

Dalton Transactions

An international journal of inorganic chemistry incorporating Acta Chemica Scandinavica
rsc.li/dalton

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

ISSN 1477-9226 CODEN DTARAF 53(15) 6475–6840 (2024)



Cover
See Zhao-Hui Zhou *et al.*,
pp. 6529–6536.

Image reproduced by
permission of Zhao-Hui Zhou
from *Dalton Trans.*, 2024, **53**,
6529.



Inside cover
Daniel B. Leznoff *et al.*,
pp. 6537–6546.

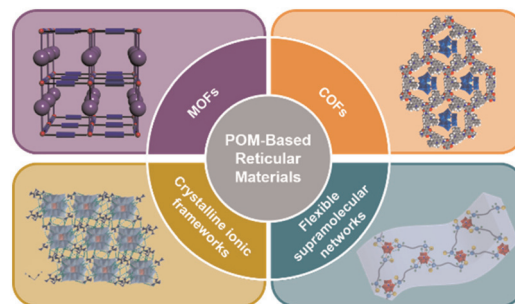
Image reproduced by
permission of Steven R. Kidd
from *Dalton Trans.*, 2024, **53**,
6537.

FRONTIER

6488

Polyoxometalate-based reticular materials for proton conduction: from rigid frameworks to flexible networks

Xiang Li, Shengchao Chai and Haolong Li*

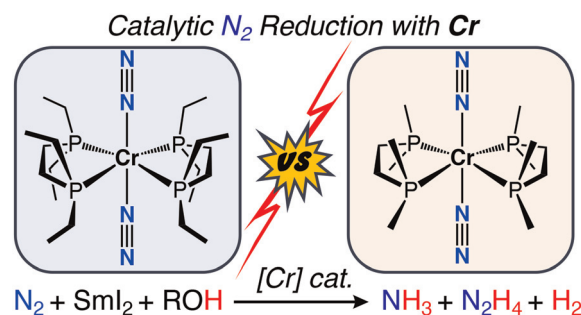


COMMUNICATIONS

6496

Catalytic dinitrogen reduction to hydrazine and ammonia using $\text{Cr}(\text{N}_2)_2(\text{diphosphine})_2$ complexes

Charles H. Beasley, Olivia L. Duletski,
Ksenia S. Stankevich, Navamoney Arulsamy and
Michael T. Mock*



Advance your career in science

with professional recognition that showcases
your **experience, expertise and dedication**

Stand out from the crowd

Prove your commitment
to attaining excellence in
your field

Gain the recognition you deserve

Achieve a professional
qualification that inspires
confidence and trust

Unlock your career potential

Apply for our professional
registers (RSci, RSciTech)
or chartered status
(CChem, CSci, CEnv)

Apply now

rsc.li/professional-development

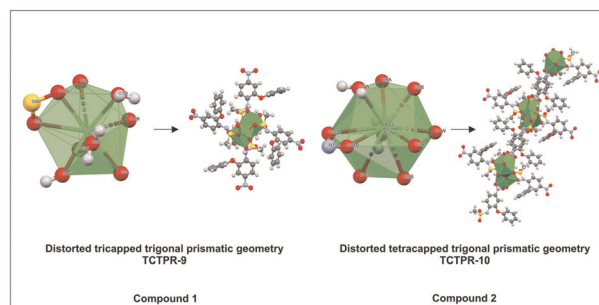


COMMUNICATIONS

6501

Structural insight and *in silico* prediction of the pharmacokinetic parameters and toxicity of alkaline earth metal compounds strontium and barium with the non-steroidal anti-inflammatory drug nimesulide

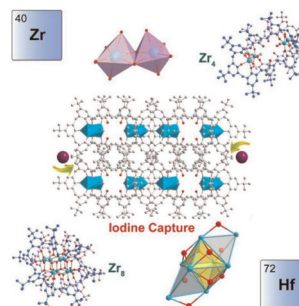
Małgorzata Rybczyńska and Artur Sikorski*



6507

Construction of zirconium/hafnium-oxo clusters based on a new protection-calix[8]arene

