

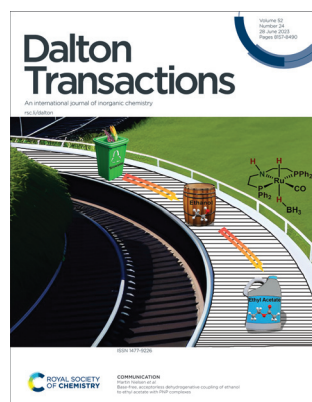
Dalton Transactions

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(24) 8157-8490 (2023)



Cover
See Martin Nielsen *et al.*,
pp. 8193–8197.

Image reproduced
by permission of
Rajib Pramanick, Zhenwei Ni,
Rosa Maria Padilla Paz, Mike
Steffen Bernhard Jørgensen
and Martin Nielsen from
Dalton Trans., 2023, **52**, 8193.



Inside cover
See Rui Wang, Qiaoling Kang,
Dongyun Li *et al.*,
pp. 8211–8221.

Image reproduced by
permission of Xiong Wang,
Rui Wang, Qiaoling Kang,
Feng Gao, Miaogen Chen,
Yang Xu, Hongliang Geac
and Dongyun Li from
Dalton Trans., 2023, **52**, 8211.

EDITORIAL

8170

Metallocycles and metallocages

Lin Xu,* Cally J. E. Haynes* and James E. M. Lewis*

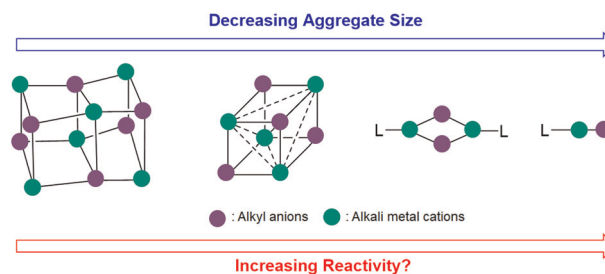


PERSPECTIVE

8172

The quest for organo-alkali metal monomers: unscrambling the structure–reactivity relationship

Nathan Davison* and Erli Lu*



Editorial Staff

Executive Editor

Sally Howells

Deputy Editor

Mike Andrews

Development Editors

Michelle Canning, Emily Cuffin-Munday

Editorial Production Manager

Susannah Davies

Publishing Editors

Debora Giovannelli, 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, 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

Chair

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, USA
Warren Piers, University of Calgary, Canada
Wolfgang Tremel, Johannes Gutenberg-Universität, Germany
Takashi Uemura, University of Tokyo, Japan
Li-Min Zheng, Nanjing University, China

Members

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, USA

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

Jennifer Love, University of British Columbia, Canada

Laurent Maron, Université de Toulouse, France

Stuart Macgregor, Heriot Watt University, UK

Ellen Matson, Rochester University, USA

Marinella Mazzanti, Ecole Polytechnique

Fédérale de Lausanne (EPFL), Switzerland

Nils Metzler-Nolte, Ruhr-Universität Bochum, Germany

Barbara Milani, Università 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,

China

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

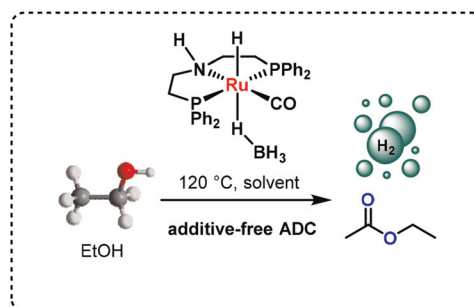


COMMUNICATIONS

8193

Base-free, acceptorless dehydrogenative coupling of ethanol to ethyl acetate with PNP complexes

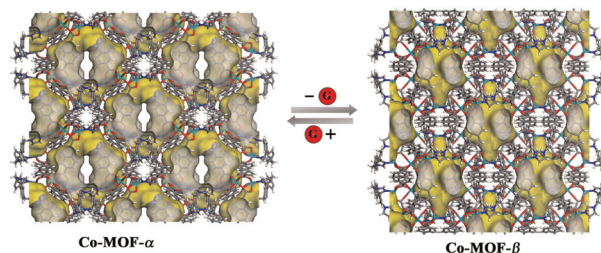
Zhenwei Ni, Rosa Padilla, Rajib Pramanick, Mike S. B. Jørgensen and Martin Nielsen*



