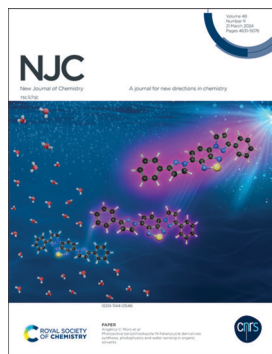


IN THIS ISSUE

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Cover

See Angélica V. Moro *et al.*, pp. 4680–4689.

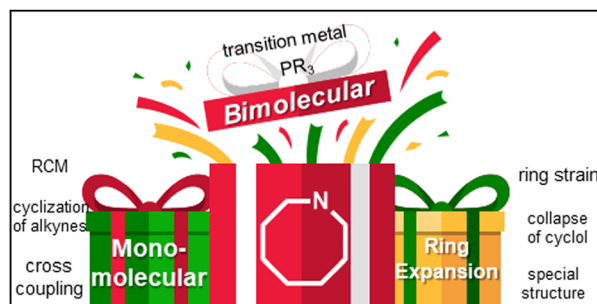
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PERSPECTIVE

4645

Recent progress in the construction of eight-membered nitrogen-heterocycles

Jia Li, Ziyang Dong and Changgui Zhao*

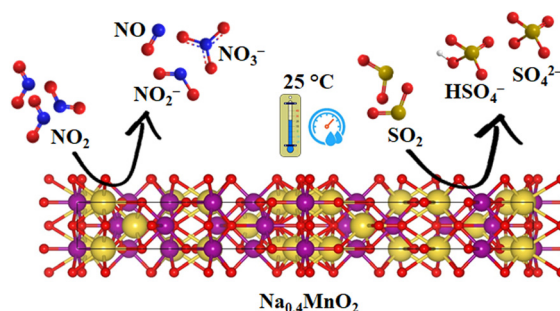


COMMUNICATIONS

4670

Chemisorption of SO₂ and NO₂ gas over Na_{0.4}MnO₂ in ambient conditions: an experimental and theoretical study

Nishesh Kumar Gupta,* Kaptan Rajput, Srungarpu N. Achary, Rushikesh P. Dhavale, Bijal R. Mehta, Debesh R. Roy and Kwang Soo Kim*



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COMMUNICATIONS

4675

Internal Coulombic assistance in intermolecular frustrated Lewis pair activation of dihydrogen

Alicia Rey Planells, Arturo Espinosa Ferao,*
Rainer Streubel* and Antonio Frontera

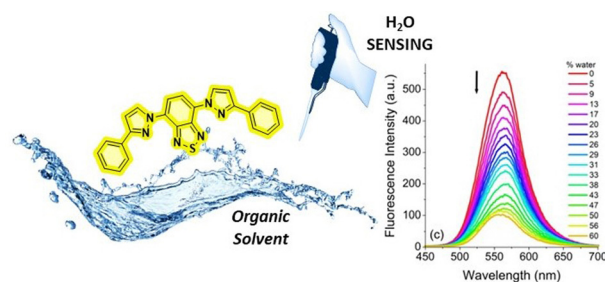


PAPERS

4680

Photoactive benzothiadiazole-N-heterocycle derivatives: synthesis, photophysics and water sensing in organic solvents

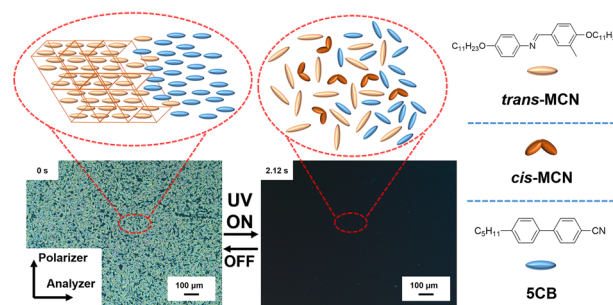
Camila P. Ebersol, Natali P. Debia, Hamilton C. Zimba,
Emmanuel S. Moraes, Diogo S. Lüdtkke,
Fabiano S. Rodembusch and Angélica V. Moro*



4690

Photoinduced solid-to-liquid transition of an *N*-benzylideneaniline derivative towards smart glass