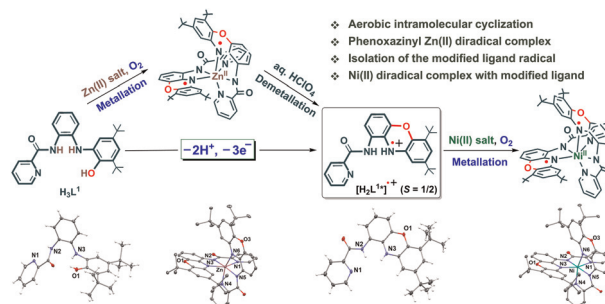
Fei-Fei Wang* and Baoshan Hou*



6515

Phenoxazinyl Zn(II) diradical complex formed via redox-driven cyclization of a 2-aminophenol-based N₃O ligand. Isolation of the modified N₃ ligand radical and its Ni(II) complex

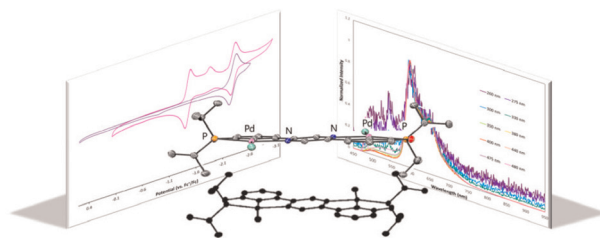
Narottam Mukhopadhyay, Arunava Sengupta, Francesc Lloret and Rabindranath Mukherjee*



6520

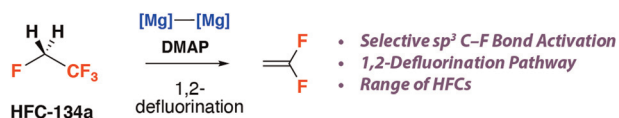
A bis(PCN) palladium pincer complex with a remarkably planar 2,5-diarylpyrazine core

Derek W. Leong, Yanwu Shao, Zhen Ni, Nattamai Bhuvanesh and Oleg V. Ozerov*



COMMUNICATIONS

6524

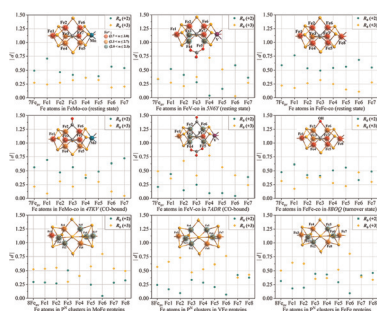


Defluorination of HFCs by a magnesium reagent

Daniel J. Sheldon, Joseph M. Parr and Mark R. Crimmin*

PAPERS

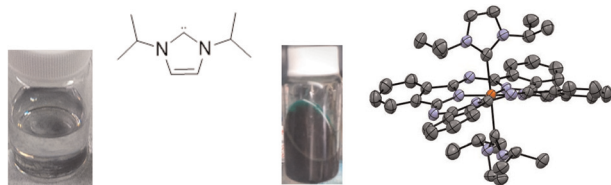
6529



Analyses of the electronic structures of FeFe-cofactors compared with those of FeMo- and FeV-cofactors and their P-clusters

Zhen-Lang Xie, Wan-Ting Jin and Zhao-Hui Zhou

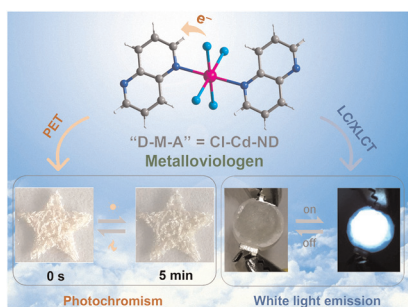
6537



Inducing ring distortions in unsubstituted metallophthalocyanines using axial N-heterocyclic carbenes

Steven R. Kidd, Wen Zhou, Jeffrey J. Warren* and Daniel B. Leznoff*

6547



Photochromism and single-component white light emission from a metalloviologen complex based on 1,5-naphthyridine

Ning-Ning Zhang,* Ya-Nan Zhang, Li Li, Zhen-Yu Li, Ya-Tong Liu, Yunyun Dong, Yong Yan* and Ming-Sheng Wang

