

## IN THIS ISSUE

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### Cover

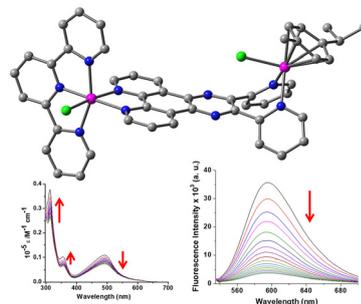
See Anwesha Mohanty and Srikanta Patra, pp. 15999–16007. Image reproduced by permission of Anwesha Mohanty and Srikanta Patra from *New J. Chem.*, 2025, 49, 15999.

## PAPERS

15999

### Synthesis, characterization, computational and DNA interaction studies of mono- and dinuclear Ru(II) complexes containing terpyridine and *p*-cymene ligands

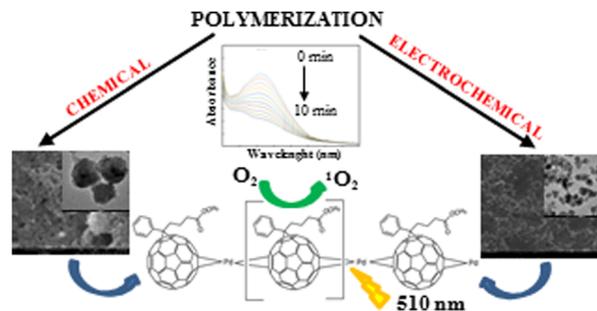
Anwesha Mohanty and Srikanta Patra\*



16008

### Photoinduced formation of singlet oxygen with PCBM–Pd polymer in solution and at the surface

Monika Wysocka-Żółta,\* Agata Blacha-Grzechnik,\* Joanna Breczko, Diana M. Bobrowska, Adam Mizera and Krzysztof Winkler



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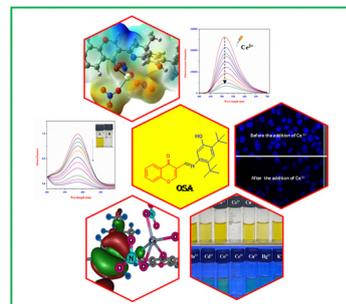
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16019

### A smartphone-assisted highly sensitive hormone-derived fluorescent receptor for rare-earth cerium metal ion detection: environmental monitoring and cancer cell imaging

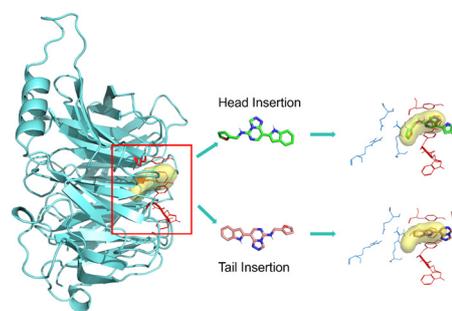
Saravana Kumar Prathiba, Karuppaiyan Kaviya, Ramar Rajamanikandan\* and Kailasam Saravana Mani\*



16029

### Subpocket complementarity and polar interactions dictate dual binding modes of EED inhibitors: insights from molecular dynamics, steered MD, and free energy calculations

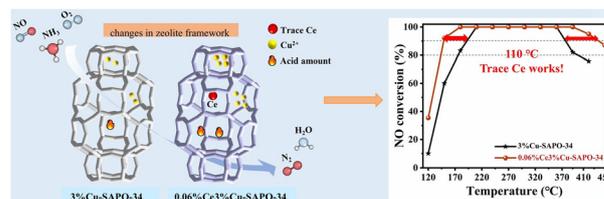
Lvzhou Zhu, Hao Zhang, Lipeng Xu, Pengyin Zhang, Jianan Ju, Shuai Yao, Yaming Shan\* and Song Wang\*



16044

### Trace Ce-modified x%Ce3%Cu-SAPO-34 zeolites prepared by a one-pot method and applied for enhanced NH<sub>3</sub>-SCR denitration activity