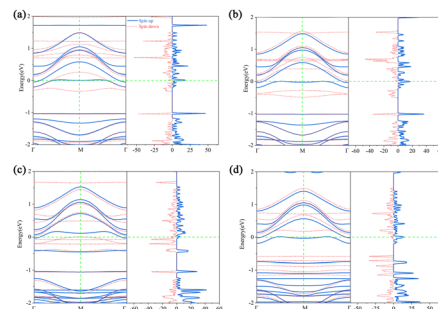
Jing Hu and Haifeng Yu*



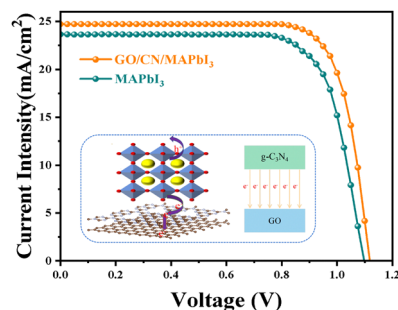
4699

Potential applications of C₂N-h2D/BN nanoribbon adsorption of transition metals in spintronic devices and magnetic storage devices

Zhihao Wang, Dong Fan, Maoye Yin, Hengshuai Li,*
Haiquan Hu, Feng Guo, Zhenbao Feng, Jun Li,
Dong Zhang, Zhi Li and Minghui Zhu



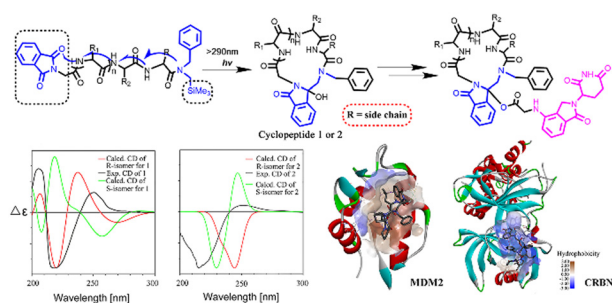
4708



A novel heterojunction layer-assisted interfacial defect control strategy for high-performance solar cells

Zihui Liang, Qiangqiang Cui, Yijun Zhou, Cheng Zeng, Fengxiang Chen, Li Zhao* and Changhai Yi*

4717

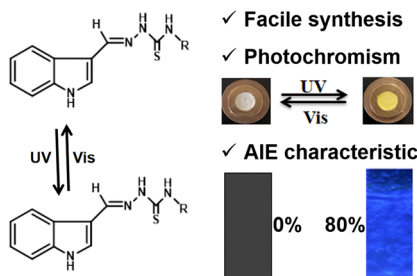


Design, synthesis, and anti-tumor activity of cyclic peptide–lenalidomide conjugated small molecules

Tingting Li, Tong Li, Xiong Zhang, Hongyu Xu, Yutian Xie, Rui Yan, Xiaodan Wu, Yingxue Jin* and Zhiqiang Wang*

4726

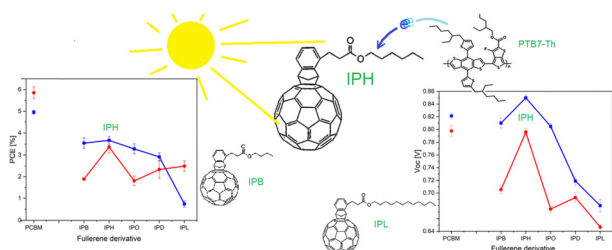
Indole thiosemicarbazone derivatives



Solid-state photochromic properties of indole thiosemicarbazones with aggregation-induced emission

Ying Cao, Yuanyuan Che, Lang Liu,* Yakun Tang and Yuming Yu

4735



Impact of the aliphatic side chain length on photovoltaic properties of fullerenes functionalized with 3-(1-indenyl)propionic acid esters

Piotr Piotrowski, Wojciech Mech, Andrzej Kaim, Rafał Bożek, Maria Kamińska and Krzysztof P. Korona

