

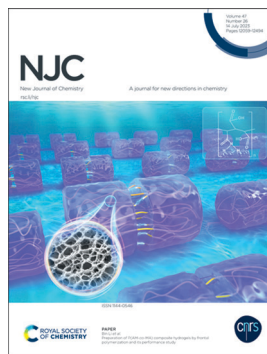
## IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 47(26) 12059-12494 (2023)



### Cover

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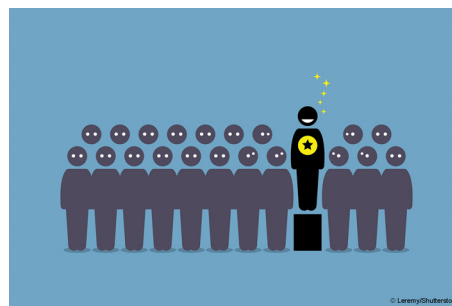
### Inside cover

See Bin Li *et al.*, pp. 12101–12108. Image reproduced by permission of Bin Li, Wenrui Hao, Jizhen Liu, Mengjing Zhou, Xiaojia Xu and Aolin Wu from *New J. Chem.*, 2023, 47, 12101.

## EDITORIAL

12074

### Outstanding Reviewers for *New Journal of Chemistry* in 2022

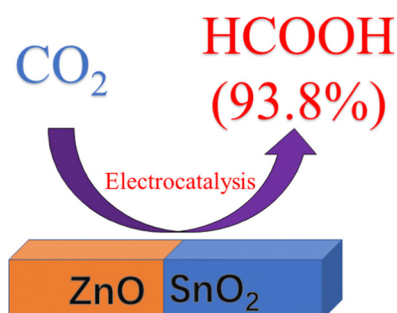


## COMMUNICATIONS

12075

### Highly selective reduction of CO<sub>2</sub> to HCOOH by a ZnO/SnO<sub>2</sub> electrocatalyst with heterogeneous interfaces

Jing-Nan He, Xin Ding,\* Qi Liu and Yan Gao\*



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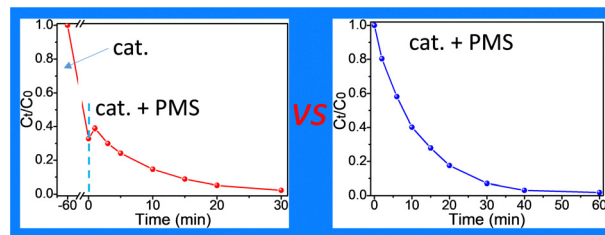


## COMMUNICATIONS

12080

### Insights into the degradation of organic pollutants via peroxymonosulfate activation over highly adsorptive carbon

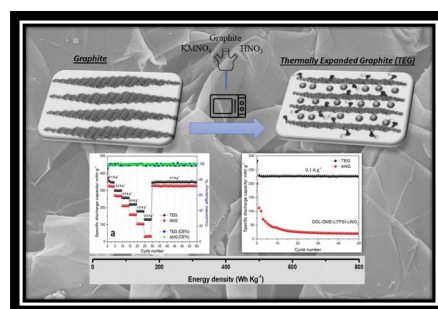
Shuchang Wu,\* Min Zhao, Zhijun Xia, Jiangyong Diao\* and Zilai Xie



12085

### Thermally expanded graphite: a promising anode electrode in the current and next-generation LIBs

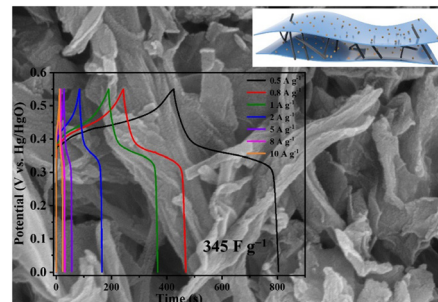
Sarmin Hamidi, Kasra Askari and Pejman Salimi\*



12089

### Fabrication of a 3D bacterial cellulose intercalated MoS<sub>2</sub>@rGO nanocomposite for high performance supercapacitors

Jingyang Tian,\* Ruihua Hao, Chundi Yang, Xiangbin Ge, Xueyang Tang, Zhirui Liu, Jingwei Wang, Minghui Cao, Yuanping Jiang and Chong Lin\*