8198

A 2D flexible cobalt-MOF: reversible solid-state structural transformation, two-step and gate-opening adsorption behaviours, and selective adsorption of C₂H₂ over CO₂ and CH₄

Shan-Shan Wang, Yu-Jie Liang, Wei Guo, Yue Yin, Xiao-Yu Li, Quan-Qing Xu, Ai-Xin Zhu* and Bo Huang*



8204

Upcycling rust and plastic waste into an Fe MOF for effective energy storage applications: transformation of trash to treasure

Rakesh Deka, Diptangshu Datta Mal and Shaikh M. Mobin*

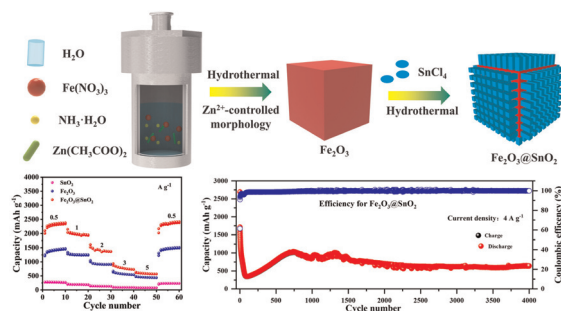


PAPERS

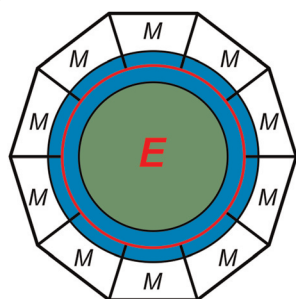
8211

Epitaxial growth of hexahedral Fe₂O₃@SnO₂ nano-heterostructure for improved lithium-ion batteries

Xiong Wang, Rui Wang,* Qiaoling Kang,* Feng Gao, Miaogen Chen, Yang Xu, Hongliang Ge and Dongyun Li*



8222



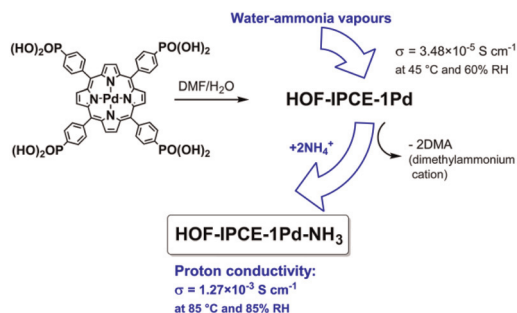
$$8-N^{\text{eff}}(E)$$

Octet rule for
polar-covalent
multiatomic bonding

Polarity-extended 8 – N^{eff} rule for semiconducting main-group compounds with the TiNiSi-type of crystal structure

Riccardo Freccero,* Yuri Grin and Frank R. Wagner*

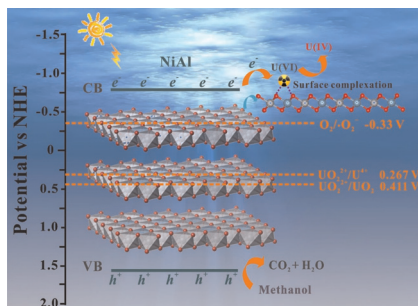
8237



An anionic porphyrinylphosphonate-based hydrogen-bonded organic framework: optimization of proton conductivity through the exchange of counterions

Ekaterina A. Zhigileva, Yulia Yu. Enakieva,* Anna A. Sinelshchikova, Vladimir V. Chernyshev, Ivan N. Senchikhin, Konstantin A. Kovalenko, Irina A. Stenina, Andrey B. Yaroslavtsev, Yulia G. Gorbunova and Aslan Yu. Tsvadze