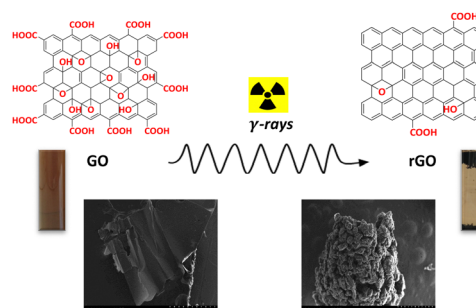


PAPERS

4749

Radiation induced reduction of graphene oxide: a dose effect study

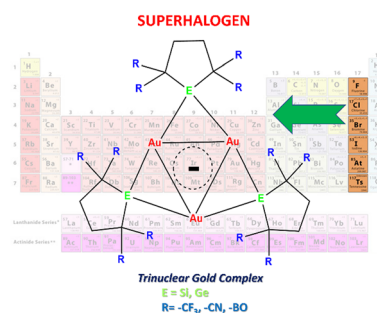
Souad Abou Zeid, Selma Bencherif, Rasta Ghasemi, Rituporn Gogoi, Yamina Chouli, Matthieu Gervais, Diana Dragoe, Jalal Ghilane, Prem Felix Siril and Samy Remita*



4765

Understanding the bonding and aromaticity of $[\text{Au}_3\{\text{C}_4\text{H}_4(\text{X})_4\text{E}\}_3]^-$ ($\text{X} = \text{CF}_3, \text{CN}, \text{BO}$; $\text{E} = \text{Si}, \text{Ge}$): trinuclear gold superhalogens

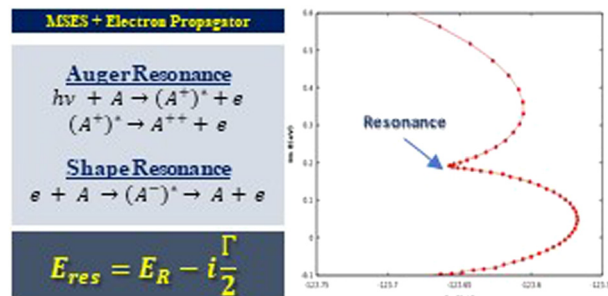
Subhra Das, Swapan Sinha, Gourisankar Roymahapatra, Mesias Orozco-Ic,* Gobinda Chandra De* and Santanab Giri*



4772

Use of the dilated electron propagator in conjunction with the modified smooth exterior scaling method to characterize $^2\text{S Be}^+ (1s^{-1})$, $^2\text{S Ne}^+ (1s^{-1})$ Auger and $^2\text{P Be}^-$ shape resonances

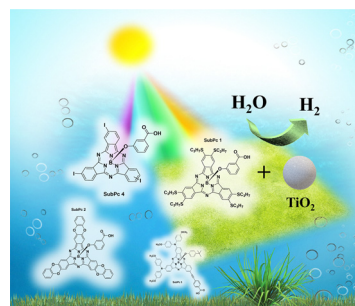
Mwdansar Banuary, Deepak Kumar and Ashish Kumar Gupta*



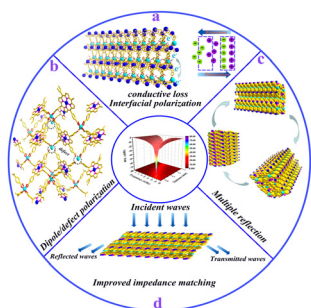
4783

Solar light-driven hydrogen evolution by co-catalyst-free subphthalocyanine-sensitized photocatalysts

Şifa Dogan, Buket Güntay, Perihan Kübra Demircioglu, Yigit Osman Akyıldız, Hasan Aydın, Emre Aslan,* Mustafa Can, Imren Hatay Patir* and Mine Ince*



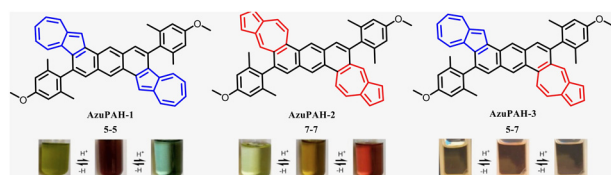
4789



Bimetallic porphyrin MOF derived CuIn particles/carbon composites as ideal microwave absorbers