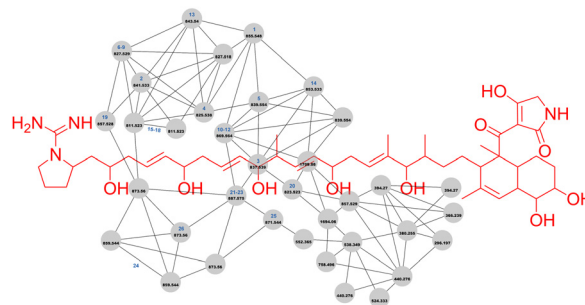


## PAPERS

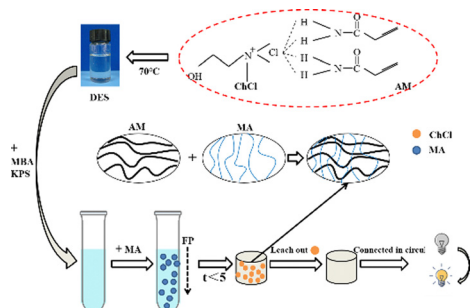
12093

### Dissecting the biosynthesis of the polyketide alkaloid lycdicamycin using a complex metabolic network

Heqian Zhang, Xiaojie Li, Shiyu Pan, Jiaquan Huang\* and Zhiwei Qin\*



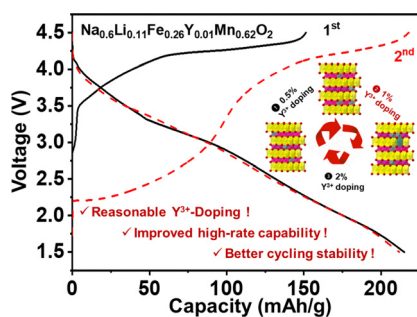
12101



### Preparation of P(AM-co-MA) composite hydrogels by frontal polymerization and its performance study

Bin Li,\* Wenrui Hao, Jizhen Liu, Mengjing Zhou, Xiaojia Xu and Aolin Wu

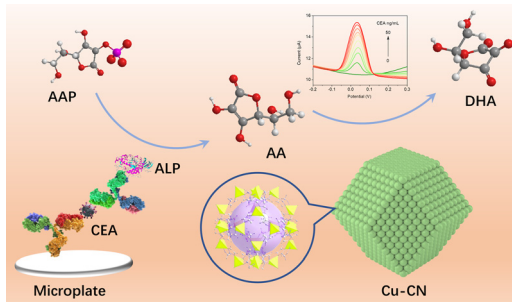
12109



### A Y-doped P2- $\text{Na}_{0.6}\text{Li}_{0.11}\text{Fe}_{0.27}\text{Mn}_{0.62}\text{O}_2$ cathode with improved high-rate capability and cycling stability for Na-ion batteries

Ming-Hui Cao,\* Ren-Yan Li, Fen-Fen Huang, Xin-Yin Cai, Miao Cui, Shi-Ya Lin, Jing-Yang Tian, Yuan-Ping Jiang, Zulipiya Shadike\* and Zheng-wen Fu\*

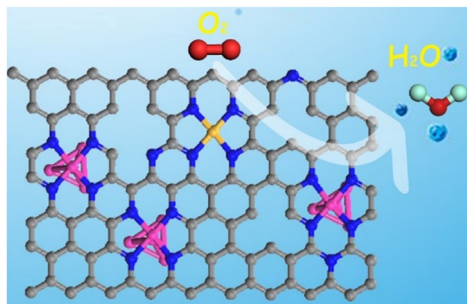
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### Electrochemical immunoassay based on an atomically Cu-dispersed nitrogen-doped carbon electrode for screening carcinoembryonic antigen

Chaoqun Huang, Yinan Li, Fan Cai, Hongbin Zhong, Fengling Zhang, Weimin Zhong, Lin Yao\* and Jiyi Huang\*

12123



### Secondary doping of Mn/Co bimetallic ZIF-derived catalysts for the oxygen reduction reaction

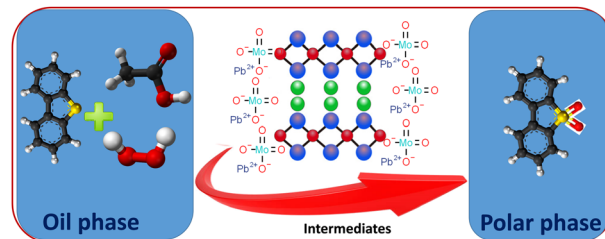
Lingli Guo, Yuekun Hu, Xiaowei Zhao, Xingkai Peng, Xinghua Zhang, Xiaofei Yu, Xiaojing Yang, Zunming Lu and Lanlan Li\*



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### Superior stability and activity of a $\text{PbMoO}_4/\text{BiOBr}$ nanocomposite for enhanced catalytic oxidative desulfurization of actual fuel