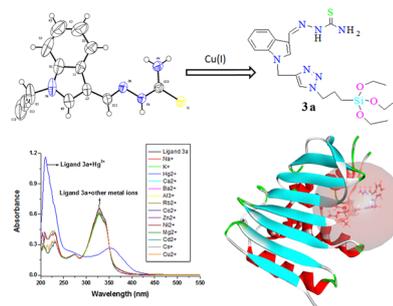
Min Qiang, Boyuan Chen, Yanhong Shao and Zhibin Li\*



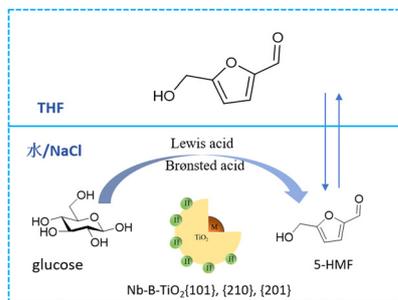
16056

### 'Click' generated indole appended thiosemicarbazone–triazole cojoined organosilane: a sensor for the recognition of Hg<sup>2+</sup> ions, *in silico* docking and *in vitro* cytotoxic evaluation

Gurjaspreet Singh,\* Sushma,\* Harshbir Kaur, Anurag Dalal, Subash Chandra Sahoo, Jandeep Singh, Nancy George, Maria Angeles Esteban\* and Cristóbal Espinosa-Ruíz



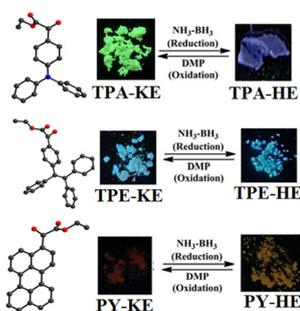
16070



### Synergistic effect of metal-doped TiO<sub>2</sub> for glucose dehydration

Xiang Liu, Ao Luo, Yiran Li, Yuqi Cao, Tingting Ma, Su Wang and Wei He\*

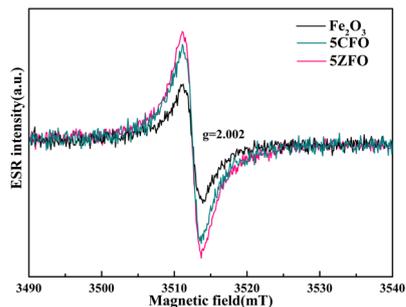
16075



### Reversible fluorescence redox switching in activated carbonyl-functionalized fluorophores through the conversion of $\alpha$ -keto esters and $\alpha$ -hydroxy esters

Deepanjaly K. Sivadas, Sasikala Ravi, Ramanathan Padmanaban, Dohyun Moon,\* Savarimuthu Philip Anthony\* and Vedichi Madhu\*

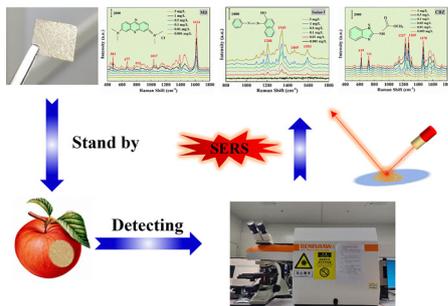
16086



### Conversion of Fe<sub>2</sub>O<sub>3</sub> from n to p type via transition metal (Cu, Zn) doping for the preparation of high-performance acetone sensors

Qixuan Qin,\* Yizhuo Fan and Wei Wang

16097



### Long-chain thiol-regulated hierarchical flower-like silver nanoparticles self-assembled on filter paper as highly sensitive flexible SERS substrates for pesticide residue detection

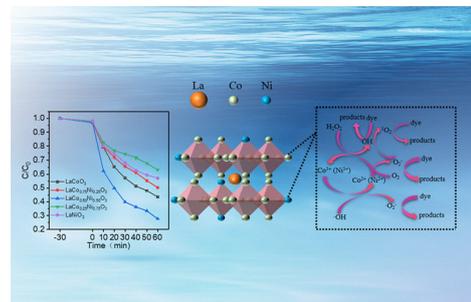
Yunpeng Shao,\* Wenlong Deng, Yue Niu, Zicheng Zhang, Jiwei Song, Yuan Yao and Linyu Mei



