

IN THIS ISSUE

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Cover

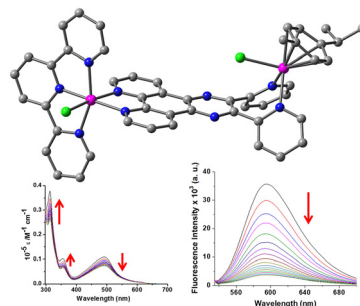
See Anwesha Mohanty and Srikanta Patra, pp. 15999–16007. Image reproduced by permission of Anwesha Mohanty and Srikanta Patra from *New J. Chem.*, 2025, 49, 15999.

PAPERS

15999

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

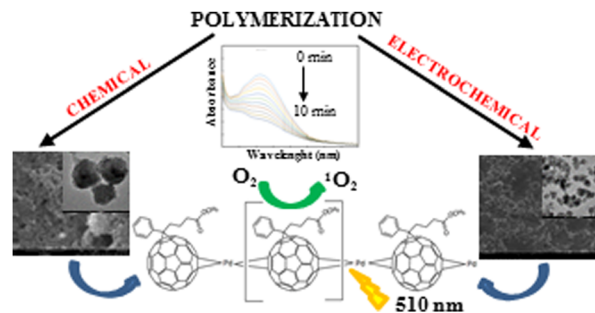
Anwesha Mohanty and Srikanta Patra*



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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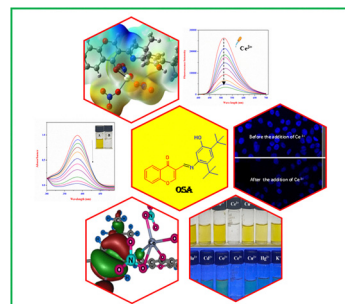
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16019

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

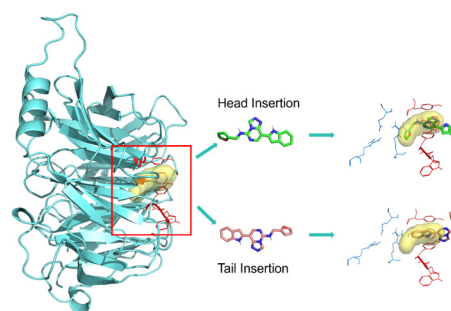
Saravana Kumar Prathiba, Karuppaiyan Kaviya, Ramar Rajamanikandan* and Kailasam Saravana Mani*



16029

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

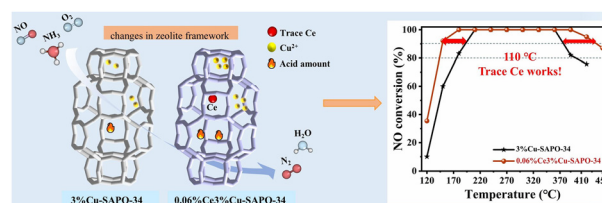
Lvzhou Zhu, Hao Zhang, Lipeng Xu, Pengyin Zhang, Jianan Ju, Shuai Yao, Yaming Shan* and Song Wang*



16044

Trace Ce-modified x%Ce3%Cu-SAPO-34 zeolites prepared by a one-pot method and applied for enhanced NH₃-SCR denitration activity

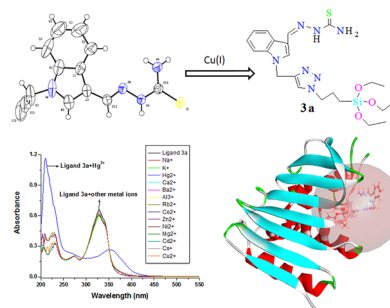
Min Qiang, Boyuan Chen, Yanhong Shao and Zhibin Li*



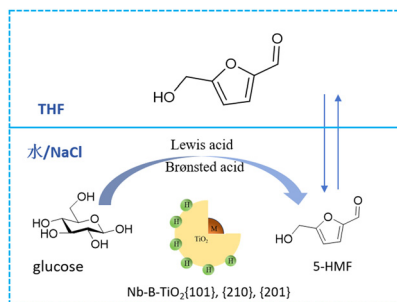
16056

'Click' generated indole appended thiosemicarbazone–triazole cojoined organosilane: a sensor for the recognition of Hg²⁺ 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