Pan Pan,* Sheng Wang, Xuesong Wei, Guangjie Hu, Shihao Li, Mingming Li* and Yi-Si Feng*

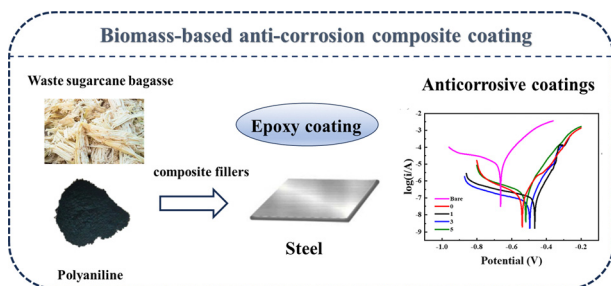
4801



Exploring C–C bond formation reactions for expanding azulene derivatives linked at the 2- and/or 6-positions

Pierre Mathey, Israel Fernández and Jean-François Morin*

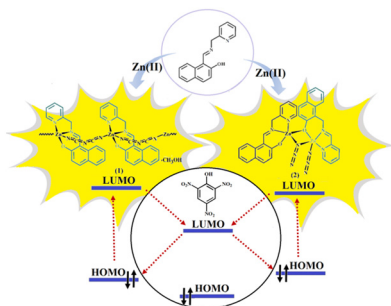
4810



Fabrication of polyaniline/waste sugarcane bagasse composite fillers for excellent anti-corrosion protective coatings

Sidi Yu, Yuansong Liu, Rongcan Mo, Ya Li, Zhongyang Zhou,* Liangkun Zhang, Bing Fan and Yuegang Cao

4821



Tridentate chelating ligand based fluorescent Zn(II) coordination compounds for highly selective detection of picric acid

Dama Saren, Ennio Zangrando, Horst Puschmann and Subal Chandra Manna*

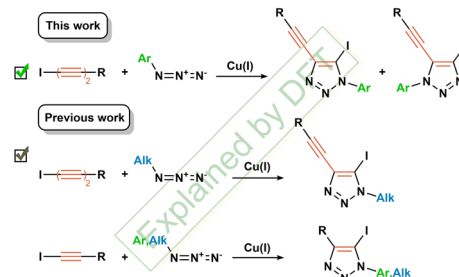


4831

Cu-catalyzed cycloaddition of aryl azides to 1-iodobuta-1,3-dienes: an experimental and quantum chemical study of unusual regiochemistry

Anastasia I. Govdi, Natalia A. Danilkina, Andrey A. Shtyrov, Mikhail N. Ryazantsev, Mia D. Kim, Mariya A. Kryukova and Irina A. Balova*

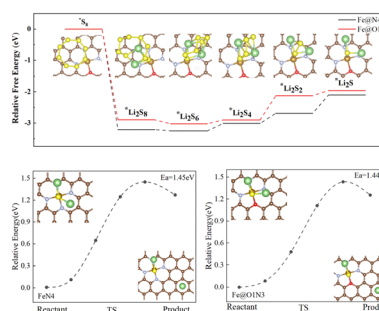
CuAAC Quiz: in which reaction(s) the regiochemistry is correct?



4846

Fe@ON₃ as an electrocatalyst for efficient sulfur reduction

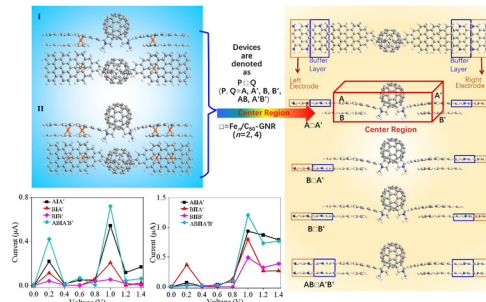
Jie Sun, Hongyi Zhang, Chengdong Wei, Hongtao Xue and Fuling Tang*



4854

NDR and spin-polarized transport properties of magnetic Fe sandwiched C₆₀-GNR single molecule devices: theoretical insight