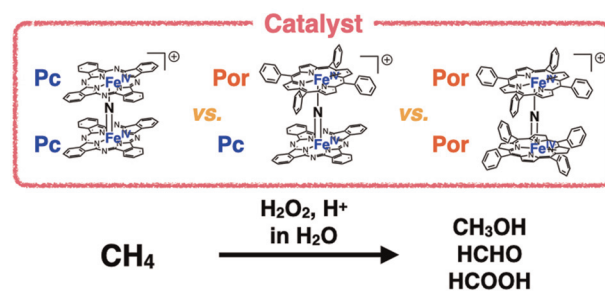


PAPERS

6556

Effect of porphyrin ligands on the catalytic CH₄ oxidation activity of monocationic μ -nitrido-bridged iron porphyrinoid dimers by using H₂O₂ as an oxidant

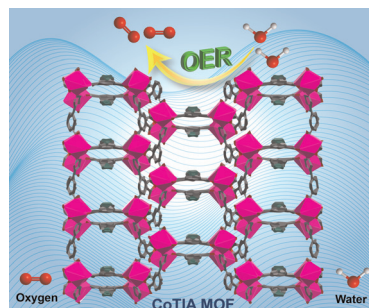
Yasuyuki Yamada,* Yusuke Miwa, Yuka Toyoda, Yoshiki Uno, Quan Manh Phung and Kentaro Tanaka*



6568

A series of isostructural metal–organic frameworks for an enhanced electro-catalytic oxygen evolution reaction

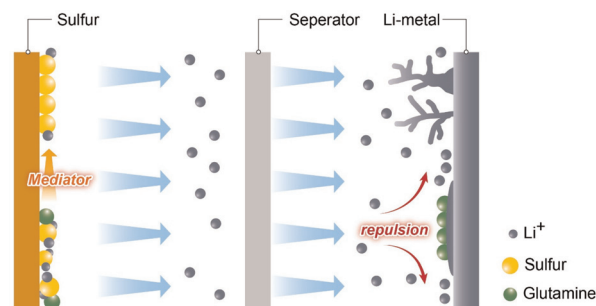
Pampa Jhariat, Abdul Kareem, Priyanka Kumari, Shafeeq Sarfudeen, Premchand Panda, Sellappan Senthilkumar and Tamas Panda*



6575

Cationic charge effect of glutamine repulsion adsorbate on Li metal surfaces for highly stable lithium–sulfur batteries

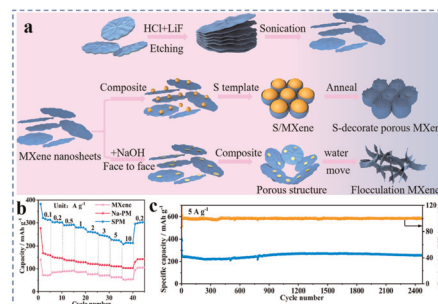
Chaehyeong Lee, Jin Won Kim and Jaeyoung Lee*



6583

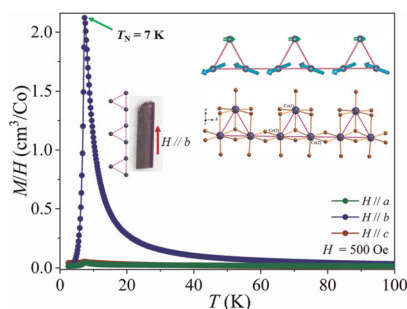
Efficient sulfur atom-doped three-dimensional porous MXene-assisted sodium ion batteries

Linlin Zhang, Yiguang Chen, Lianghao Yu,* Xin Tao, Lan Tang, Liangzheng Ye, Yu Liu, Lu Han, Hengzheng Li, Yihan Ling,* Guang Zhu* and Huile Jin



PAPERS

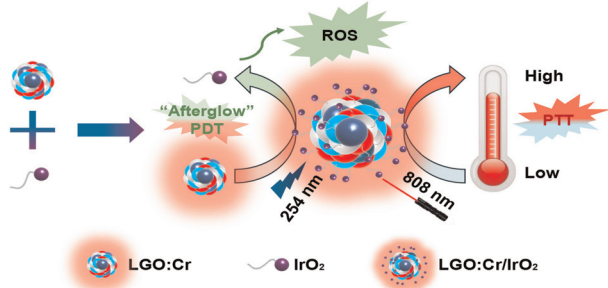
6592



Large magnetic anisotropy of a decorated spin-chain system $\text{K}_2\text{Co}_3(\text{MoO}_4)_3(\text{OH})_2$

Bhakti K. Patel, Feng Ye, W. L. N. C. Liyanage, C. Charlotte Buchanan, Dustin A. Gilbert, Joseph W. Kolis and Liurukara D. Sanjeewa*