16105

### Enhancement of Fenton-like degradation performance of organic dyes by constructing Ni substitution at the B-site for $\text{LaCo}_x\text{Ni}_{1-x}\text{O}_3$ perovskite catalysts

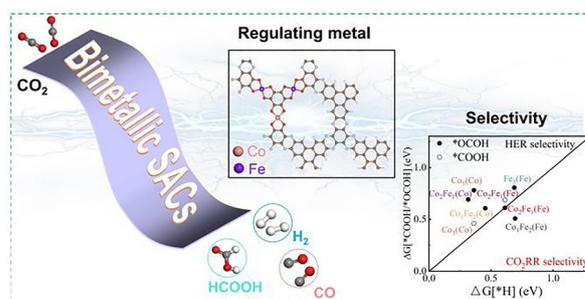
Han Zhang, Quanyu Suo, Ruiduo Zhao, Xia Zhang and Shushu Huang\*



16113

### Design of bimetallic single-atom catalysts and theoretical study of $\text{CO}_2$ reduction reaction

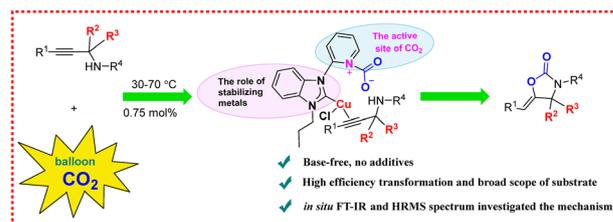
Yang Liu, Zhao-Di Yang\* and Guiling Zhang



16122

### Base-free catalytic systems achieved *via* the design of copper complexes: synthesis of 2-oxazolidinones from propargylic amines and $\text{CO}_2$

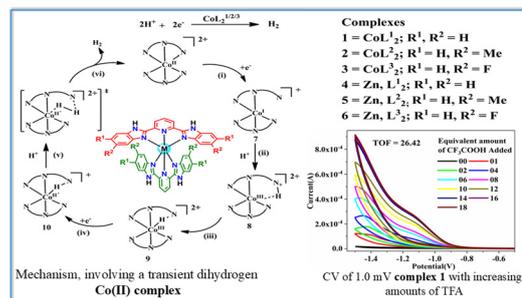
Sheng Tao, Zhi-Hong Du, Chun-Bo Bo, Min Li, Fei Chen\* and Ning Liu\*



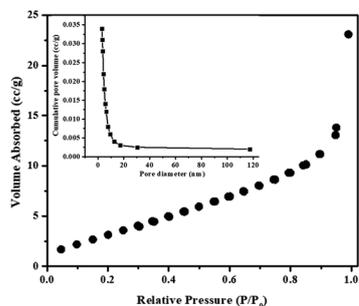
16134

### Electrocatalytic proton reduction by mononuclear cobalt complexes of bis(benzimidazolyl)pyridine ligands: experimental and theoretical study

Sahanwaj Khan, Swaraj Sengupta, Md. Adnan Khan, Narayan Ch. Jana, Bidraha Bagh and Subhendu Naskar\*



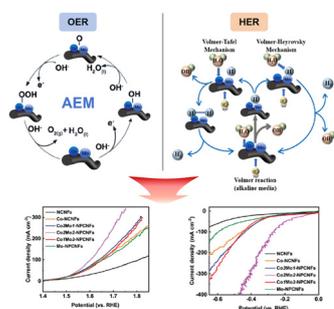
16145



**Biogenic synthesis of zinc oxide nanoparticles using cell-free extract of *Spirogyra crassa* (Kütz.) Kütz. for sustainable biomedical and environmental applications**