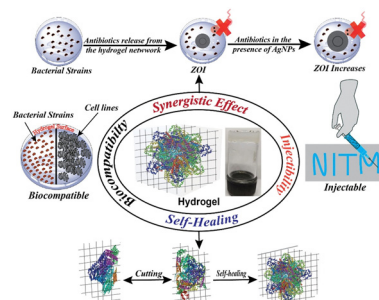
Xiaohui Liu, Yan Shang,* Yangyang Hu, Zhaodi Yang, Ya Wang, Lei Pei, Hong Yu, Munir Ur Rehman, Yuqi Dong, Lu Han and Guiling Zhang*



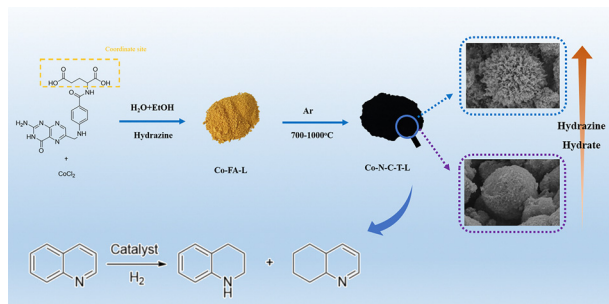
4865

A protein-based self-healing hydrogel for prolonged antimicrobial drug delivery with synergistic activity

Amarjyoti Mondal, Smarak Islam Chaudhury, Sona Lyndem, Subinoy Rana, Dasuklang Lyngdoh Nongbri, Kripamony Aguan and Atanu Singha Roy*



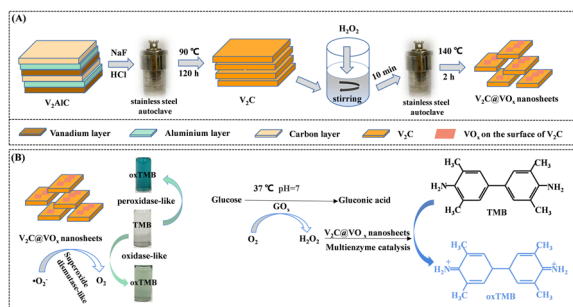
4880



Co–N–C catalysts derived from folic acid and mediated by hydrazine hydrate for selective hydrogenation of quinoline

Xuejiao Rong, Hua Li, Ligong Chen,* Binwei Yuan, Anni Guo, Zhaoshuo Jiang, Guoyi Bai and Bowei Wang*

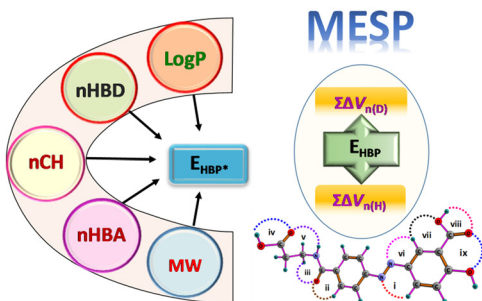
4886



Facile preparation of $\text{V}_2\text{C}@/\text{VO}_x$ nanosheets with excellent multi-enzyme activity and their colorimetric sensing application

Haiyan Wang,* Cheng Liu, Yue Zhao, Xinyu Luo, Pengjie Yin, Fuyou Du* and Guangsheng Zeng*

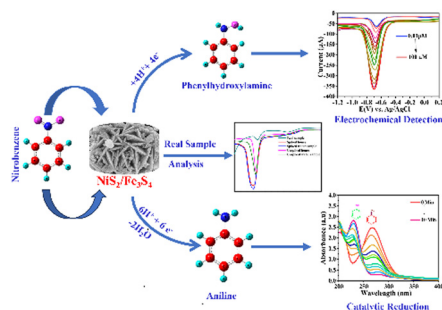
4896



Quantifying the hydrogen-bond propensity of drugs and its relationship with Lipinski's rule of five

Mambatta Haritha, Manikandan Sreerag and Cherumuttathu H. Suresh*

4909



Electrochemical detection and catalytic reduction of nitrobenzene using a bimetallic $\text{NiS}_2/\text{Fe}_3\text{S}_4$ magnetic heterostructure: an innovative approach for environmental remediation

