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 52(44) 16069-16540 (2023)



See Magdalena Rowińska-Żyrek et al., pp. 16140-16150.

Image reproduced by permission of Kinga Garstka and Magdalena Rowińska-Żyrek from Dalton Trans., 2023. 52. 16140.



Inside cover

See Adinarayana Doddi et al., pp. 16151-16158.

Image reproduced by permission of Adinaravana Doddi from Dalton Trans., 2023, 52, 16151.

PERSPECTIVE

16085

Recent advances in the nanoarchitectonics of metal-organic frameworks for light-activated tumor therapy

Huijuan Duan, Fang Wang, Weizhe Xu, Gang Sheng, Zhaogang Sun* and Honggian Chu*

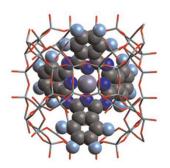


FRONTIER

16103

Zeolite encapsulated organometallic complexes as model catalysts

Ethan P. Iaia, Ademola Soyemi, Tibor Szilvási* and James W. Harris*



Editorial Staff

Executive Editor

Sally Howells-Wyllie

Deputy Editor

Mike Andrews

Development Editors Michelle Canning, Emily Cuffin-Munday

Editorial Production Manager

Susannah Davies

Publishing Editors

Debora Giovanelli, Helen Lunn, Samuel Oldknow, Kate Tustain

Editorial Assistant

Daphne Houston

Publishing Assistant Huw Hedges

Publisher

Jeanne Andres

For queries about submitted articles please contact Susannah Davies, Editorial Production Manager in the first instance. E-mail dalton@rsc.org

For pre-submission queries please contact Sally Howells-Wyllie, Editor. Email dalton-rsc@rsc.org

Dalton Transactions (electronic: ISSN 1477-9234) is published 48 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road Cambridge, UK CB4 0WF.

All orders, with cheques made payable to the Royal Society of Chemistry, should be sent to the Royal Society of Chemistry Order Department, Royal Society of Chemistry Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK

Tel +44 (0)1223 432398; E-mail orders@rsc.org

2023 Annual (electronic) subscription price: £4441; US\$7972. Customers in Canada will be subject to a surcharge to cover GST. Customers in the EU subscribing to the electronic version only will be charged VAT.

If you take an institutional subscription to any Royal Society of Chemistry journal you are entitled to free, site-wide web access to that journal. You can arrange access via Internet Protocol (IP) address at www.rsc.org/ip

Customers should make payments by cheque in sterling payable on a UK clearing bank or in US dollars payable on a US clearing bank.

Whilst this material has been produced with all due care, the Royal Society of Chemistry cannot be held responsible or liable for its accuracy and completeness, nor for any consequences arising from any errors or the use of the information contained in this publication. The publication of advertisements does not constitute any endorsement by the Royal Society of Chemistry or Authors of any products advertised. The views and opinions advanced by contributors do not necessarily reflect those of the Royal Society of Chemistry which shall not be liable for any resulting loss or damage arising as a result of reliance upon this material. The Royal Society of Chemistry is a charity, registered in England and Wales, Number 207890, and a company incorporated in England by Royal Charter (Registered No. RC000524), registered office: Burlington House, Piccadilly, London W1J 0BA, UK, Telephone: +44 (0) 207 4378 6556.

Advertisement sales:

Tel +44 (0) 1223 432246; Fax +44 (0) 1223 426017; E-mail advertising@rsc.org

For marketing opportunities relating to this journal, contact marketing@rsc.org

Dalton Transactions

An international journal for high quality, original research in inorganic and organometallic chemistry incorporating Acta Chemica Scandinavica

rsc.li/dalton

Editorial Board

Russell Morris, University of St Andrews, UK

Associate Editors

Paola Ceroni, University of Bologna, Italy Vadapalli Chandrasekhar, Indian Institute of Technology Kanpur, India Maarit Karpinnen, Aalto University, Finland

Mi Hee Lim, Korea Advanced Institute of

Science and Technology, South Korea Neal Mankad, University of Illinois at Chicago, Warren Piers, University of Calgary, Canada