Vinay Kumar, Sandeep Kaushal\* and Yadvinder Singh\*

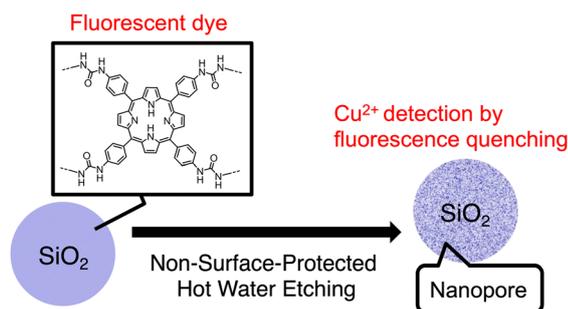
16160



**Harnessing Co/Mo dual-atom synergy on N,P-carbon nanofibers for superior bifunctional water splitting**

Ruidan Duan, Jiawei Fan, Jianhang Ding, Linzhou Zhuang\* and Zhi Xu\*

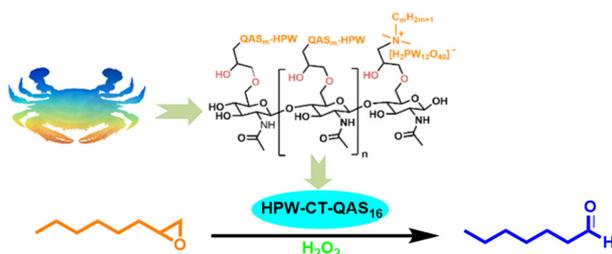
16172



**Synthesis of nanoporous silica nanoparticles encapsulating porphyrin derivatives by non-surface-protected hot water etching for their fluorescent sensing of metal ions in water**

Yoshio Nakahara,\* Ami Kawashima, Natsuki Terashima, Mitsuru Watanabe, Toshiyuki Tamai and Setsuko Yajima

16180



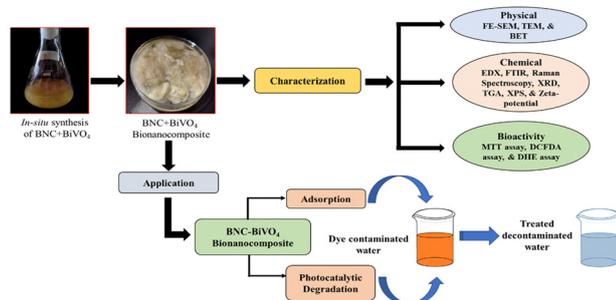
**Selective oxidative cleavage of epoxides to aldehydes by chitin quaternary ammonium phosphotungstate as a recycle catalyst**

Tengfei Niu,\* Xile Xia, Ziyi Wei, Xiao Yu and Zhongjian Tian\*





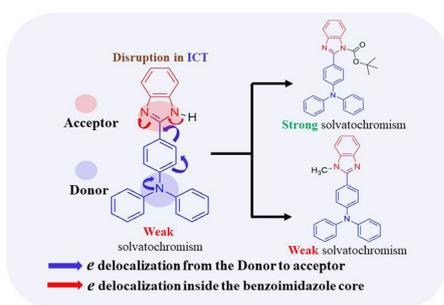
16235



### Biofabrication of a bismuth vanadate/bacterial nanocellulose adsorbent: a photocatalytic mesoporous composite for efficient removal of a fluorochrome pollutant

Bendangtula Walling, Pranjal Bharali,\* D. Ramachandran, Kanagasabai Viswanathan, Nipu Dutta, Naorem Shanta Singh, Swapnali Hazarika, Rajiv K. Srivastava, Balamurali Mahalakshmi, Jeganathan Manivannan and Viphezolie Sorhie

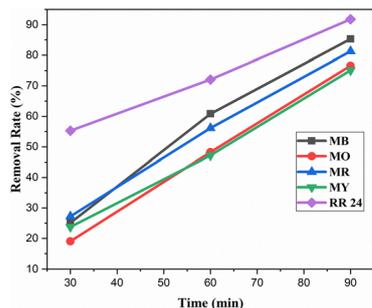
16256



### Substituent effect on the solvatochromic behaviour of benzoimidazole based donor-acceptor type fluorescent molecules

Souvik Santra and Nikhil Guchhait\*

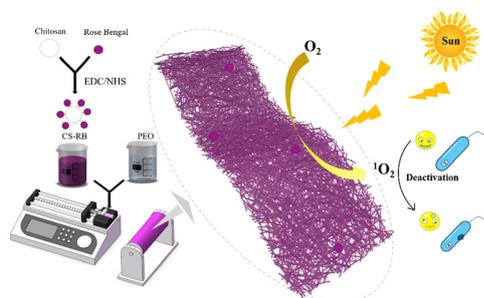
16271



### Synergistic effects of the pyrite and graphitic carbon nitride-based bio-polymer composite for enhancing the photocatalytic degradation of reactive red-24 dye