Irfan Nazir, Zia Ul Haq, Arshid Bashir, Aaliya Qureashi, Firdous Ahmad Ganaie, Kaniz Fatima, Sheikh Irfan, Ghulam Nabi Dar and Altaf Hussain Pandith*

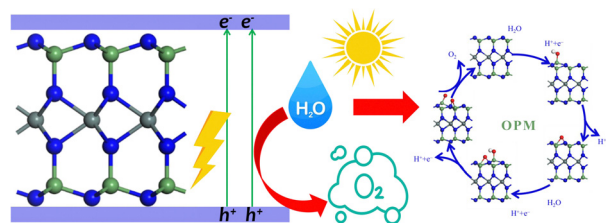


PAPERS

4922

Computational study of two-dimensional SnGe_2N_4 as a promising photocatalyst for the oxygen evolution reaction

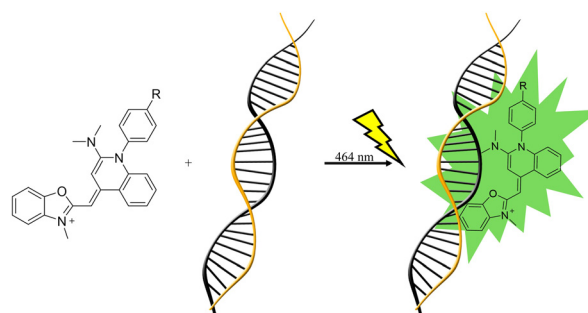
Noor Ul Ain, Arooba Kanwal, Abdul Jalil,* Chang-Fu Dee,* Tingkai Zhao, Syed Raza Ali Raza and Ishaq Ahmad



4931

Modifying the terminal phenyl group of monomethine cyanine dyes as a pathway to brighter nucleic acid probes

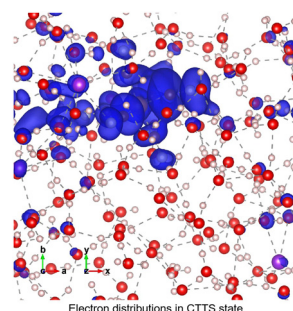
Johanna M. Alaranta, Arto M. Valkonen, Sailee S. Shroff, Varpu S. Marjomäki, Kari Rissanen and Tanja M. Lahtinen*



4936

Interpreting the charge transfer to solvent state in the photoionization of potassium ferrocyanide in an aqueous solution

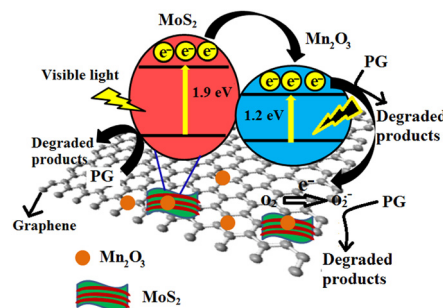
Zhijian Hu, Songqiu Yang,* Yan Zhang, Huaxin Liu, Hongming Yin and Jianyong Liu



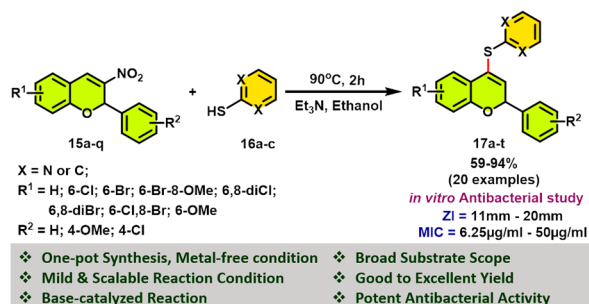
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MOF-derived Mn_2O_3 -decorated MoS_2 -graphene composite for visible light-assisted degradation of environmentally hazardous penicillin G in water

Md Rakibuddin* and Rajakumar Ananthakrishnan*



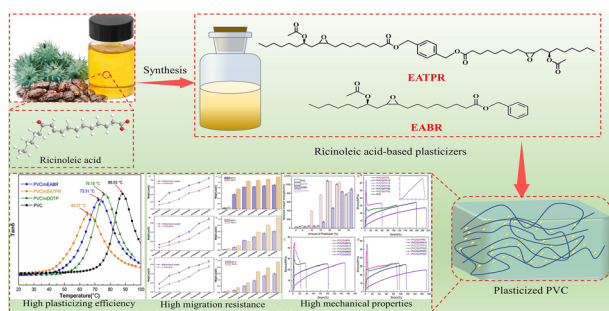
4953



Base catalyzed one-pot thia-Michael addition-oxidation reaction of hetero-aromatic thiols to 2-aryl-3-nitro-2H-chromenes and their antibacterial evaluation