Universität, Germany Takashi Uemura, University of Tokyo, Japan Li-Min Zheng, Nanjing University, China

Wolfgang Tremel, Johannes Gutenberg-

Jaqueline Kiplinger, Los Alamos National Laboratory, USA Sascha Ott, Uppsala University, Sweden

Advisory Board

Simon Aldridge, University of Oxford, UK Santiago Alvarez, University of Barcelona, Spain

John Arnold, University of California, Berkeley, USA

Mu-Hyun Baik, KAIST, Korea Jitendra Bera, IIT Kanpur, India Eszter Borbas, Uppsala University, Sweden Holger Braunschweig, Universität Würzburg, Germany

Xian-He Bu, Nankai University, China Raffaella Buonsanti, École Polytechnique Fédérale de Lausanne, Switzerland Claire Carmalt, University College London, UK Eric Clot, University of Montpellier 2, France Catherine Constable-Housecroft, University of Basel, Switzerland

Amitava Das, Indian Institute of Science and Education Research Kolkata, India Jillian Dempsey, University of North Carolina, USA

Anjana Devi, Ruhr-University Bochum, Germany Rasika Dias, University of Texas at Arlington,

Jairton Dupont, University of Nottingham, UK

William Evans, University of California, Irvine, USA

Harry B. Gray, California Institute of Technology, USA Zijian Guo, Nanjing University, China Michael Hayward, University of Oxford, UK Todd W. Hudnall, Texas State University, USA

Ilich Ibarra, National Autonomous University of Mexico, Mexico Cameron Jones, Monash University, Australia Masako Kato, Hokkaido University, Japan Takahiko Kojima, University of Tsukuba, Japan Jian-Ping Lang, Suzhou University, China

Stuart Macgregor, Heriot Watt University, UK Celia Machado Ronconi, Federal Fluminense University, Brazil

Jennifer Love, University of British Columbia,

Laurent Maron, Université de Toulouse, France Ellen Matson, Rochester University, USA Marinella Mazzanti, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland Nils Metzler-Nolte, Ruhr-Universität Bochum, Germany

Barbara Milani, Universita di Trieste, Italy Georgii Nikonov, Brock University, Canada

Seiji Ogo, Kyushu University, Japan Chris Orvig, University of British Columbia, Canada

Gerard Parkin, Columbia University, USA Eric Rivard, University of Alberta, Canada Douglas Stephan, University of Toronto, Canada

Matthias Tamm, Technische Universität Braunschweig, Germany

Jinkui Tang, Changchun Institute of Applied Chemistry, China Thomas Teets, University of Houston, USA

Christine Thomas, The Ohio State University, USA Ajay Venugopal, Indian Institute of

Science Education and Research Thiruvananthapuram, India Claudio N. Verani, Wayne State University, USA Wai-Yeung Wong, Hong Kong Baptist University, China Zhiguo Xia, South China University of Technology, China

Zuowei Xie, Chinese University of Hong Kong

Lin Xu, East China Normal University, China

Information for Authors

Full details on how to submit material for publication in Dalton Transactions are given in the Instructions for Authors (available from http://www.rsc.org/authors). Submissions should be made via the journal's homepage: rsc.li/dalton

Authors may reproduce/republish portions of their published contribution without seeking permission from the Royal Society of Chemistry, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation)-Reproduced by permission of the Royal Society of Chemistry

This journal is @ The Royal Society of Chemistry 2023. Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

Registered charity number: 207890

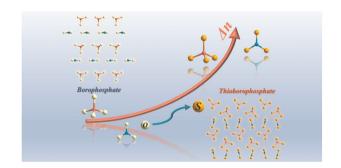


COMMUNICATIONS

16113

Ba₃(BS₃)(PS₄): the first alkaline-earth metal thioborate-thiophosphate with strong optical anisotropy originating from planar [BS3] units

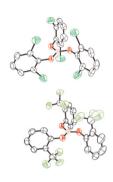
Jiazheng Zhou, Linan Wang, Hongshan Wang, Ling Luo, Junjie Li* and Feng Yu*