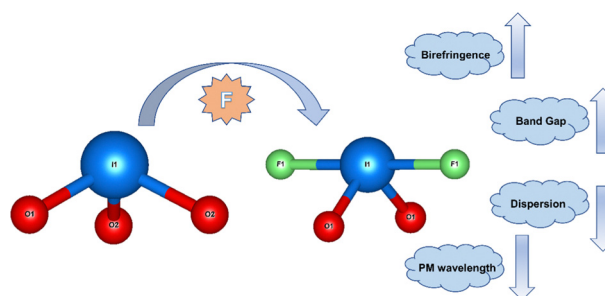
Asmaa. A. Abdelrahman, Heba M. Salem,\*  
Doaa. I. Osman and Abdelrahman M. Rabie\*



12145

### Enhancement of birefringence and refractive index dispersion optimization from iodates to fluorooxiodates

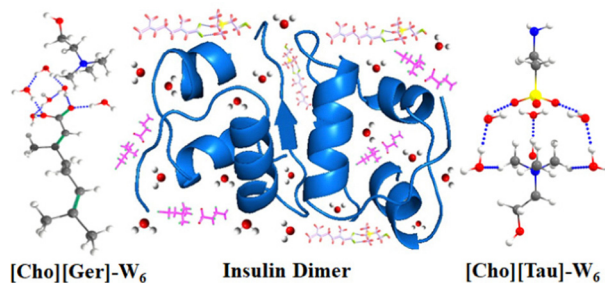
Shibin Wang, Jie Zhang, Jianbang Chen, Peng Han,  
Na Lei and Xuchu Huang\*



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### Effect of mixtures of ionic liquids and water on the structure and stability of the insulin dimer: a combined DFT and MD simulation study

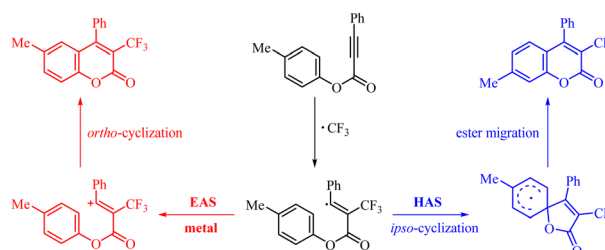
N. Giri Lakshman, S. M. Esther Rubavathy, S. Priyanka,  
K. Palanisamy and M. Prakash\*



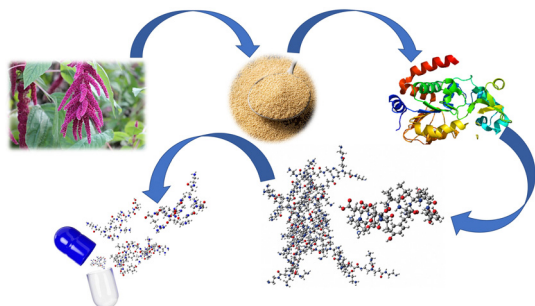
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### Mechanistic insight for tunable regioselective cyclization of aryl propiolates with radicals: *ipso-* versus *ortho-* cyclization

Meryem Fıstıkçı



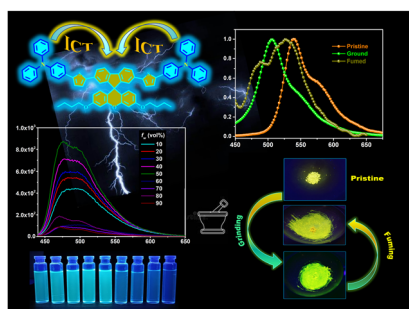
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### Theoretical–experimental prediction of the selectivity between polyamidoamine dendrimers and bioactive peptides derived from amaranth seeds

Alejandro Fajardo De La Rosa, Oscar Hernández-Meléndez, J. Manuel Saniger-Blesa, Ma. Inés Nicolás-Vázquez\* and Eduardo Bárzana\*

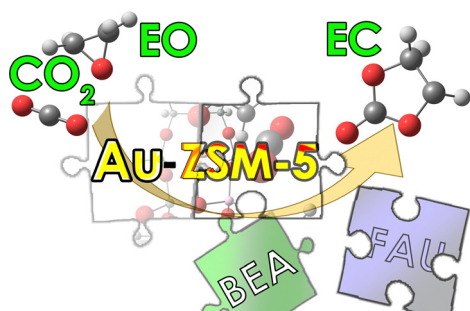
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### Rational design of spiro[fluorene-9,9'-xanthene] based molecule for aggregation induced emission (AIE) and mechanochromism (MC): synthesis and theoretical investigation