Barsha Samanta, Bhabani Shankar Panda, Seetaram Mohapatra,* Sabita Nayak, Debdutta Bhattacharya and Chita Ranjan Sahoo

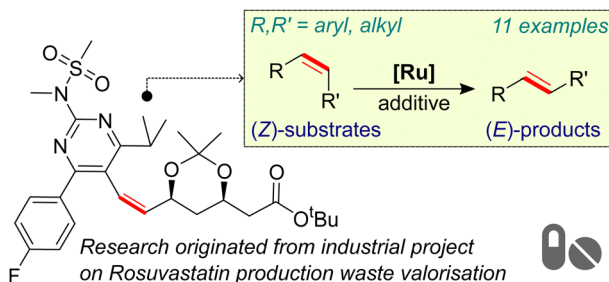
4960



Novel environmentally sustainable plasticizers based on ricinoleic acid for polyvinyl chloride: structure and properties

Y. Y. Jiang, F. X. Gao, L. Ren,* Q. Liu, T. Song, Y. D. Shen, W. N. Du, Y. B. Wang and M. Y. Zhang*

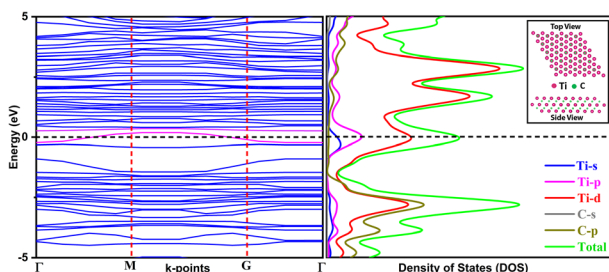
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From trials on rosuvastatin production waste valorization to development of new catalytic methods for Z → E isomerization of alkenes

Agata Tyszk-Gumkowska, Błażej Peta, Kamil Kosik, Emil Szepeński, Anna Kajetanowicz* and Karol Grela*

4982



Validating superior electrochemical properties of Ti₃C₂ MXene for supercapacitor applications through first-principles calculations

Sheheera Irfan, Yasir A. Haleem,* Muhammad Usman,* Naseeb Ahmad, Muhammad Arshad, Muhammad Imran Irshad, Muhammad Farooq Saleem, Muhammad Habib, Rashid Khan and Serdar Altin

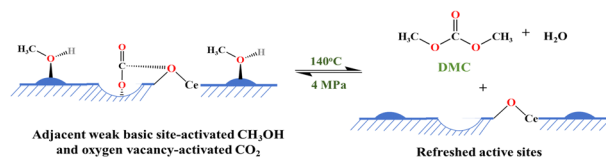


PAPERS

4995

Characterization of alkaline earth metal-doped CeO₂ nanocatalysts and their catalytic activities in the synthesis of dimethyl carbonate through a reaction between methanol and CO₂

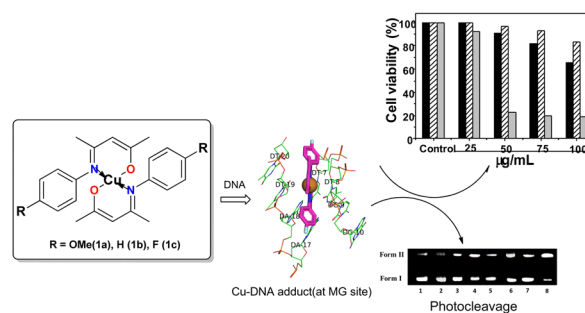
Aili Wang, Hao Wang, Mengyi Ji and Hengbo Yin*



5008

Evaluating the substitution effects of bis(β-iminoenolate)copper(II) complexes on their photophysical, DNA binding/photocleavage, and cytotoxic activities