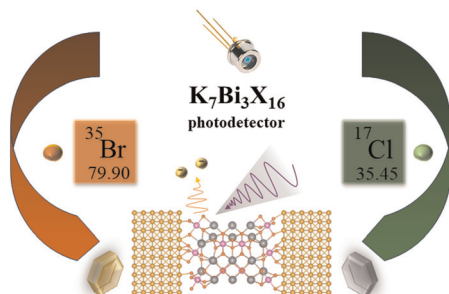
6601



A multi-functional nano-platform based on $\text{LiGa}_{4.99}\text{O}_8:\text{Cr}_{0.01}/\text{IrO}_2$ with near infrared-persistent luminescence, "afterglow" photodynamic and photo-thermal functions

Xiangyu Liu, Rujie Xi, Yanfang Hu, Yong Wang and Abdulkader Abdulkayum*

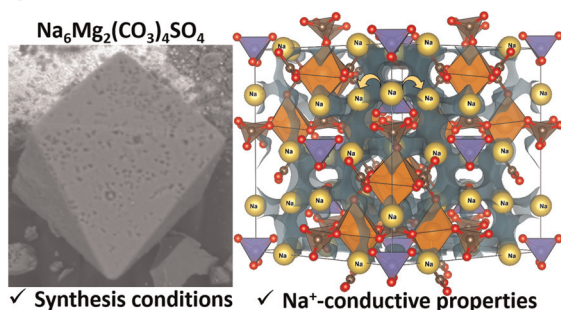
6609



Emerging lead-free all inorganic perovskite single crystals $\text{K}_7\text{Bi}_3\text{X}_{16}$ ($\text{X} = \text{Cl}, \text{Br}$) toward photodetector application

Wenjian Yang, Jingshen Zhang, Hui Xiong, Jing Lan, Songyang Yuan, Mengdi Zhan, Ziyu Tan, Wenzhe Li* and Jiandong Fan*

6618



Comprehensive study of the synthetic tychite, $\text{Na}_6\text{Mg}_2(\text{CO}_3)_4\text{SO}_4$: synthesis, structure and conductive properties

Alexander A. Shindrov* and Yelizaveta A. Morkhova*

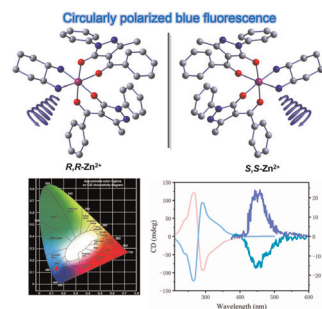


PAPERS

6625

Circularly polarized blue fluorescence based on chiral heteroleptic six-coordinate *bis*-pyrazolonate- Zn^{2+} complexes

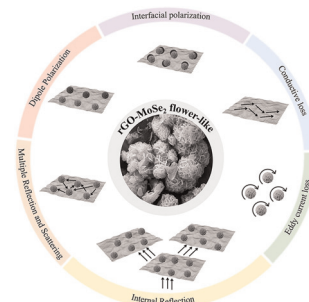
Jiaxiang Liu, Yuzhen Zhao, Zhe Zhang, Manni Li, Wenqi Song, Wentao Li* and Zongcheng Miao*



6631

Preparation of rGO/MoSe₂ nanocomposites for enhanced microwave absorption of whole X and Ku bands

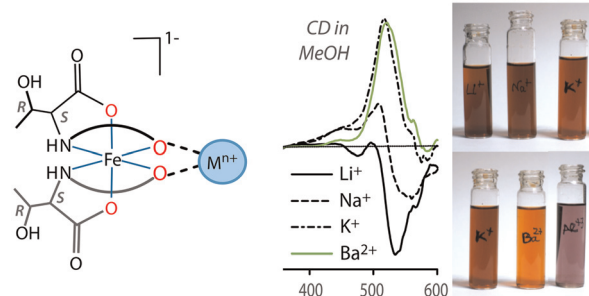
Farzad Farahmandzadeh, Hoda Hekmatara* and Mehdi Molaei*



6642

Water-soluble chiral coordination polymers of Li^+ , Na^+ , K^+ , and Ba^{2+} with an anionic iron(III) complex of a L-threonine derivative and a significant red shift of visible spectra with Al^{3+} salt