16118

Reactivity of a series of triaryl borates, B(OArx)3, in hydroboration catalysis

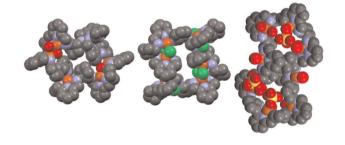
Tomasz Sokolnicki, Mashael M. Alharbi, Yara van Ingen, Shahnaz Rahim, Milan Pramanik, Alberto Roldan, Jędrzej Walkowiak* and Rebecca L. Melen*



16123

Hexa- and octanuclear copper(II) complexes with a tetraeicosaaza amine macrocycle

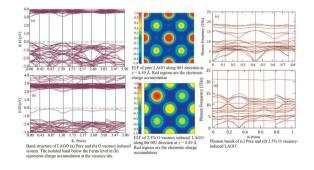
Dominika Fedorowicz, Katarzyna Ślepokura, Julia Kłak, Maciaj Witwicki and Janusz Gregoliński*



16128

The role of oxygen defects in the electronic, optical and phonon dispersion of the LAGO perovskite: a density functional theory investigation

Chaithanya P. Bhat, Ashwin K. Godbole and Debashis Bandyopadhyay*

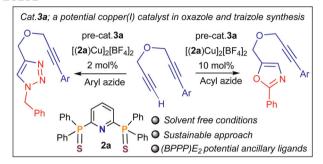


16140

Metal coordination to solute binding proteins exciting chemistry with potential biological meaning

Kinga Garstka, Denise Bellotti, Joanna Watły, Henryk Kozłowski, Maurizio Remelli and Magdalena Rowińska-Żyrek*

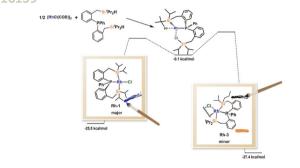
16151



Dicationic copper(ı) complexes bearing ENE (E = S, Se) pincer ligands; catalytic applications in regioselective cyclization of 1,6-diynes

Bhagyashree Das, Amiya Kumar Sahoo, Shyam Kumar Banjare, Subhra Jyoti Panda, Chandra Shekhar Purohit and Adinarayana Doddi*

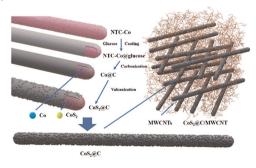
16159



Unexpected alkyl isomerization at the silicon ligand of an unsaturated Rh complex: combined experiment and theory

Niroshani S. Abeynayake, Nghia Le, Gabriela Sanchez-Lecuona, Bruno Donnadieu, Charles Edwin Webster* and Virginia Montiel-Palma*

16167



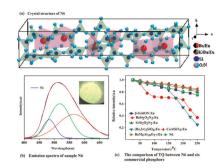
CoS2@C catalyzes polysulfide conversion to promote the rate and cycling performances of lithium-sulfur batteries

Yufei Zhang, Xinhang Liu, Qi Jin, Fengfeng Han, Zhiguo Zhang, Xitian Zhang* and Lili Wu*

16173

Oxynitride K₂Ba_{6.72}Si₁₆O_{40-1.5v}N_v:0.28Eu²⁺ phosphor with high thermal stability realized by crystal field engineering

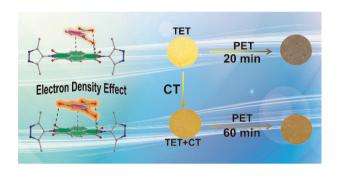
Aijun Mao, * Xinwei Wang, Yali Guo, Xuejie Zhai and Pai Lv



16184

Electron density effect of aromatic carboxylic acids in naphthalenediimide-based coordination polymers: from thermal electron transfer and charge transfer to photoinduced electron transfer

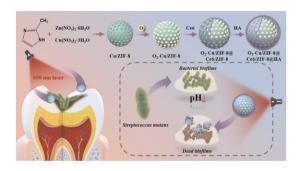
Gao-Peng Li,* Jing Zhang, Wan-Wan Ren, Si-Nan Wang, Ying-Xia Wang, Yun-Long Fu* and Yao-Yu Wang*