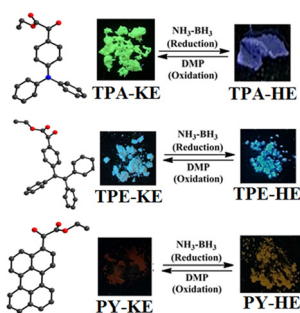
16070



Synergistic effect of metal-doped TiO₂ for glucose dehydration

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

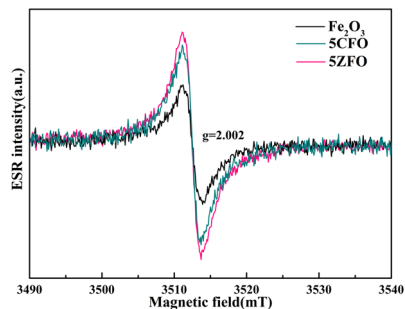
16075



Reversible fluorescence redox switching in activated carbonyl-functionalized fluorophores through the conversion of α -keto esters and α -hydroxy esters

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

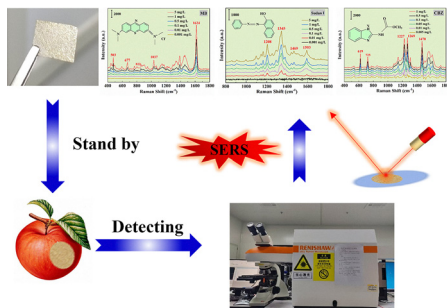
16086



Conversion of Fe₂O₃ 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

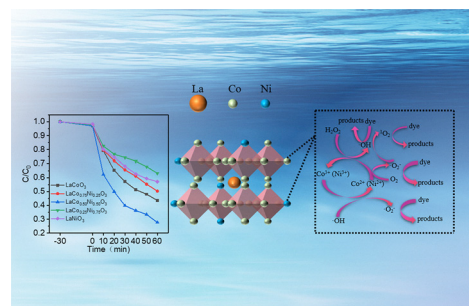
Yunpeng Shao,* Wenlong Deng, Yue Niu, Zicheng Zhang, Jiwei Song, Yuan Yao and Linyu Mei



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

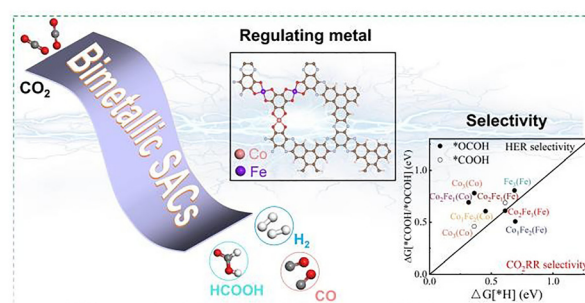
Han Zhang, Quanyu Suo, Ruiduo Zhao, Xia Zhang and Shushu Huang*



16113

Design of bimetallic single-atom catalysts and theoretical study of CO_2 reduction reaction

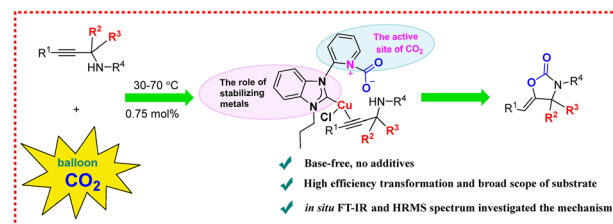
Yang Liu, Zhao-Di Yang* and Guiling Zhang



16122

Base-free catalytic systems achieved *via* the design of copper complexes: synthesis of 2-oxazolidinones from propargylic amines and CO_2

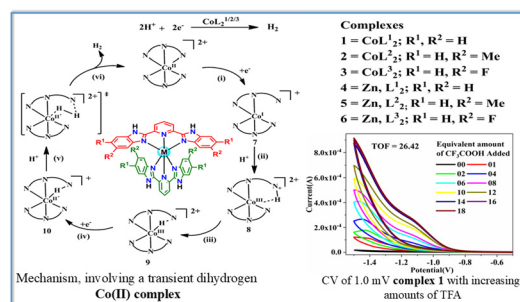
Sheng Tao, Zhi-Hong Du, Chun-Bo Bo, Min Li, Fei Chen* and Ning Liu*