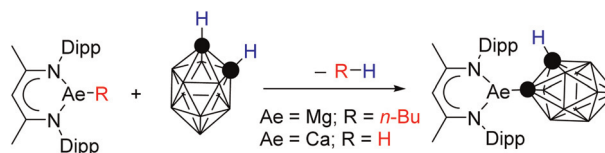
Chanreingam Long and Manabendra Ray*



6653

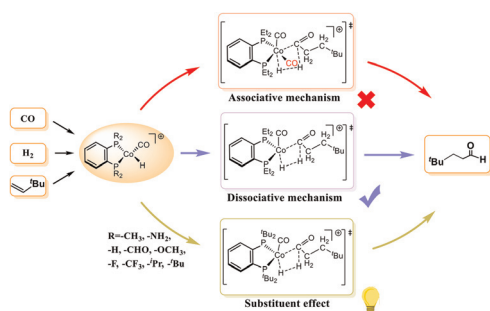
From alkaline earth to coinage metal carboranyls

Kyle G. Pearce, Louis J. Morris, Thomas P. Robinson, Andrew L. Johnson,* Mary F. Mahon and Michael S. Hill*



PAPERS

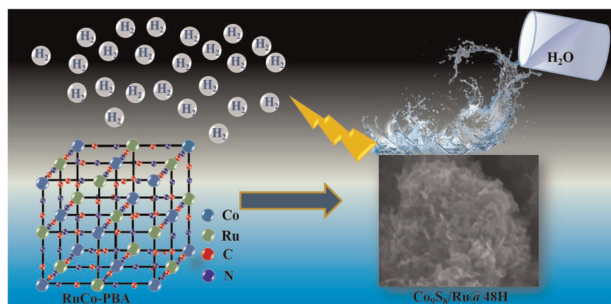
6660



Theoretical study on hydroformylation catalyzed by cationic cobalt(II) complexes

Shuo Zhang, Zhewei Li, Hexiang Qi, Yaqi Zhao, Yanhui Tang, Anqi Liu, Min Pu and Ming Lei*

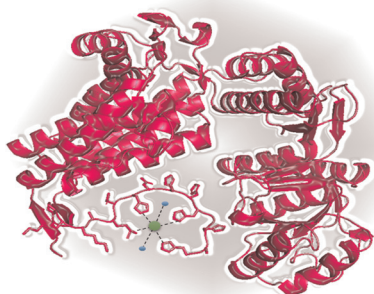
6667



Ruthenium-doped cobalt sulphide electrocatalyst derived from a ruthenium–cobalt Prussian blue analogue (RuCo-PBA) for an enhanced hydrogen evolution reaction (HER)

Manisha Sadangi and J. N. Behera*

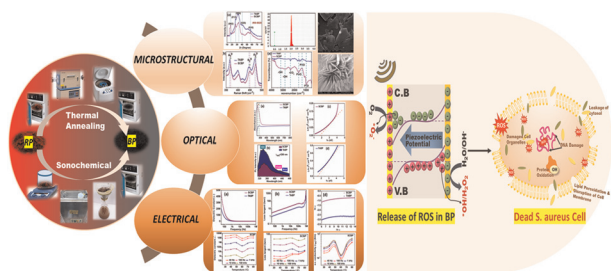
6676



Beyond copper: examining the significance of His-mutations in mycobacterial GroEL1 HRCT for Ni(II) complex stability and formation

Anna Rola, Arian Kola, Daniela Valensin, Oscar Palacios, Merce Capdevila, Elżbieta Gumienna-Kontecka and Sławomir Potocki*

6690



Sonochemically synthesized black phosphorus nanoparticles: a promising candidate for piezocatalytic antibacterial activity with enhanced dielectric properties

Piyali Halder, Indrajit Mondal, Neelanjana Bag, Alapan Pal, Somen Biswas, Souvik Sau, Biplab Kumar Paul, Dheeraj Mondal,* Brajadulal Chattopadhyay* and Sukhen Das*