16189

Oxygen-carrying acid-responsive Cu/ZIF-8 for photodynamic antibacterial therapy against cariogenic Streptococcus mutans infection

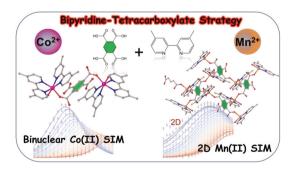
Ruifeng Wang, Qiyuan Pan, Fang Li, Jingying Guo, Yaru Huo, Chao Xu, Manwen Xiong, Ziyong Cheng, Min Liu* and Jun Lin*



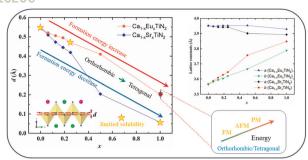
16197

Binuclear cobalt(II) and two-dimensional manganese(II) coordination compounds self-assembled by mixed bipyridine-tetracarboxylic ligands with single-ion magnet properties

Dong-Qing Wu,* Kusum Kumari, Yi Wan, Xueling Gao, Mengxi Guo, Genyan Liu, Dong Shao,* Bin Zhai and Saurabh Kumar Singh*



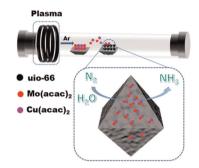
16206



$KCoO_2$ -type layered nitrides $Ca_{1-x}Eu_xTiN_2$: structural stability, electrical properties and Eu coordination chemistry

Junwei Liu, Bowen Zhang, Shenglin Lu, Xing Ming* and Xiaojun Kuang*

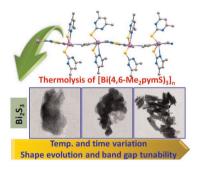
16217



Double-single-atom MoCu-embedded porous carbons boost the electrocatalytic N_2 reduction reaction

Zhiya Han, Chenbao Lu, Senhe Huang, Xinyu Chai, Zhenying Chen, Xintong Li, Jilong Wang, Jingshun Zhang,* Boxu Feng,* Sheng Han* and Rongbin Li*

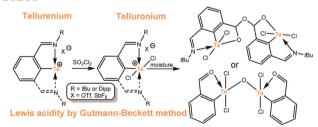
16224



Controlled synthesis of photoresponsive bismuthinite (Bi₂S₃) nanostructures mediated through a new 1D bismuth-pyrimidylthiolate coordination polymer as a molecular precursor

Atharva Yeshwant Kulkarni, Gourab Karmakar, Alpa Y. Shah, Sandeep Nigam, Gayatri Kumbhare, Adish Tyagi,* Raymond J. Butcher, Rohit Singh Chauhan* and N. Naveen Kumar

16235



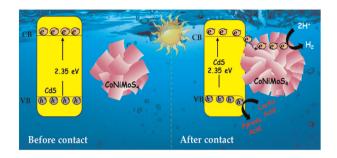
N-Coordinated tellurenium(II) and telluronium(IV) cations: synthesis, structure and hydrolysis

Martin Hejda, Lukáš Doležal, Jan Blahut, Emanuel Hupf, Jiří Tydlitát, Roman Jambor, Aleš Růžička, Jens Beckmann* and Libor Dostál*

16249

Positioning hydrogen reaction sites by constructing CdS/CoNiMoS₄ heterojunctions for efficient photocatalytic hydrogen evolution

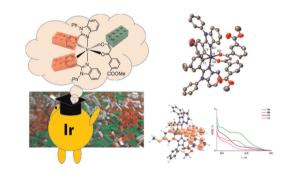
Pooia Varma, Rama Krishna Chava, Chunli Liu, Tae Kyu Kim and D. Amaranatha Reddy*



16261

Rational design of efficient photosensitizers based on cyclometalated iridium(III) complexes with 2-arylbenzimidazole and aromatic 1,3-diketone ligands