Sadia Aroob, Muhammad Babar Taj,\* Antoniadou Maria, Ismat Bibi, Muhammad Imran Khan\* and Abeer M. Beagan\*

16288



### Preparation and characterization of rose bengal modified chitosan/polyethylene oxide nanocomposite membranes with photodynamic antimicrobial properties

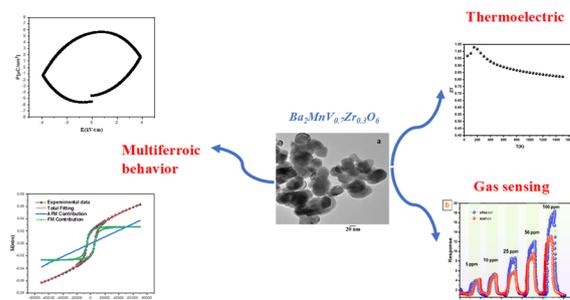
Ming Huang, Yingfeng Wang,\* Yuhang Zhu, Maoli Yin, Zhipeng Ma and XiaoJuan Li\*



16295

### Multifunctional properties of a novel $\text{Ba}_2\text{MnV}_{0.7}\text{Zr}_{0.3}\text{O}_6$ multiferroic double perovskite

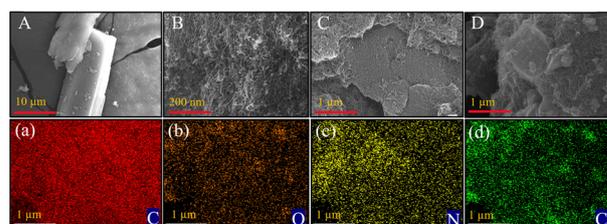
A. Mabrouki,\* Olfa Messaoudi, Afrah Bardaoui, Amajd S. Aljaloud, Latifah Alfahid and E. Dhahri



16307

### A novel electrochemical biosensor based on a heterojunction-structured COF/ $\text{Co}_3\text{O}_4$ /MWCNT: enabling the detection of dopamine and uric acid in complex matrices

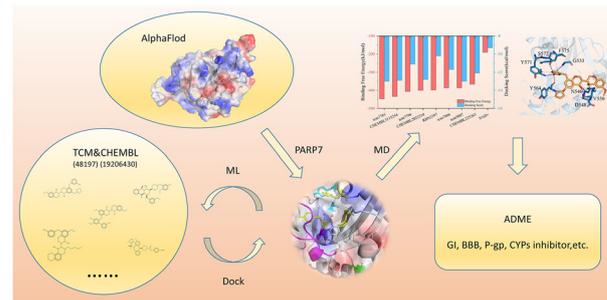
Ya-Xin Li, Dong-Mei Ma,\* Xing-Ming Zhao,\* Jun Xiang, Fu-Fa Wu and Rong-Da Zhao



16320

### Large-scale identification of PARP7 inhibitors via computational modeling and simulation

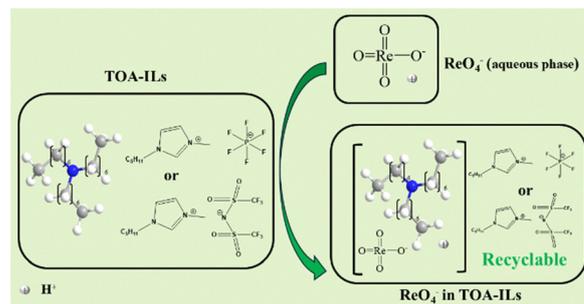
Xiaochen Yang, Baolin Liu and Daixi Li\*



16333

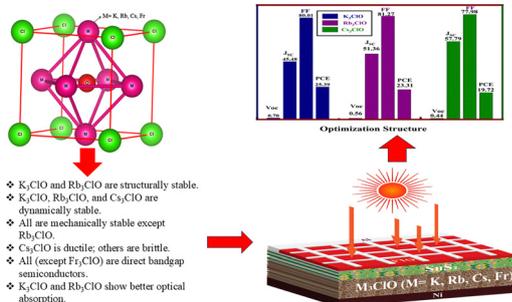
### Solvent extraction of rhenium(VII) from aqueous solution using an ionic liquid system