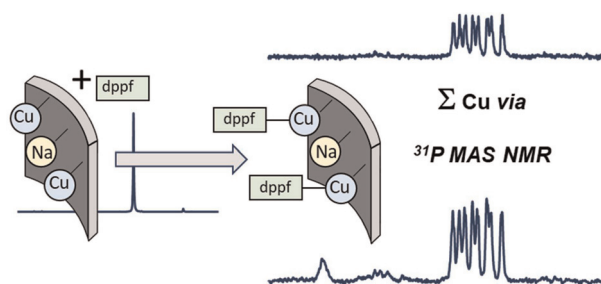


PAPERS

6709

Cu(dppf) complexes can be synthesized from Cu-exchanged solids and enable a quantification of the Cu-accessibility by ^{31}P MAS NMR spectroscopy

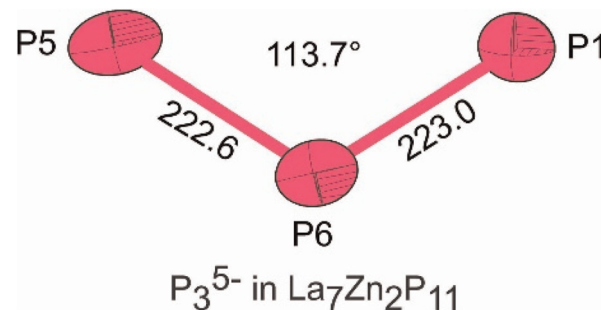
Elif Kaya, Daniel Dittmann, Maximilian Schmidt and Michael Dyballa*



6720

Triclinic $\text{La}_7\text{Zn}_2\text{P}_{11}$ with P_3^{3-} , P_2^{4-} , and P_3^{5-} units: a combined study by ^{31}P solid-state NMR spectroscopy and single crystal X-ray diffraction

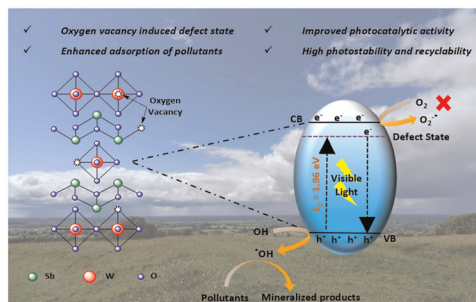
Jutta Kösters, Christopher Benndorf, Tobias Uesbeck, Thomas Wiegand, Hellmut Eckert,* Hannes Lincke and Rainer Pöttgen*



6731

Tuning of surface oxygen vacancies for enhancing photocatalytic performance under visible light irradiation in Sb_2WO_6 nanostructures

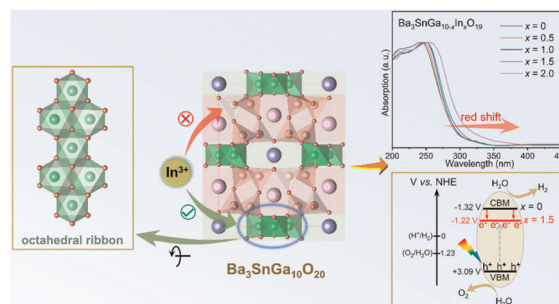
Manisha Sharma, Rahul Singh, Anitya Sharma and Venkata Krishnan*



6747

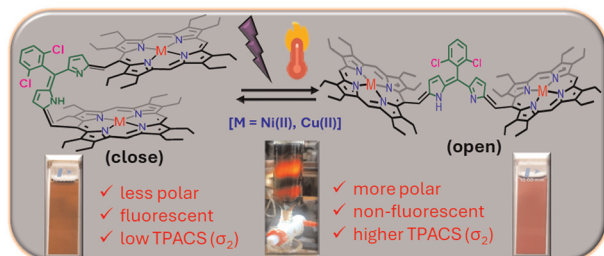
$\text{Ba}_3\text{SnGa}_{10-x}\text{In}_x\text{O}_{20}$ ($0 \leq x \leq 2$): site-selective doping, band structure engineering and photocatalytic overall water splitting

Weihua Li, Guangxiang Lu, Yanhong Ding, Rihong Cong* and Tao Yang*



PAPERS

6758



Reversible open–closed conformational switching of nano-size metalloporphyrin dimers triggered by light and temperature

Syed Jehanger Shah, Ajitesh Singh, Debabrata Goswami, Masatoshi Ishida and Sankar Prasad Rath*