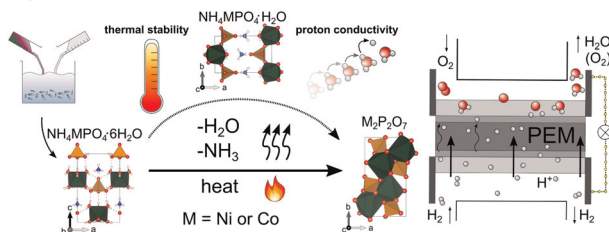
8247



Adsorption-photoreduction behaviors and mechanisms of layered double hydroxide loaded on uranium(vi) removal

Qian Ling, Peiling Kuang, Xin Zhong* and Baowei Hu*

8262



Thermally processed Ni- and Co-struvites as functional materials for proton conductivity

Stephanos Karafiludis,* Biswajit Bhattacharya, Ana Guilherme Buzanich, Friedrich Fink, Ines Feldmann, Johan E. ten Elshof, Franziska Emmerling and Tomasz M. Stawski*

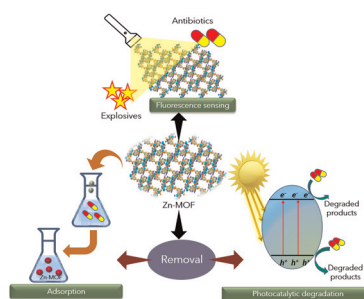


PAPERS

8275

Amino decorated adenine based metal–organic framework for multi-faceted applications

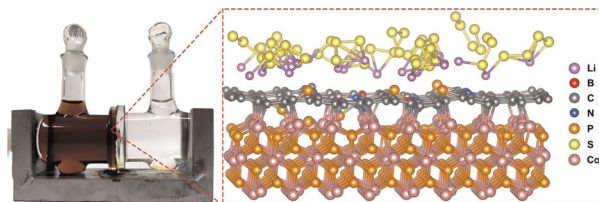
Alehegn Eskemech, Diksha Gambhir, Harpreet Kaur, Anirban Karmakar and Rik Rani Koner*



8284

Synthesis of CoP@B,N,P co-doped porous carbon by a supramolecular gel self-assembly method for lithium–sulfur battery separator modification

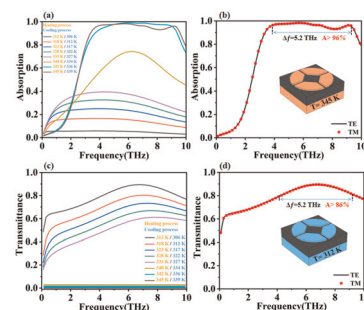
Zhenpu Shi, Yunqi Huang, Juhong Xu, Yudong Pang, Lan Wang, Wanli Zhao, Hongyun Yue, Zongxian Yang, Shuting Yang* and Yanhong Yin*



8294

Active thermally tunable and highly sensitive terahertz smart windows based on the combination of a metamaterial and phase change material

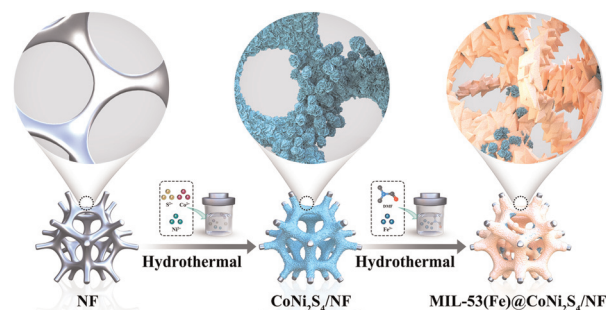
Zhipeng Zheng, Wenchao Zhao, Zao Yi,* Liang Bian, Hua Yang, Shubo Cheng, Gongfa Li, Liangcai Zeng, Hailiang Li and Peipei Jiang