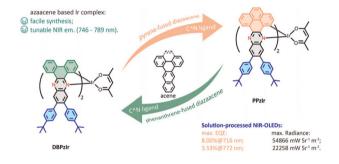
Sergei V. Tatarin, Elizaveta A. Meshcheriakova, Sergey A. Kozyukhin, Victor V. Emets and Stanislav I. Bezzubov*



16276

Azaacene containing iridium(III) phosphors: elaboration of the π -conjugation effect and application in highly efficient solution-processed near-infrared OLEDs

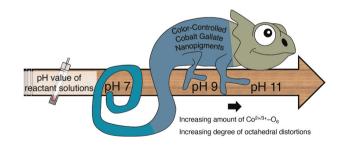
Min Li, Li Wang, Caifa You,* Denghui Liu, Kai Zhang and Weiguo Zhu*



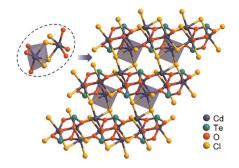
16285

Color-controlled nonstoichiometric spinel-type cobalt gallate nanopigments prepared by supercritical hydrothermal synthesis

Bo Xie, Chiya Numako, Takashi Naka and Seiichi Takami*



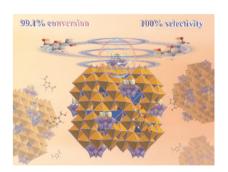
16297



Synthesis, structure and characterization of $Cd_2TeO_3Cl_2$ with unprecedented $[Cd_2O_6Cl_4]$ octahedral dimers

Linan Wang, Chen Bai, Yingying Kong, Maqsood Iqbal, Yu Chu* and Junjie Li*

16303



Enhanced catalysis of a vanadium-substituted Keggin-type polyoxomolybdate supported on the M_3O_4/C (M = Fe or Co) surface enables efficient and recyclable oxidation of HMF to DFF

Yun-Dong Cao, Wen-Xia Mu, Mengdi Gong, Lin-Lin Fan,* Jie Han, Hong Liu,* Bin Qi and Guang-Gang Gao*

16315 | Sywo: 1.0Eu* | Sywo: 1.0Eu*

Limited energy migration and circumscribed multiphonon relaxation produced non-concentration quenching in a novel dazzling red-emitting phosphor

Yue Wang, Kexin Zhao, Bohuai Shao, Chuang Wang* and Ge Zhu*

16326 RO HC (3a)Ме (3b) Ag₂CO₃ .CI Εt (3c) (3d) H_2O Bu (3e) 60 °C (3f) Pe 24 h

Not the usual suspect – an unexpected organometallic product during the synthesis of cytotoxic platinum(II) complexes

Thomas Maier, Judith Wutschitz, Natalie Gajic, Michaela Hejl, Klaudia Cseh, Sebastian Mai, Michael A. Jakupec, Mathea S. Galanski* and Bernhard K. Keppler*

16336

Green synthesis of carbon-supported ultrafine ZnS nanoparticles for superior lithium-ion batteries

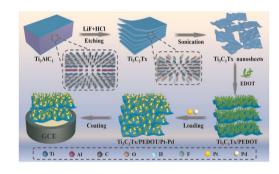
Ying-Yi Han, Xuefei Zhang, Bi-Cui Chen, Pei-Wen Huang, Yun Chai, Xiao-Hui Wu* and Zailai Xie*



16345

PEDOT-embellished Ti₃C₂Tx nanosheet supported Pt-Pd bimetallic nanoparticles as efficient and stable methanol oxidation electrocatalysts

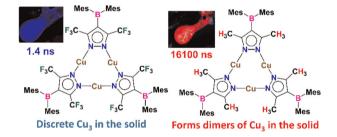
Shuyue Xie, Fangfei Liu, Tursun Abdiryim,* Xiong Liu, Ruxangul Jamal,* Yanyan Song, Mariyam Niyaz, Yajun Liu, Hujun Zhang and Xinsheng Tang



16356

Filling the gap with a bulky diaryl boron group: fluorinated and non-fluorinated copper pyrazolates fitted with a dimesityl boron moiety on the backbone

Mukundam Vanga, Benjamin T. Diroll,* Álvaro R. Muñoz-Castro* and H. V. Rasika Dias*