Babar Suraj Shivaji, Lal Chand, Jaipal Devesing Girase and Surya Prakash Singh\*

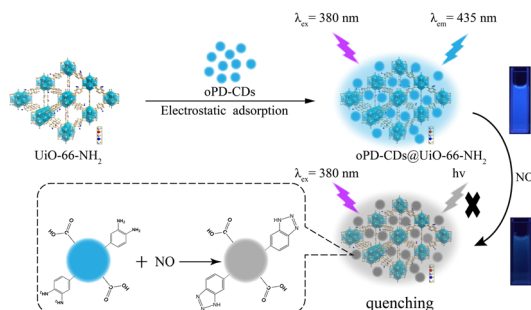
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### Effects of Lewis acid strength of monovalent coinage metals and zeolite frameworks on catalytic CO<sub>2</sub> cycloaddition with ethylene oxide: A DFT study

Winyoo Sangthong and Jakkapan Sirijaraensre\*

12200



### An oPD-CD doped zirconium-based metal–organic frame composite fluorescence probe for efficient and selective detection of nitric oxide

Botao Zhang, Liyun Ding,\* Yumei Zhang, Shiyuan Wang, Xingdong Jiang, Fei Ma and Jue Zhao



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## Producing green hydrogen in an efficient way using a nexus of a waste-biomass derived catalyst and a cost-effective & scalable electrode platform

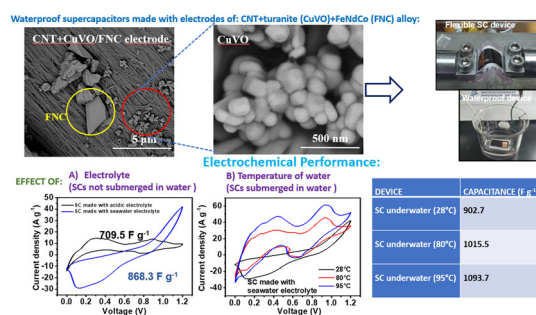
Kirti, Amravati S. Singh, Kinjal B. Patel, Ashish A. Patil, Ankush V. Biradar\* and Divesh N. Srivastava\*



12217

## CNT/turanite/FeNdCo-alloy electrodes to enhance the capacitance of waterproof/eco-friendly supercapacitors

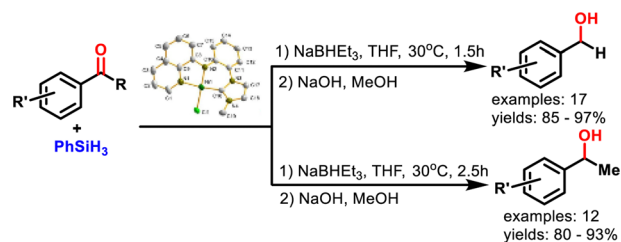
Marco Balderas-Soto, Edgar Giovanni Villabona-Leal, Anvar A. Zakhidov, Arturo I. Mtz-Enriquez, Pedro Salas, Andrea Molina, Horacio Flores-Zuñiga and Jorge Oliva\*



12229

## Synthesis of [CNN] pincer nickel(II) NHC chlorides and their catalytic effects on the hydrosilylation of aldehydes and ketones under mild conditions

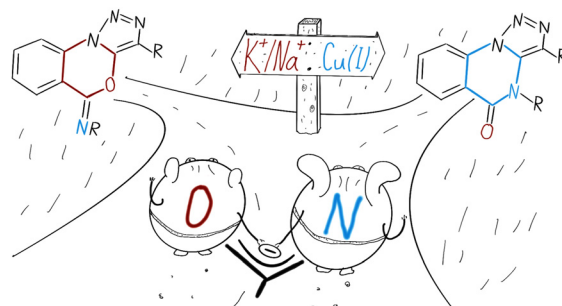
Shaobo Cao, Shangqing Xie, Qingshuang Li, Xiaoyan Li, Hongjian Sun,\* Olaf Fuhr and Dieter Fenske



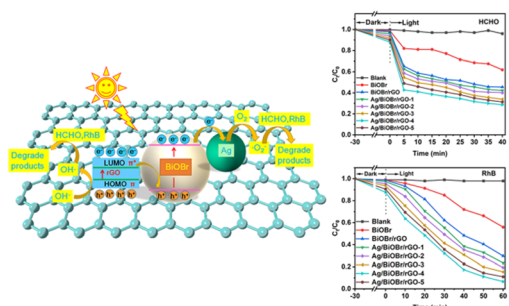
12239

## Divergent cyclization of 2-(5-iodo-1,2,3-triazolyl)benzamides toward triazole-fused lactams and cyclic imidates

Yury N. Kotovshchikov,\* Stepan S. Tatevosyan, Gennadij V. Latyshev,\* Zoya R. Kugusheva, Nikolay V. Lukashev and Irina P. Beletskaya