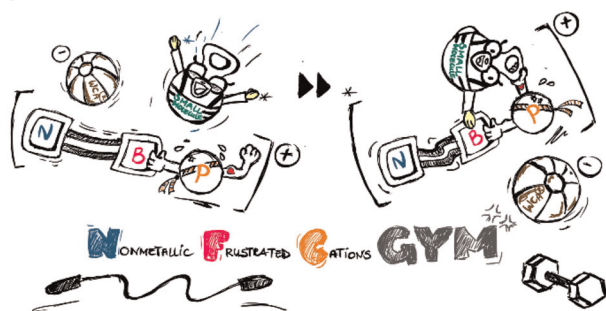
8302

A hybrid of MIL-53(Fe) rhombus and conductive CoNi₂S₄ nanosheets as a synergistic electrocatalyst for the oxygen evolution reaction

Weidong Liu, Lijun Wang and Yaqiong Gong*



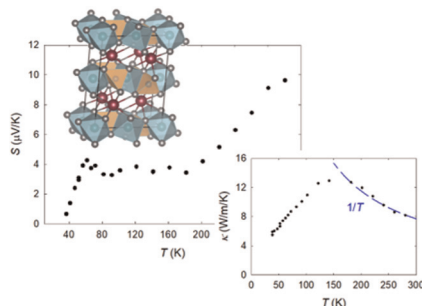
8311



Application of nonmetallic frustrated cations in the activation of small molecules

Kinga Kaniewska-Laskowska,* Marcin Czapla, Jarosław Chojnacki and Rafał Grubba*

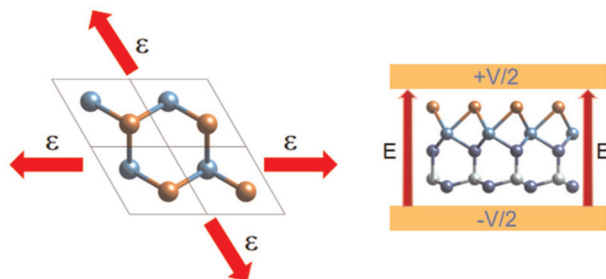
8316



Structure, electrical and thermal properties of single-crystal BaCuGdTe₃

Wilarachige D. C. B. Gunatilleke, Winnie Wong-Ng, Teiyan Chang, Yu-Sheng Chen and George S. Nolas*

8322



First principles prediction of two-dimensional Janus STiXY₂ (X = Si, Ge; Y = N, P, As) materials

Zhen Gao, Xin He, Wenzhong Li, Yao He* and Kai Xiong

8332



Interesting chemical and physical features of the products of the reactions between trivalent lanthanoids and a tetradentate Schiff base derived from cyclohexane-1,2-diamine

I. Mylonas-Margaritis,* Z. G. Lada, A. A. Kitos, D. Maniaki, K. Skordi, A. J. Tasiopoulos, V. Bekiari, A. Escuer, J. Mayans,* V. Nastopoulos,* E. G. Bakalbassis,* D. Papaioannou* and S. P. Perlepes*

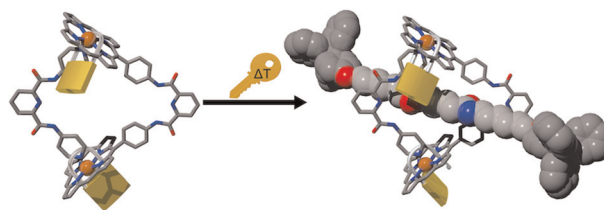


PAPERS

8344

A robust heterodimeric bis-Rh(III)–porphyrin macrocycle for the self-assembly of a kinetically stable [2]–rotaxane

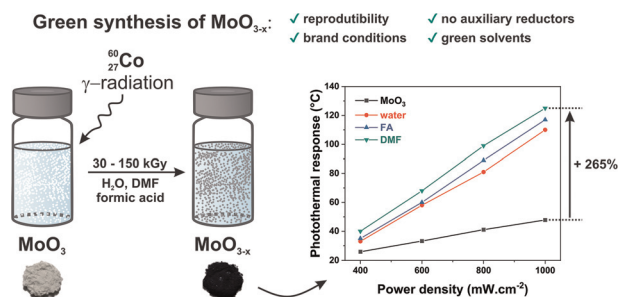
Naoyuki Hisano,* Virginia Valderrey, Gemma Aragay and Pablo Ballester*