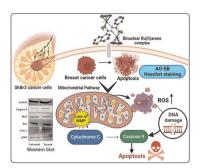


16364

Synthesis of nitrogen mustards on cobalt(III)

Rasika J. Kariyawasam, Ramin Zibaseresht, Matthew I. J. Polson, Joanna C. C. Houlihan, Jan L. Wikaira and Richard M. Hartshorn*

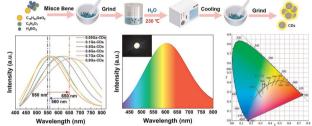
16376



Naphthoyl benzhydrazine-decorated binuclear arene Ru(II) complexes as anticancer agents targeting human breast cancer cells

Arunachalam Abirami, Umapathy Devan, Rengan Ramesh,* Arockiam Antony Joseph Velanganni and Jan Grzegorz Małecki

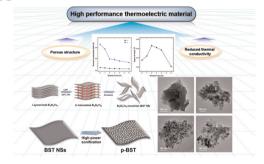
16388



Bright solid-state luminescence and hightemperature resistance of Ga-doped carbon dots with ultra-wideband white emission for light-emitting diodes

Xiao Gao, Hongquan Yu,* Zhanwen Han, Baojiu Chen,* Jiashi Sun and Xiangping Li

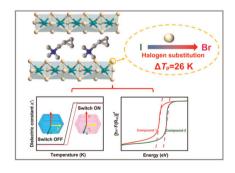
16398



Highly porous thermoelectric composites with high figure of merit and low thermal conductivity from solution-synthesized porous Bi₂Si₂Te₆ nanosheets

Dabin Park, Minsu Kim and Jooheon Kim*

16406



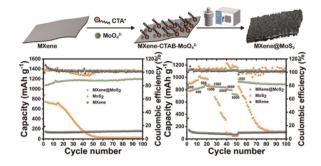
The halogen substitution strategy of inorganic skeletons triggers dielectric and band gap regulation of hybrid perovskites

Xiao-Tong Sun, Ying-Yu Zhang, Yan Han, Xiao-Ping Wang, Jie Li, Jun-Yi Li, Hao-Fei Ni, Da-Wei Fu* and Zhi-Xu Zhang*

16413

Few-layer MoS₂ nanosheets vertically supported on Ti₃C₂-MXene sheets promoting lithium storage performance

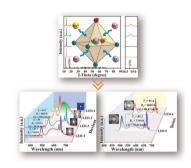
Hankun Tan, Lei Zhang, Kaiyue Gao, Li Sun,* Yihe Zhang* and Feng Xie



16421

Optical enhancement of highly efficient organicinorganic oxyfluoride red phosphors via the cation co-doping strategy

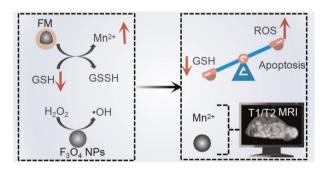
Xiaoyi Liu, Haiming Cheng, Hu Wang, Zhu Wen, Guixia Liu,* Shengda Liu, Dan Li, Jinxian Wang, Wensheng Yu and Xiangting Dong



16433

Dual-targeting nanotheranostics for MRI-guided enhanced chemodynamic therapy of hepatoma via regulating the tumor microenvironment

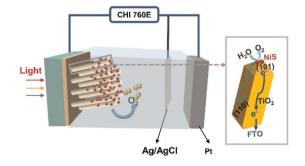
Jinwu Liu, Hong Qu, Lifeng Hang, Yiqiang Sun, Wuming Li, Yiyu Chen, Hong Li, Wei Wen,* Yanqiu Feng* and Guihua Jiang*



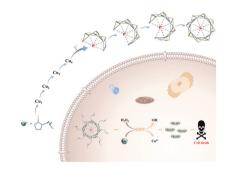
16442

Enhanced photoelectrochemical performance of NiS-modified TiO₂ nanorods with a surface charge accumulation facet