Dawei Fang, Jia Li, Jie Yang, Donglu Fu,\* Jie Wei\* and Zongren Song\*



## PAPERS

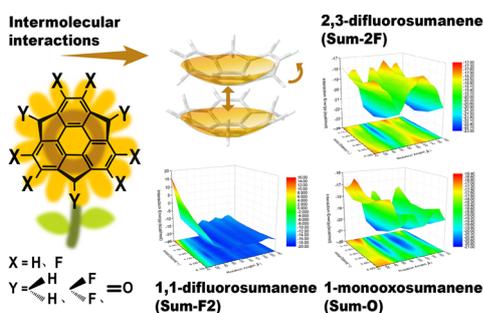
16340



### First-principles design and photovoltaic evaluation of alkali-based $M_3ClO$ anti-perovskites for high-efficiency lead-free solar cells

Md. Sakib Hasan Saikot, Rifat Rafiu, Md. Azizur Rahman,\*  
 Imtiaz Ahamed Apon, Ali El-Rayyes, Mohd Taukeer Khan,  
 Zubair Ahmad and Mohd Shkir

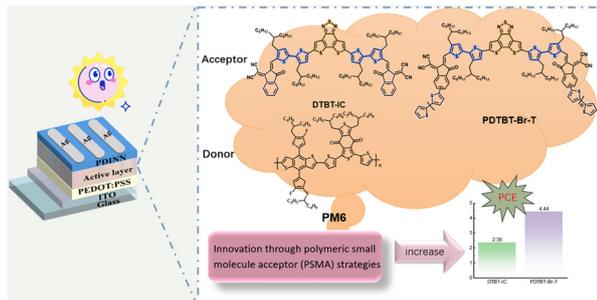
16370



### Unraveling the substituent impact of fluorinated & oxidized sumanene derivatives on stacking interactions and charge transport

Xi Chen, Shuo Xu, Xinpeng Liu, Huan Wang, Simeng Gao  
 and Fu-Quan Bai\*

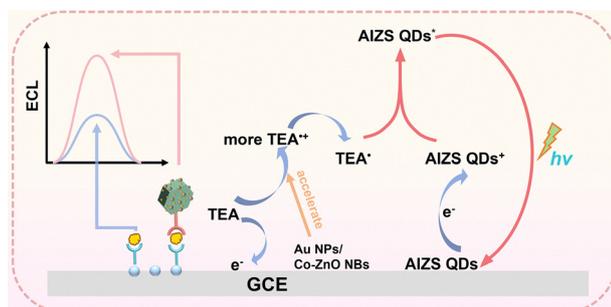
16382



### Synthesis of dithieno[3,2-*b*:2',3'-*d*]benzo[1,2-*c*][1,2,5]thiadiazole-cored polymerized small-molecule acceptors with ordered backbone stacking and their application in all-polymer solar cells

Tiantian Wang, Jianhong Wei, Furong Shi,\* Hejie Wang,  
 Jinye He, Xudong Lv, Yuan Zhou, Pengzhi Guo,\*  
 Chenglong Wang and Yangjun Xia

16390



### A signal-amplified electrochemiluminescence immunosensor based on AgInZnS QDs with Au NPs/Co-ZnO NBs as a co-reaction accelerator for the detection of CA242

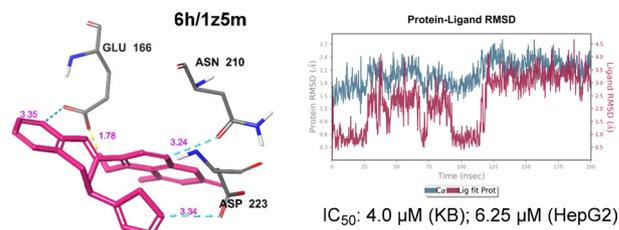
Jie Zhang, Baokun Han, Xiaofei Sun, Shuangna Wang,  
 Xinyue Wang, Yushu Lin, Yuying Liu, Feng Tang,\*  
 Qing Liu\* and Shujun Wang\*