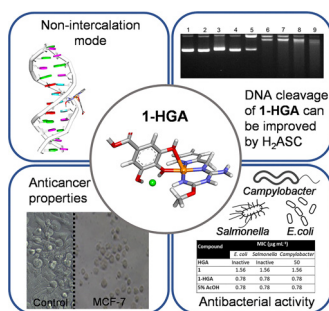
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### Ternary Ag/BiOBr/rGO nanoflower composite as a high-efficiency photocatalyst for formaldehyde and rhodamine B degradation

Gang Yan,\* Lijun Zhou, Baolin Yang, Hongliang Hu, Xiangwei Guo and Hongkai Zhao

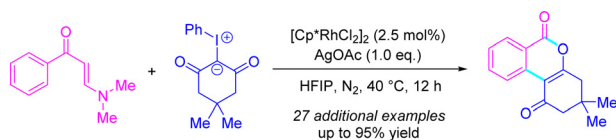
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### The effect of gallic acid on the copper(II) complex of *N*-(methylpyridin-2-yl)-amidino-*O*-methylurea: crystal structure, DNA interactions, *in vitro* cytotoxicity and antibacterial activity

Prangtip Nonkuntod, Jaurusup Boonmak, Thanaset Senawong, Chaiyaporn Soikum, Prapansak Chaveerach, Athis Watwiangkham, Suwit Suthirakun and Unchulee Chaveerach\*

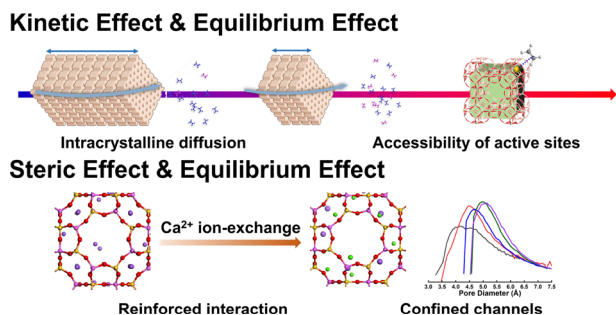
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### Rh(III)-catalyzed cascade annulation reaction of *N,N*-dimethyl enaminones with iodonium ylides to give substituted isocoumarins

Mingshuai Zhang, Longkun Chen, Donghan Liu, Zhuoyuan Liu, Jiuzhong Huang,\* Xiang Li\* and Fuchao Yu\*

12279



### Unraveling the separation mechanisms of the LTA zeolite depending on the regulated particle size and pore structure for efficient ethylene/ethane separation

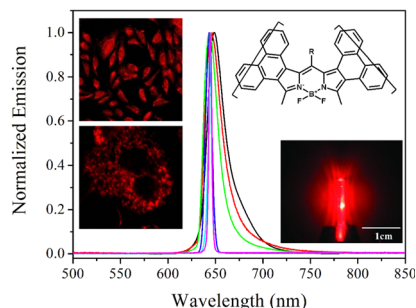
Chaowen Liu, Mudi Xin, Xuejing Zhang, Chunlu Wang, Limei Qiu and Guangtong Xu\*



12287

### A series of $\pi$ -expanded coplanar BODIPY dyes with deep-red emission: Synthesis, optical properties, and application in amplified spontaneous emission

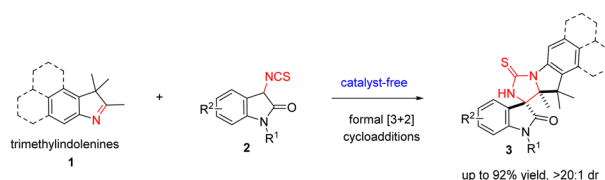
Yang Wang,\* Lei Xie, Qinning Sun and Liang Liu



12296

### Trimethylindolenines as C–N synthons for the assembly of spiro[oxindole-thioximidazolidine-indoline] hybrids in formal [3+2] cycloadditions

Wen-Hui Zhang, Zi-Yue Chen, Ren-Ming Liu, Xiong-Wei Liu, Bo-Wen Pan,\* Jian Zhou, Ying Zhou, You-Ping Tian and Xiong-Li Liu\*