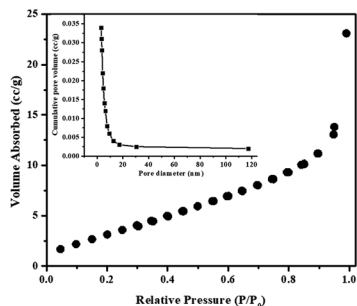
16134

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*



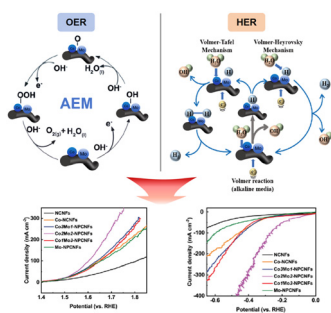
16145



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*

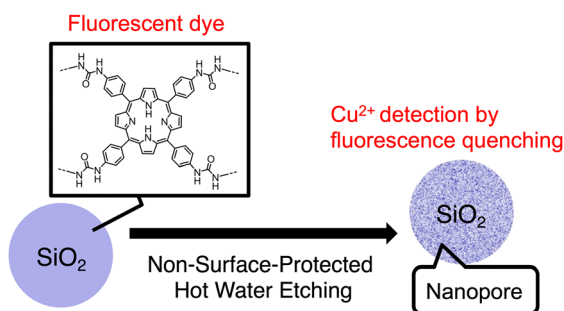
16160



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*

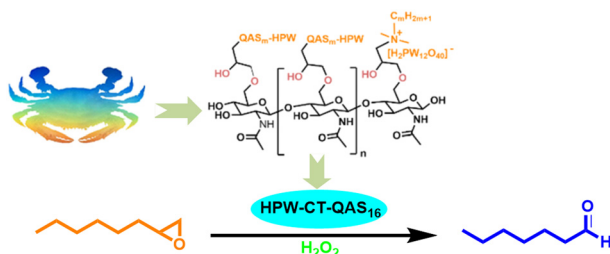
16172



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

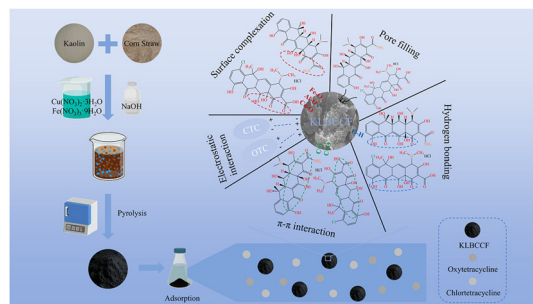
Tengfei Niu,* Xile Xia, Ziyi Wei, Xiao Yu and Zhongjian Tian*



16187

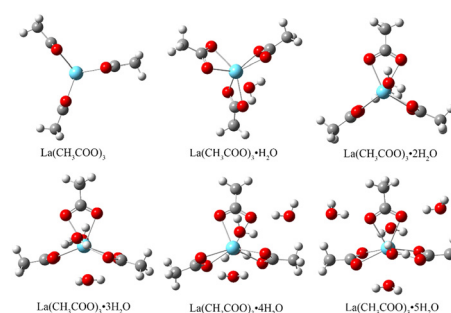
Study on the adsorption performance of modified kaolin/corn straw biochar for oxytetracycline and chlortetracycline

Yufei Liang, Lihong Zhao* and Liangbin Chen



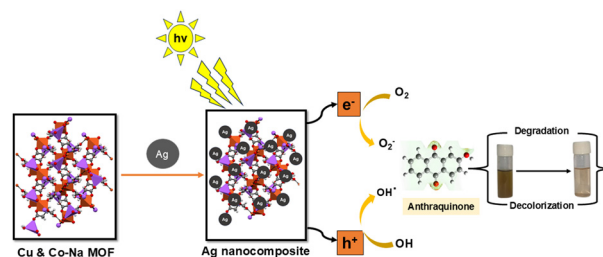
16199

The investigation of ion association characteristics in lanthanum acetate solution using density functional theory and molecular dynamics simulations

Caocheng Li, Wen Fang, Si Yang, Yuefei Zhang,*
Lian Zou, Fang Zhou* and Ruan Chi

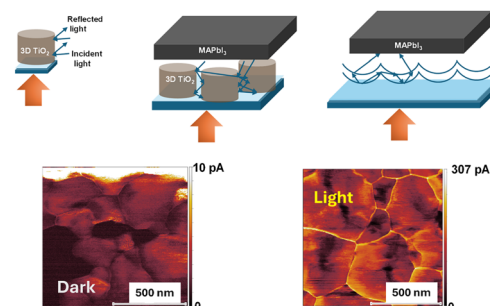
16213

Silver anchored Cu–Na and Co–Na atrane MOFs as photocatalysts for the visible-light-driven degradation and decolorization of a hydroxyanthraquinone dye