8353

Synthesis and photothermal performance of non-stoichiometric molybdenum oxide (MoO_{3-x}) prepared by gamma radiation

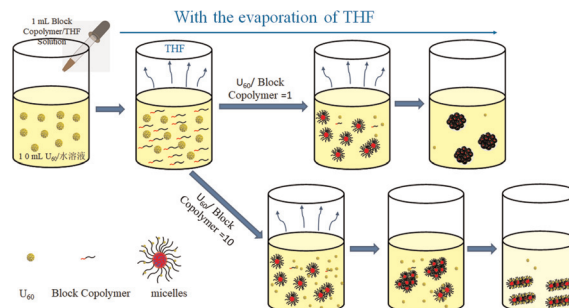
Diane C. A. Lima,* Aldebarã F. Ferreira, Stterferson E. Silva, Severino Alves, Junior, Felipe L. N. Sousa and Walter M. de Azevedo*



8361

Hydrogen bonding and phase separation cooperatively guide the self-assembly of U₆₀ and the polymer to fabricate multiscale nanostructures

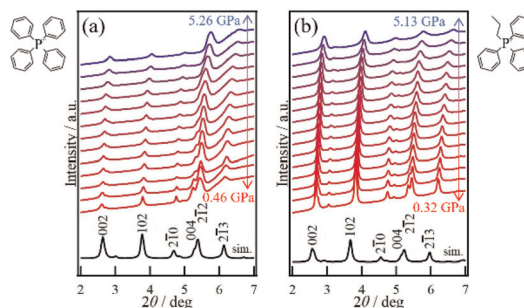
Jie Hu,* Yingxuan Mei, Huiwen Wu, Yan Zhao, Dongping Wu, Nan Ye, Peng Yi, Yu Yang and Minmeng Liao



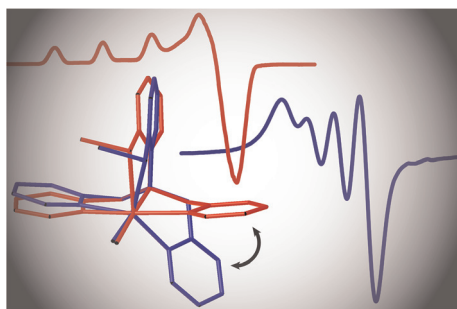
8368

⁵⁷Fe Mössbauer spectroscopy and high-pressure structural analysis for the mechanism of pressure-induced unique magnetic behaviour in (cation) [Fe^{II}Fe^{III}(dto)₃] (cation = Ph₄P and ⁿPrPh₃P; dto = 1,2-dithiooxalato)

Ryosuke Taniai, Tsubasa Endo, Takuya Kanetomo,* Atsushi Okazawa, Hirokazu Kadobayashi, Saori I. Kawaguchi and Masaya Enomoto*



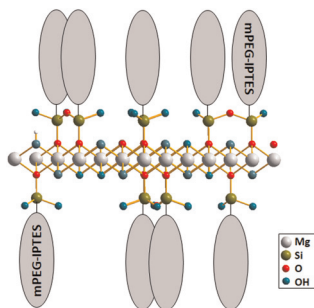
8376



Conformational dynamics in a copper(II) coordination complex

Paul J. Griffin, Matthew J. Dake, Alesandro D. Remolina and Lisa Olshansky*

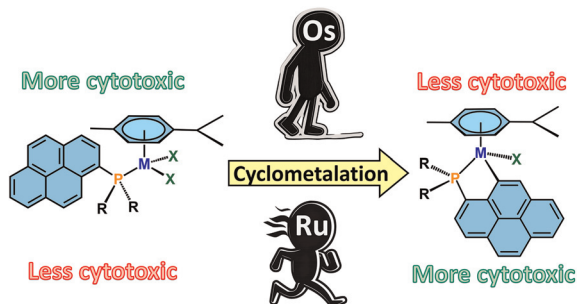
8384



In situ preparation of compounds using silanized mPEG inspired by talc-like structures