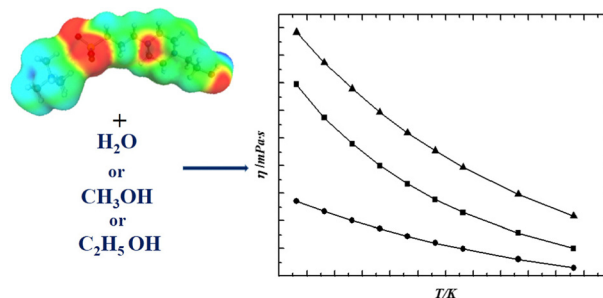


- The first example of trimethylindolenines serving as C–N synthons in [3+2] cycloadditions
- The creation of three crowded adjacent quaternary stereocentres on pent/hexacyclic spirocyclic structures

12304

### Mixtures of the [TMA][EPPS] ionic liquid with methanol, ethanol, or water: thermophysical properties and molecular interactions

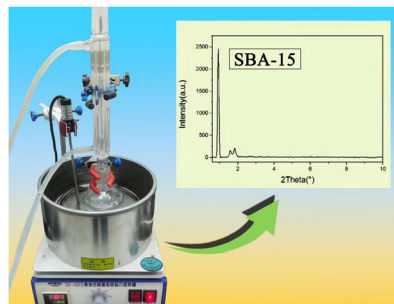
Asalil Mustain, Bhupender S. Gupta, Mohamed Taha\* and Ming-Jer Lee\*



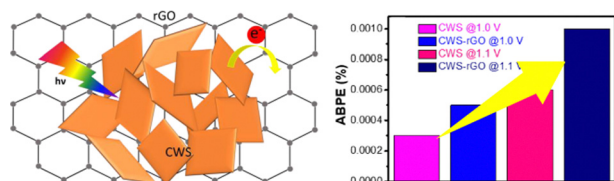
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### A reflux system for SBA-15 synthesis for the selective hydrogenation of cinnamyl aldehyde

Guofeng Wang, Wenwen Gao, Dong Yun,\* Chuanzhi Xu,\* Zhen Li\* and Chungu Xia



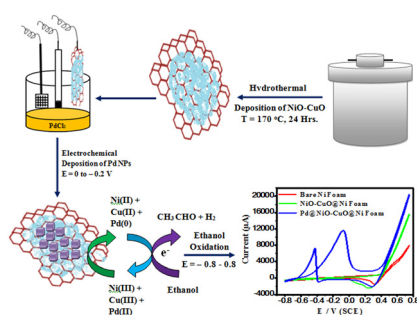
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### Reduced graphene oxide–copper thio tungstate composite for enhanced photoelectrochemical performance

Preeti Dagar and Ashok K. Ganguli\*

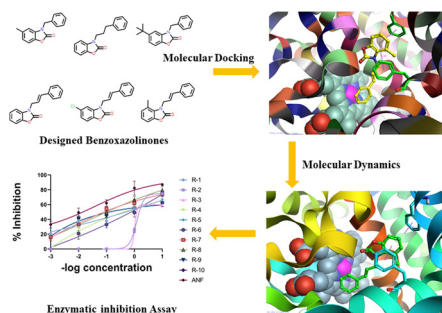
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### Highly dispersed Pd nanoparticles on NiO–CuO nanocomposite for efficient ethanol sensing

Jagdish C. Bhangoji, Ulka B. Suryavanshi,\*  
Gurudas P. Mane, Gurmeet C. Wadhawa,  
Nagesh D. Pawar and Suresh S. Shendage\*

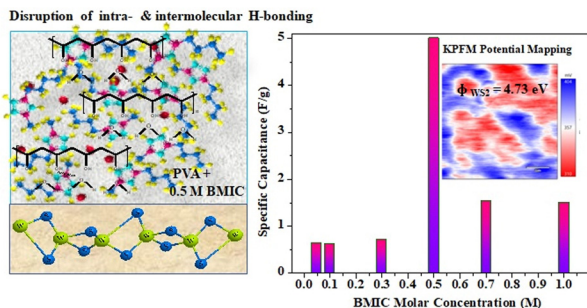
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### Identification of potential benzoxazolinones as CYP1B1 inhibitors via molecular docking, dynamics, waterswap, and *in vitro* analysis

Baddipadige Raju, Himanshu Verma, Gera Narendra,  
Gurleen Kaur, Subheet Kumar Jain and Om Silakari\*

12350



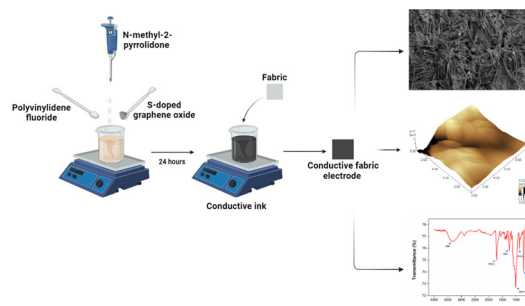
### Ionic liquid gel electrolyte with a WS<sub>2</sub> electrode for highly stable high-voltage solid-state supercapacitors