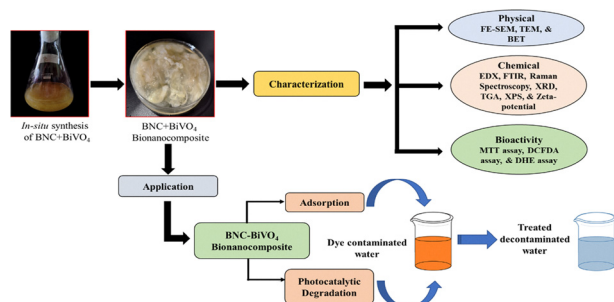
Sahil Sharma, Jyoti Rohilla, Sahil Thakur, Raghubir Singh*
and Varinder Kaur*

16226

Unveiling the nanoscale photocurrent behavior in perovskite films on photonic-structured TiO₂

Jenny Boane, Shrabani Panigrahi,* Tomás Calmeiro,
Edgar Coimbra, Ivan M. Santos, Elvira Fortunato,
Rodrigo Martins, Manuel J. Mendes* and Hugo Águas

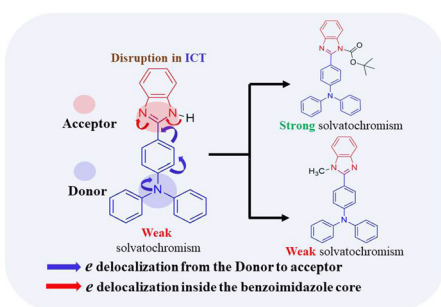
16235



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

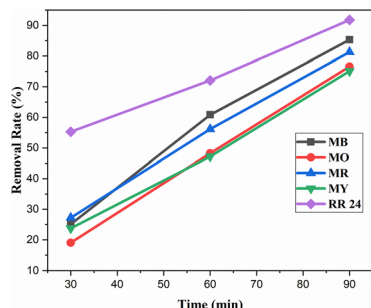
16256



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

Souvik Santra and Nikhil Guchhait*

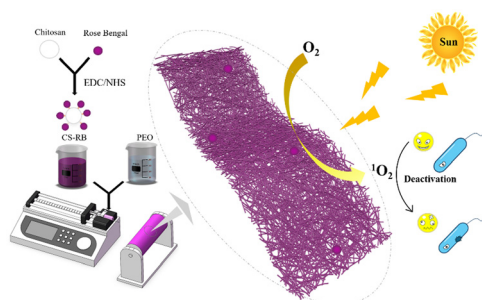
16271



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

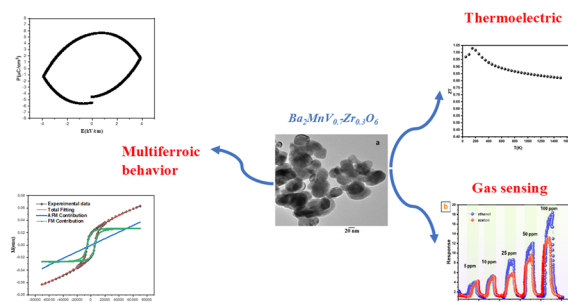
Ming Huang, Yingfeng Wang,* Yuhuan Zhu, Maoli Yin, Zhipeng Ma and XiaoJuan Li*



16295

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

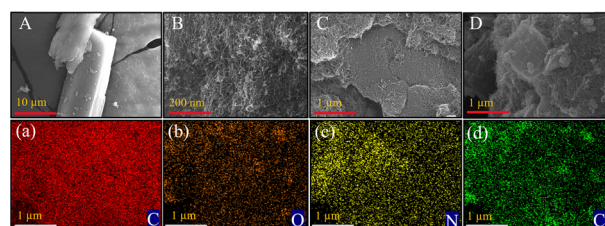
A. Mabrouki,* Olfa Messaoudi, Afrah Bardaoui, Amajd S. Aljaloud, Latifah Alfahid and E. Dhahri



16307

A novel electrochemical biosensor based on a heterojunction-structured COF/ Co_3O_4 /MWCNT: enabling the detection of dopamine and uric acid in complex matrices

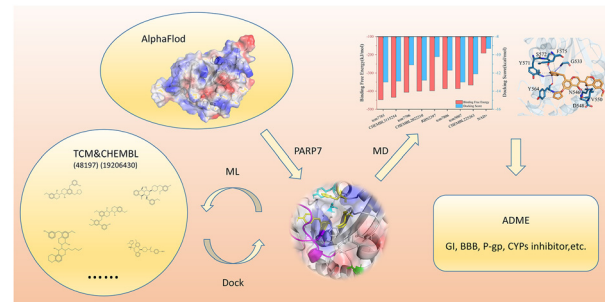
Ya-Xin Li, Dong-Mei Ma,* Xing-Ming Zhao,* Jun Xiang, Fu-Fa Wu and Rong-Da Zhao