Liva Dzene,* Anne-Sophie Schuller, Frédéryck Tidas, Séverinne Rigolet, Jocelyne Brendlé and Christelle Delaite

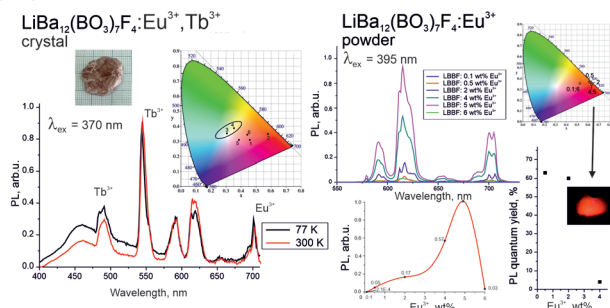
8391



Cytotoxicity of osmium(II) and cycloosmated half-sandwich complexes from 1-pyrenyl-containing phosphane ligands

Dana Josa, David Aguilà, Pere Fontova, Vanessa Soto-Cerrato, Piedad Herrera-Ramírez, Laia Rafols, Arnald Grabulosa* and Patrick Gamez*

8402



LiBa₁₂(BO₃)₇F₄ (LBBF) crystals doped with Eu³⁺, Tb³⁺, Ce³⁺: structure and luminescence properties

Tatyana B. Bekker,* Alexey A. Ryadun, Alexey V. Davydov and Sergey V. Rashchenko

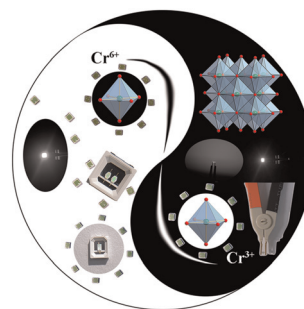


PAPERS

8414

A broadband near-infrared Cr³⁺-doped phosphor applied to near-infrared light-emitting diodes: enhanced luminescence and thermal stability by annealing

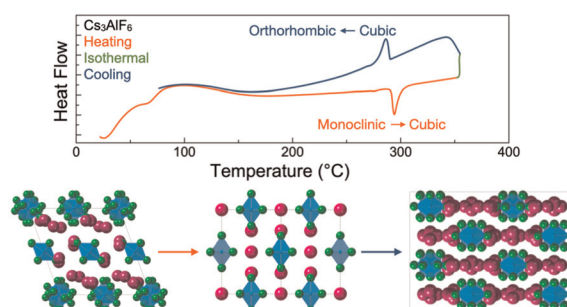
Tao Tan, Ran Pang,* Shangwei Wang, Haiyan Wu, Jiutian Wang, Su Zhang, Chengyu Li* and Hongjie Zhang



8425

Polymorphism in A₃MF₆ (A = Rb, Cs; M = Al, Ga) grown using mixed halide fluxes

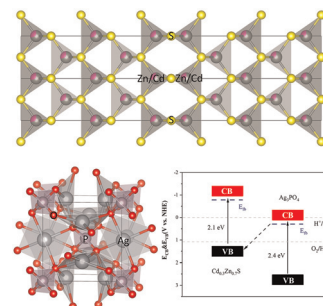
Gregory Morrison, Lakshani W. Masachchi, Hunter B. Tisdale, Tiejian Chang, Virginia G. Jones, K. Pilar Zamorano, Logan S. Breton, Mark D. Smith, Yu-Sheng Chen and Hans-Conrad zur Loye*



8434

Defective Cd_{0.3}Zn_{0.7}S twin crystal/Ag₃PO₄ Z-scheme heterojunctions toward optimized visible-light-driven photocatalytic hydrogen evolution

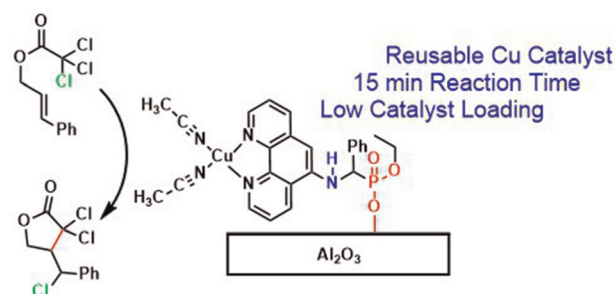
Jie Chen, Haitao Yu,* Ying Xie,* Zhenzi Li and Wei Zhou*