Priyanka Rani, Rajdeep Banerjee, Prama Adhya,  
Samit K Ray, Anupam Midya\* and Dipak K Goswami\*

12360

### Heteroatom-doped graphene oxide-based conductive ink: synthesis, characterization and investigation of the conductivity properties for flexible sensor technology

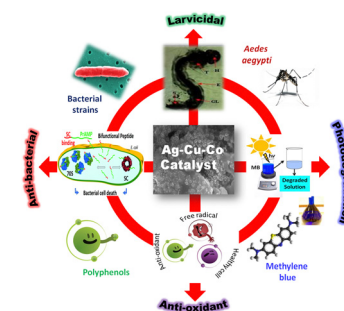
Selen Uruc, Ebrar Dokur, Rabianur Kurteli, Ozge Gorduk and Yu cel Sahin\*



12375

### Fabrication of a bifunctionalized *Calotropis gigantea* inspired Ag–Cu–Co trimetal oxide for the remediation of methylene blue, and its larvicidal and antibacterial applications

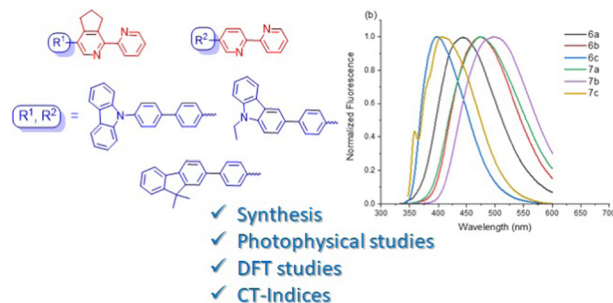
A. Nivetha, C. Sakthivel, J. Hemalatha, C. Senthamil and I. Prabha\*



12393

### Carbazole/fluorene-substituted 5-phenyl-2,2'-bipyridine D- $\pi$ -A fluorophores: photophysical data, hyperpolarizability and CT-indices

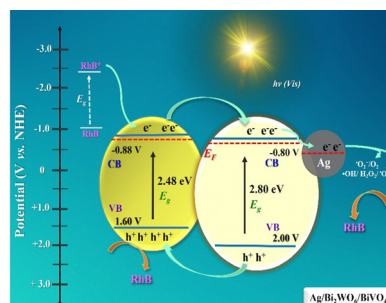
Ekaterina S. Starnovskaya, Maria I. Valieva, Rammohan Aluru, Dmitry S. Kopchuk, Albert F. Khasanov, Olga S. Taniya, Alexander S. Novikov, Alexey A. Kalinichev, Sougata Santra,\* Grigory V. Zyryanov and Brindban C. Ranu



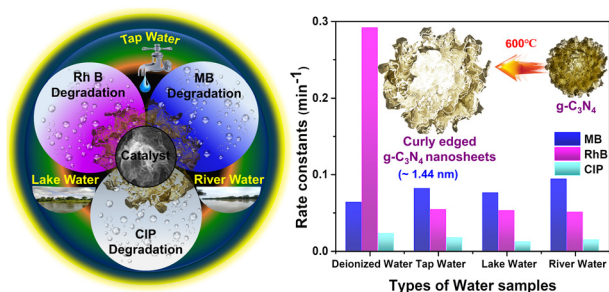
12403

### Visible-LEDs-induced photocatalytic activity of Bi<sub>2</sub>WO<sub>6</sub>/BiVO<sub>4</sub> heterojunctions prepared by a novel and green methodology

Sonia Judith Segovia-Sandoval, Esmeralda Mendoza-Mendoza,\* Araceli Jacobo-Azuara, Roberto Leyva-Ramos, Hiram Joazet Ojeda-Galván, Joelis Rodríguez-Hernández and Ignacio René Galindo-Esquivel



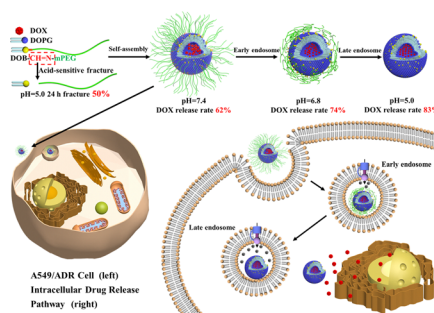
12418



### Unlocking the potential of thermally exfoliated ultrathin g-C<sub>3</sub>N<sub>4</sub> nanosheets: abundant active sites for enhanced solar photocatalysis