16397

### Synthesis, antiproliferative activity, ADMET, molecular docking, molecular dynamics simulation, and DFT study for coumarin-based 1,5-benzothiazepines

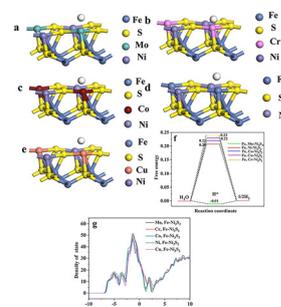
Duong Ngoc Toan,\* Dinh Thuy Van and Nguyen Dinh Thanh\*



16415

### Controllable synthesis of M and Fe co-doped Ni<sub>3</sub>S<sub>2</sub> (M = Mo, Cr, Co, Ni, Cu) catalysts for efficient urea oxidation and hydrogen production in urea electrolyte

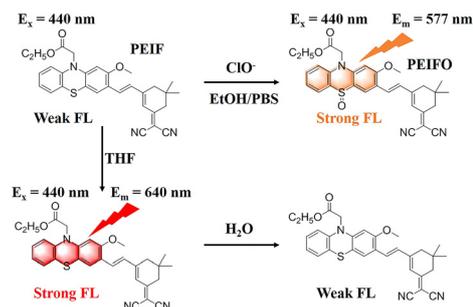
Fengchao Li, Xiaoqiang Du\* and Xiaoshuang Zhang



16423

### A novel dual-responsive fluorescent probe for moisture detection and hypochlorite sensing

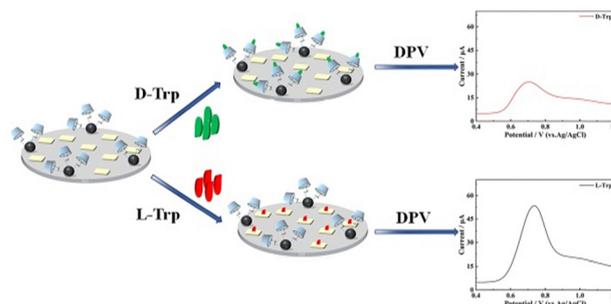
Yuehua Yuan, Siyi Shen, Chaoyi Yue, Mengqing Du, Yongjun Zhu, Yuzhen Wang, Feng Feng\* and Maozhong Tian\*



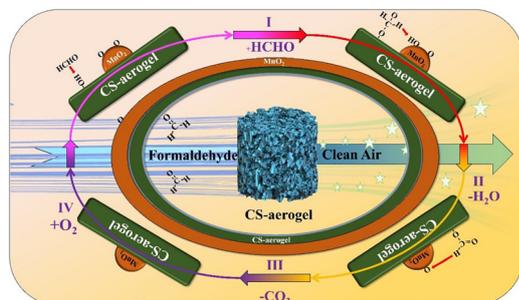
16433

### A sensitive electrochemical probe for the chiral identification of tryptophan isomers with carbon dot/chitosan composites

Mingfang Zhang, Fengxia Wang, Liang Ma, Xuewen Li, Yan Tang and Guang Yang\*



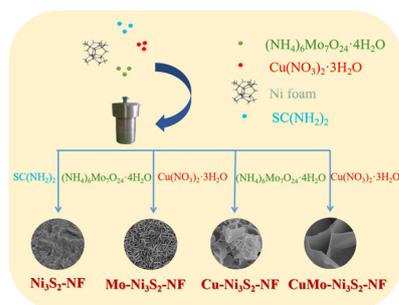
16444



### Cross-linker-free fabrication of chitosan–MnO<sub>2</sub> composite aerogels with synergistic adsorption-catalysis for high-efficiency room-temperature formaldehyde elimination

Yulong Fan, Wuyu Wang and Xuelai Zhao\*

16455



### A CuMo dual-doped Ni<sub>3</sub>S<sub>2</sub> porous ultrathin nanosheet as an efficient bifunctional electrocatalyst for urea–water electrolysis

Jiefei Li,\* Mingyang Song, Xianrong Meng and Xingyue Qi