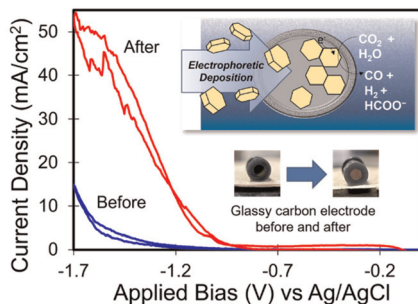
6766

Sample	Aspect
PSNa2S7	
PSNa2S5	
PSNa2S3	
PSNa2S1	
PSNa2S0,5	

Structure and morphology of red pigments based on sepiolite

I. Carrillo,* E. Atanes-Sánchez and F. Fernández-Martínez

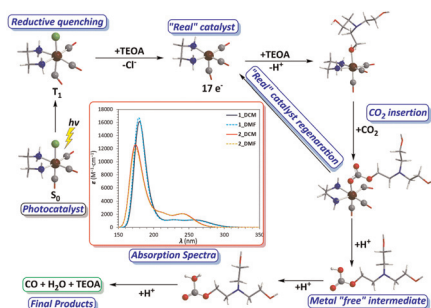
6779



Coordination of copper within a crystalline carbon nitride and its catalytic reduction of CO_2

Magnus Pauly, Ethan White, Mawuli Deegbey, Emmanuel Adu Fosu, Landon Keller, Scott McGuigan, Golnaz Dianat, Eric Gabilondo, Jian Cheng Wong, Corban G. E. Murphey, Bo Shang, Hailiang Wang, James F. Cahoon, Renato Sampaio, Yosuke Kanai, Gregory Parsons, Elena Jakubikova and Paul A. Maggard*

6791



Photocatalytic conversion of CO_2 to CO by Ru(II) and Os(II) octahedral complexes: a DFT/TDDFT study

Athanassios C. Tsipis* and Antonia A. Sarantou

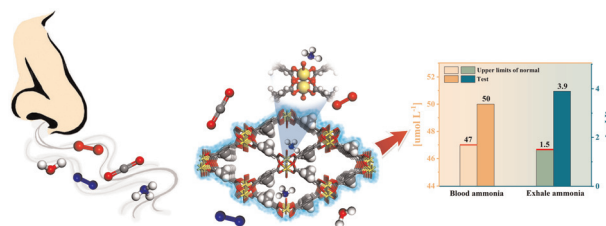


PAPERS

6802

Hydrophobic functionalization of a metal–organic framework as an ammonia visual sensing material under high humidity conditions

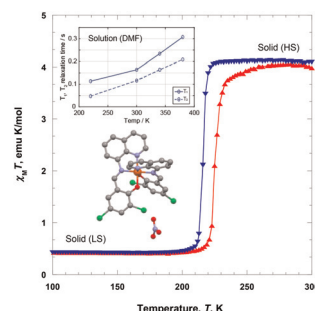
Yuxin Wang, Zhengxuan Song, Yutao Liu, Yang Chen, Jinping Li, Libo Li* and Jia Yao*



6809

Mononuclear Fe(III) complexes with 2,4-dichloro-6-((quinoline-8-ylimino)methyl)phenolate: synthesis, structure, and magnetic behavior

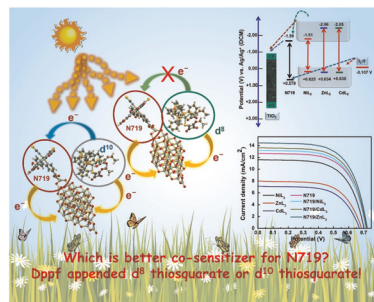
Ah Rim Jeong, Si Ra Park, Jong Won Shin,* Jihyun Kim, Ryuya Tokunaga, Shinya Hayami and Kil Sik Min*



6818

1,1'-Bis-(diphenylphosphino)ferrocene appended d⁸- and d¹⁰-configuration based thiosquarates: the molecular and electronic configurational insights into their sensitization and co-sensitization properties for dye sensitized solar cells

Aparna Kushwaha, Devyani Srivastava, Om Prakash, Gabriele Kociok-Köhn, Suresh W. Gosavi, Ratna Chauhan,* Mohd. Muddassir and Abhinav Kumar*



6830

Room temperature spin crossover properties in a series of mixed-anion Fe(NH₂trz)₃(BF₄)_{2-x}(SiF₆)_{x/2} complexes

Xinyu Yang, Alejandro Enriquez-Cabrera, Kane Jacob, Yannick Coppel, Lionel Salmon* and Azzedine Bousseksou*