Suma Das, Swapnamoy Pramanik, Ranjith G. Nair\* and Avijit Chowdhury\*

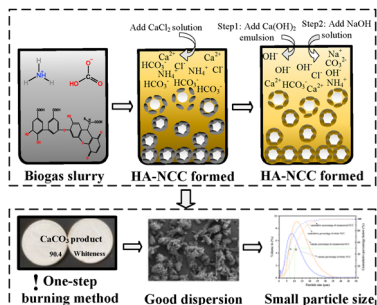
12431



### Acid-sensitive PEG-removable nanoscale liposomes for delivery of doxorubicin in A549/ADR therapy

Hailiang Chen, Chenyu Liu,\* Simiao Yu, Hengjun Zhou, Farishta Shafiq and Weihong Qiao\*

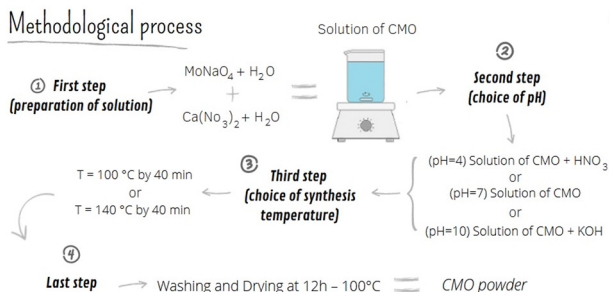
12445



### Macroscale preparation of nanosized calcium carbonate by exploiting biogas slurry synchronous metathesis encapsulation method

Fanghui Pan, Han Xiao, Fei Huang, Jingjing Lei, Hongguang Zhu\* and Jie Ma\*

12458



### Optical and electrical features of calcium molybdate scheelite solar cells

Ananda Ramires das Neves Stigger,\* Vinicius Fonseca Hernandes, Mateus Meneghetti Ferrer and Mario Lucio Moreira

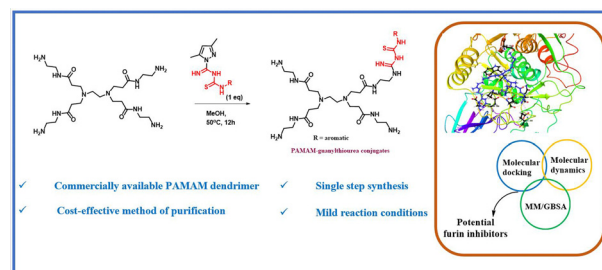


## PAPERS

12468

**PAMAM–guanylthiourea conjugates mask furin's substrate binding site: mechanistic insights from molecular docking and molecular dynamics studies assist the design of potential furin inhibitors**

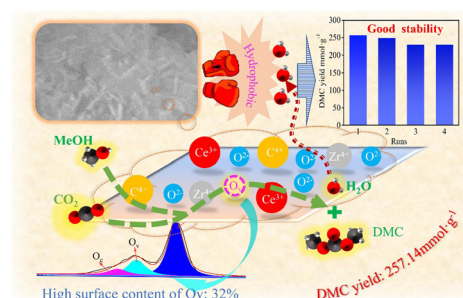
Chithra R. Nair and K. G. Sreejalekshmi\*



12477

**Hierarchically porous  $Ce_xZr_{1-x}O_2$  materials prepared by solvent volatilization for highly efficient synthesis of DMC from  $CO_2$  and methanol**

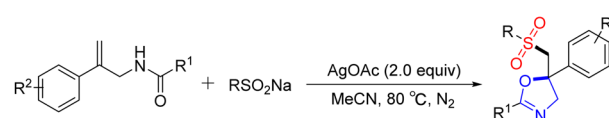
Guanling Yang, Haobo Wang, Aizhong Jia,\* Jingde Li and Yanji Wang



12487

**Silver-mediated radical cascade cyclization of *N*-allylamides with sodium sulfonates to access sulfonated oxazolines**

Zhichao Chen,\* Mu He, Hongmei Zheng, Wenting Weng,\* Lidan Sun\* and Xiaolan Xie



- facile and practical synthesis
- mild conditions
- good functional group tolerance

## CORRECTION

12492

**Correction: Triflic acid-catalyzed metal-free synthesis of (*E*)-2-cyanoacrylamides and 3-substituted azetidine-2,4-diones**

Bapurao D. Rupanawar, Santosh S. Chavan, Anil M. Shelke and Gurunath M. Suryavanshi\*