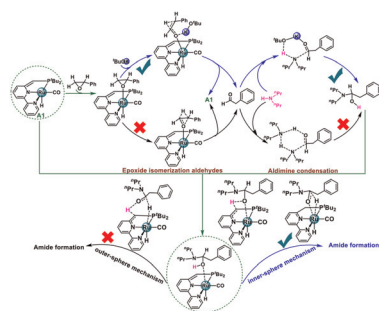
8442

Surface immobilized Cu-1,10-phenanthroline complexes with α -aminophosphonate groups in the 5-position as heterogeneous catalysts for efficient atom-transfer radical cyclizations

Sarah E. Maier, Osman Bunjaku, Elif Kaya, Michael Dyballa, Wolfgang Frey and Deven P. Estes*



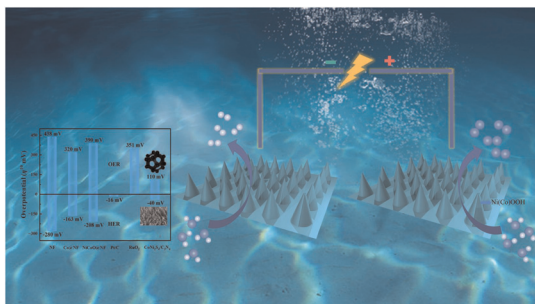
8449



Mechanistic insights into amide formation from aryl epoxides and amines catalyzed by ruthenium pincer complexes: a DFT study

Jing Wen, Zhewei Li, Yanhui Tang, Min Pu* and Ming Lei*

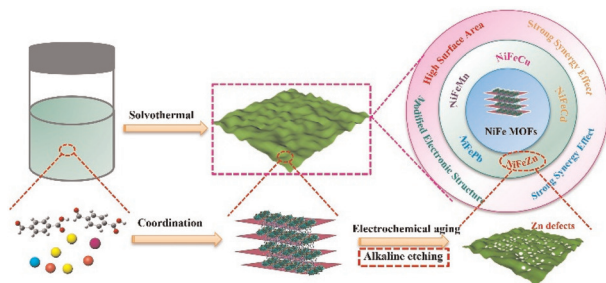
8456



Tentacle-like core–shell $\text{CoNi}_2\text{S}_4/\text{C}_3\text{N}_4$ bifunctional electrocatalysts for efficient overall alkaline water splitting

Qingfei Li, Nan Li,* Mianmian Wu, Guifang Sun, Wenjing Shen, Minghao Shi and Jiangquan Ma*

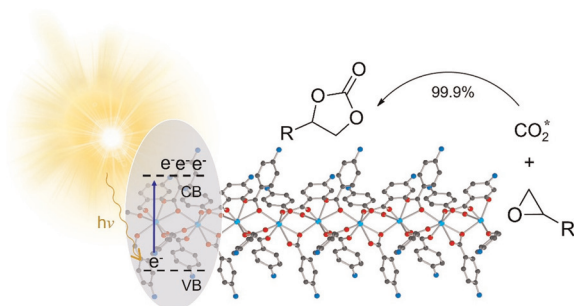
8466



Engineering defective trimetallic metal–organic framework nanosheets for advanced water oxidation electrocatalysis

Hui Xu, Cheng Wang, Guangyu He* and Haiqun Chen*

8473



Lanthanide(III) (Er/Ho) coordination polymers for a photocatalytic CO_2 cycloaddition reaction

Reem H. Alzard, Lamia A. Siddig, Abdalla S. Abdelhamid, Alejandro Perez Paz, Ha L. Nguyen, K. Sethupathi, P. K. Sreejith and Ahmed Alzamy*



CORRECTION

8488

Correction: An insight into the optical properties of a sub nanosize glutathione stabilized gold cluster

Lakshmi V. Nair, Resmi V. Nair and Ramapurath S. Jayasree*