16320

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

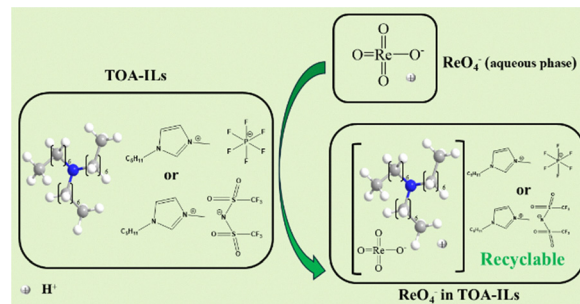
Xiaochen Yang, Baolin Liu and Daixi Li*



16333

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

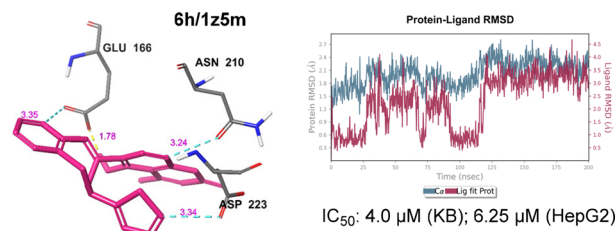
Dawei Fang, Jia Li, Jie Yang, Donglu Fu,* Jie Wei* and Zongren Song*



16397

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

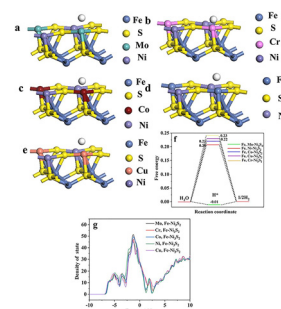
Duong Ngoc Toan,* Dinh Thuy Van and Nguyen Dinh Thanh*



16415

Controllable synthesis of M and Fe co-doped Ni₃S₂ (M = Mo, Cr, Co, Ni, Cu) catalysts for efficient urea oxidation and hydrogen production in urea electrolyte

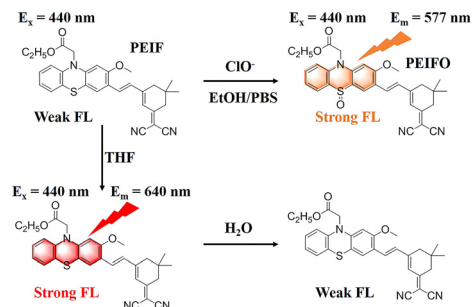
Fengchao Li, Xiaoqiang Du* and Xiaoshuang Zhang



16423

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

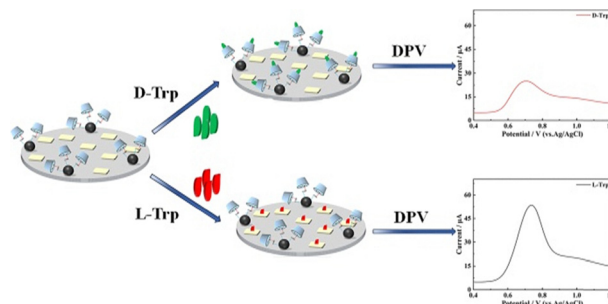
Yuehua Yuan, Siyi Shen, Chaoyi Yue, Mengqing Du, Yongjun Zhu, Yuzhen Wang, Feng Feng* and Maozhong Tian*



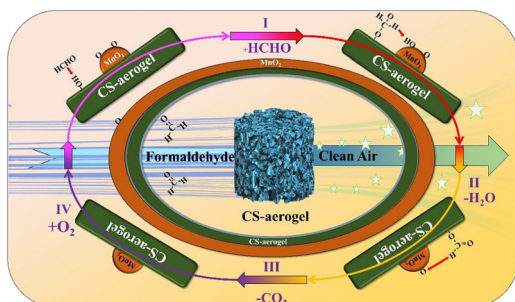
16433

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*



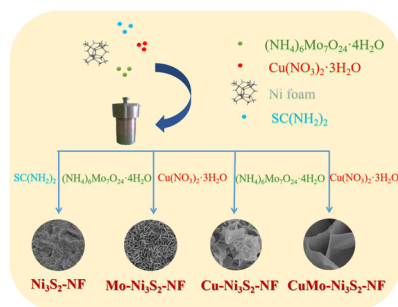
16444



Cross-linker-free fabrication of chitosan–MnO₂ 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 Ni₃S₂ porous ultrathin nanosheet as an efficient bifunctional electrocatalyst for urea–water electrolysis

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