Suyi Yang, Baoyuan Wang, Rui Zhao, Liting Wei and Jinzhan Su*



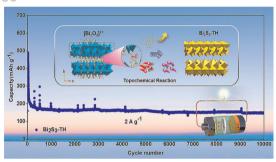
16451



Stepwise formation of a chemodynamic therapy agent of $\{Cu_8\}$ macrocyclic complex recognized by iodide ions

Sudi Huang, Jingjing Zhong, Xinyi Huang, Yuqing Jia, Zhaoguo Hong and Fu-Ping Huang*

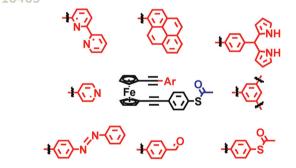
16456



A topochemical reaction induced the formation of Bi_2S_3 micro-straws from a Bi-MOF for an ultra-long Zn storage life

Lei Gou,* Kai Liang, Wen-Yan Wang, Ya-Ting Lei, Shou-Lin Xie, Ding-Kai Wei, Dong-Lin Li and Xiao-Yong Fan*

16465



A convenient synthesis of ferrocene-(ethynylphenyl)thioacetates

Troy L. R. Bennett and Nicholas J. Long*

16472

Electrophilic activation of molecular bromine mediated by I(III)

Lachlan Sharp-Bucknall, Tania, Marcus Sceney, Lachlan Barwise and Jason L. Dutton*

16480

2-(Thienyl)quinoxaline derivatives and their application in Ir(III) complexes yielding tuneable deep red emitters

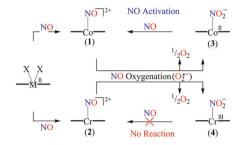
Sophie A. Fitzgerald, Ellie N. Payce, Peter N. Horton, Simon J. Coles and Simon J. A. Pope*

+ 5 other examples

16492

Mechanistic insights into nitric oxide oxygenation (NOO) reactions of {CrNO}⁵ and {CoNO}⁸

Akshaya Keerthi C. S., Sandip Das, Kulbir, Prabhakar Bhardwaj, Md Palashuddin Sk and Pankaj Kumar*

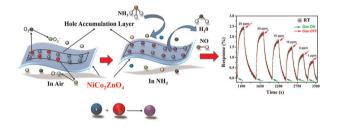


M = Cr, X = Cl; M = Co, X = CH₃CN

16500

A room-temperature gas sensor based on 2D Ni–Co–Zn ternary oxide nanoflakes for selective and sensitive ammonia detection

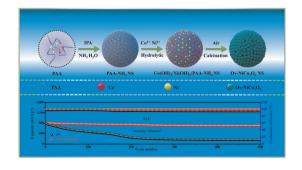
Sourav Karmakar, Avik Sett, Palash Chandra Maity, Gairik Karmakar, Rinky Sha,* Tarun Kanti Bhattacharyya and Indranil Lahiri



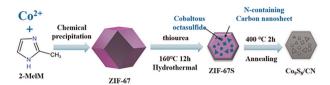
16513

A well-dispersed O_V-NiCo₂O₄ nanosphere modified separator for Li-S batteries

Yumeng Gao, Siyu Liu, Jiudi Zhang, Xiaoyang Chen, Bing Han, Yali Wang, Jianhua Guo, Zhanshuang Jin,* Junjie Li and Xudong Meng*



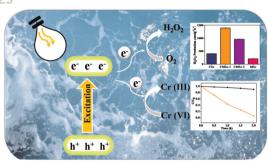
16519



Topochemical and phase transformation induced Co₉S₈/NC nanosheets for high-performance sodium-ion batteries

Yining Li, Shimei Wu, Chilin Liu, Zhiting Liu, Wei Yang, Yufei Zhang* and Haosen Fan*

16525



Compositionally engineered Cd-Mo-Se alloyed QDs toward photocatalytic H_2O_2 production and $Cr(v_1)$ reduction with a detailed mechanism and influencing parameters

Jyotirmayee Sahu, Sriram Mansingh, Bhagyashree Priyadarshini Mishra, Deeptimayee Prusty and Kulamani Parida*