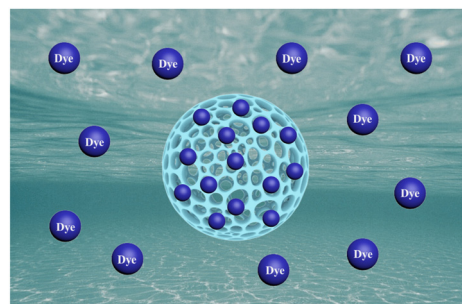
Panneerselvam Arun Prasanth, Periyappan Nantheeswaran, Kaliyan Prabakaran, Rajendran Senthilnathan, Faruck Lukmanul Hakkim, Arunachalam Jothi, Muthu Seenivasa Perumal, Veerappan Anbazhagan* and Mariappan Mariappan*



5018

Biomimetic seaweed absorbable membrane for dye adsorption in wastewater treatment

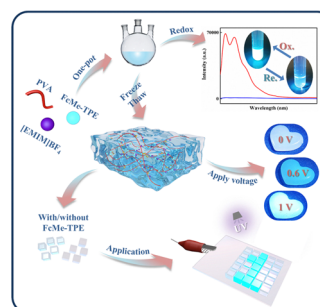
Chen Yang, Qinghong Zeng and Zhiguang Guo*



5025

Redox regulation of electrofluorochromic behavior for an AIEgen-doped PVA hydrogel based on a ferrocene derivate

Shang Zhang, Qihong Li,* Hao Liu, Xueshu Li, Xuemei Wang, Xueqin Du, Cuiling Lv, Zhaodong Wang,* Aixiang Li and Lin Niu





Thiago Galeote Tabuti, Lorena Portela Brazuna,
Joyce Gabrielle da Silva, Rebeca Bacani,
Rafael Garcia Candido, Josy Antevelli Osajima Furtini,
Carolina Ramos Hurtado, Dayane Batista Tada and
Eduardo Rezende Triboni*

Figure 1: Photocatalytic degradation of EUG and IEO.

Left: Bar Chart of % degradation at 240 min

| Photocatalyst | EUG (%) | IEO (%) |
|---------------|---------|---------|
| CuO-1 | ~75 | ~65 |
| ZnO-1 | ~78 | ~68 |
| CuO-2 | ~80 | ~70 |
| ZnO-2 | ~82 | ~72 |
| CuO-3 | ~85 | ~75 |
| ZnO-3 | ~88 | ~78 |
| CuO-4 | ~88 | ~78 |
| ZnO-4 | ~90 | ~80 |
| CuO-5 | ~92 | ~82 |
| ZnO-5 | ~95 | ~85 |

Right: Pie Chart of Opto-electrochemical parameters

| Parameter | CuO-1 | ZnO-1 | CuO-2 | ZnO-2 | CuO-3 | ZnO-3 | CuO-4 | ZnO-4 | CuO-5 | ZnO-5 |
|-------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| α | 76.32% | 23.0% | 99.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| β | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| γ | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| δ | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| ϵ | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| ζ | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| η | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| θ | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| ι | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| κ | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| λ | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| μ | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| ν | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| ξ | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| \omicron | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| π | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| ρ | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| σ | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| τ | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| υ | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| ϕ | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| χ | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| ψ | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| ω | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| φ | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| ϑ | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% | 98.33% |
| ϖ | 98.33% | 98.33% | | | | | | | | |

Photocatalytic evaluation of CuO and ZnO crystallites synthesized hydrothermally using binary eugenol/iso-eugenol mixtures: isomer effects on the capping propensity of biogenic agents

Tabee Jan, Shabnam Raheem, S. V. Sawant,
T. V. Manolikar, S. S. Sakate, S. K. Pardeshi, R. M. Jagtap*
and Masood Ahmad Rizvi*

Magnetically separable Ag@Fe₃O₄-GO nanocomposites for SERS detection, removal of organic pollutants and oil from water, and antibacterial applications

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A novel "off-on" peptide fluorescent probe for the detection of copper and sulphur ions in living cells

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Jing-cheng Hou, Jiang Wu* and Peng-cheng Lin*