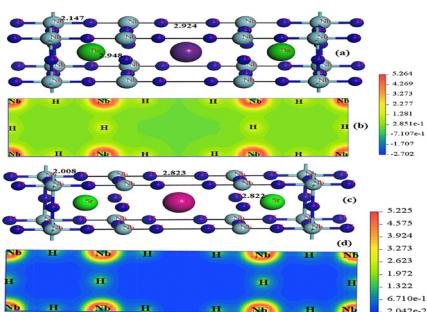
14952



### $\gamma$ -Cyclodextrin metal–organic framework enhanced the bioavailability of vitexin in rats by increasing solubility and inhibiting re-crystallization

Qing-Hua Ni, Qiao Chen, Hai-Xia Xu,\* Wen-Jun Wang, Zhong-Ping Yin and Qing-Feng Zhang\*

14961



### Study of the physical properties of hydride double perovskite $\text{CsD}_2\text{Nb}_3\text{H}_{10}$ ( $\text{D} = \text{Ba}$ and $\text{Sr}$ ) materials: computational insights for hydrogen storage applications

Abhinav Kumar,\* Lilia El Amraoui and Kais Ouni

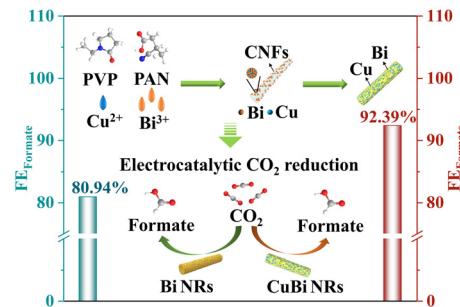


## PAPERS

14978

**Cu-modified Bi nanorods stabilize HCOO<sup>\*</sup> intermediates for efficient CO<sub>2</sub>-to-formate electrocatalytic conversion**

Yijia Guo, Xueyan Wu\* and Jixi Guo\*



14987

**High-yield bottom-up synthesis of 2D metal-organic frameworks via a solvent-free magnetic milling method as high performance anodes for lithium ion batteries**

Fan Zhang, Yunyun Zhai, Quanwei Sun, Haiqing Liu,\* Wei Wang, Zuguang Li\* and Lei Li\*

