

ChemComm

Chemical Communications

rsc.li/chemcomm

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.

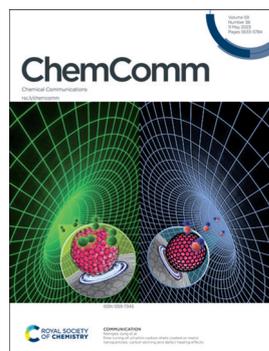
IN THIS ISSUE

ISSN 1359-7345 CODEN CHCOFS 59(38) 5633-5784 (2023)



Cover

See Linqin Jiang, Yu Qiu *et al.*, pp. 5677-5680. Image reproduced by permission of Linqin Jiang from *Chem. Commun.*, 2023, 59, 5677.



Inside cover

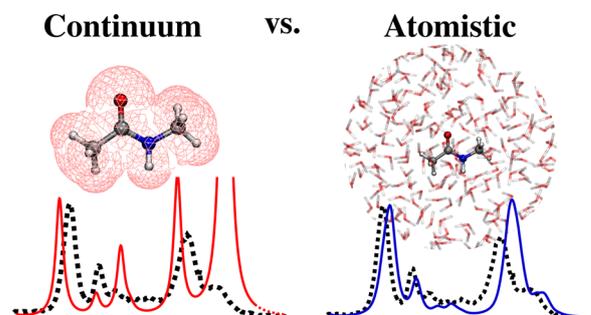
See Namgee Jung *et al.*, pp. 5681-5684. Image reproduced by permission of Namgee Jung from *Chem. Commun.*, 2023, 59, 5681.

FEATURE ARTICLES

5644

Continuum vs. atomistic approaches to computational spectroscopy of solvated systems

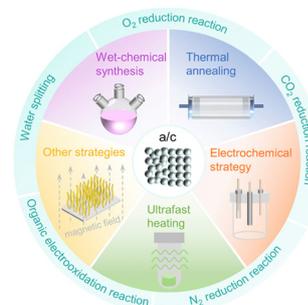
Tommaso Giovannini and Chiara Cappelli*



5661

Amorphous/crystalline heterophase electrocatalysts: synthesis, applications and perspectives

Zhichao Gong, Jingjing Liu, Gonglan Ye* and Huilong Fei*



Editorial Staff

Executive Editor

Richard Kelly

Deputy Editor

Harriet Riley

Editorial Production Manager

Helen Saxton

Development Editor

Danny Andrews, Ershad Abubacker

Senior Publishing Editor

Becky Webb

Publishing Editors

Kirstine Anderson, Matthew Bown, Laura Cooper, Hannah Fielding, Clare Fitzgerald, Anoushka Handa, Claire Harding, Alan Holder, Charlie Palmer, Rosie Rothwell, Donna Smith, Laura Smith

Editorial Assistant

Jade Holliday

Publishing Assistant

Natalie Ford

Publisher

Jeanne Andres

For queries about submitted papers, please contact Helen Saxton, Editorial Production Manager in the first instance. E-mail chemcomm@rsc.org

For pre-submission queries please contact

Richard Kelly, Executive Editor.

Email chemcomm-rsc@rsc.org

Chemical Communications (print: ISSN 1359-7345; electronic: ISSN 1364-548X) is published 100 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, UK CB4 0WE.

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: £3,553 / US\$6,258. 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

ChemComm

Chemical Communications

rsc.li/chemcomm

Editorial Board

Chair

Douglas Stephan, University of Toronto

Associate Editors

Lutz Ackermann, University of Göttingen

Daive Bonifazi, University of Vienna

Rachel Caruso, RMIT University

Fengtao Fan, Chinese Academy of Sciences

Itaru Hamachi, Kyoto University

Michael Hardie, University of Leeds

Kim Jelfs, Imperial College London

Chao-Jun Li, McGill University

Connie Lu, University of Minnesota, US

Marinella Mazzanti, EPFL, Switzerland

Amy Prieto, Colorado State University

Yang Tian, East China Normal University

Sandeep Verma, Indian Institute of

Technology Kanpur

Advisory Board

Brendan Abrahams, University of Melbourne

Polly Arnold, University of Edinburgh

Louise Berben, University of California, Davis

Penny Brothers, Australian National University

Wesley Browne, University of Groningen

Raffaella Buonsanti, EPFL

Luiz Henrique Catalani, University of São Paulo

Xiao-Ming Chen, Sun Yat-Sen University

Lifeng Chi, Soochow University

Arindam Chowdhury, Indian Institute of

Technology Bombay

Derrick Clive, University of Alberta

Seth Cohen, University of California, San Diego

Marcetta Darensbourg, Texas A&M University

Jyotirmayee Dash, Indian Association for the

Cultivation of Science

Gautam R. Desiraju, Indian Institute of

Science, Bangalore

Abhishek Dey, Indian Association for the

Cultivation of Science (IACS)

Josh Figueroa, University of California, San

Diego

Lutz Gade, University of Heidelberg

Sujit Ghosh, Indian Institute of Science

Education of Research, India

Nathan Gianneschi, University of California,

San Diego

Robert Gilliard Jr., University of Virginia

David Gonzalez-Rodriguez, Autonomous

University of Madrid

Rebecca Goss, University of

St Andrews

Mike Greaney, University of Manchester

Shaojun Guo, Peking University

Michael Hardie, University of Leeds

Amanda Hargrove, Duke University

Craig Hawker, University of California, Santa

Barbara

Feihe Huang, Zhejiang University

Todd Hudnall, Texas State University

Ilich A. Ibarra Alvarado, National University

of Mexico

Hiroshi Kageyama, Kyoto University

Jong Seung Kim, Korea University

Shu Kobayashi, University of Tokyo

Mi Hee Lim, Ulsan National Institute of

Science and Technology (UNIST)

Teck-Peng Loh, Nanyang

Technological University

Tien-Yau Luh, National Taiwan University

Doug MacFarlane, Monash University

Hiromitsu Maeda, Ritsumeikan University

Silvia Marchesan, University of Trieste

Nazario Martin, Complutense University of

Madrid

Keiji Maruoka, Kyoto University

Alexander Miller, University of North Carolina

at Chapel Hill

Wonwoo Nam, Ewha Womans University

Jean-Francois Nierengarten, University of

Strasbourg

Thalappil Pradeep, Indian Institute of

Technology Madras

S Ramakrishnan, Indian Institute of Science

Erwin Reisner, University of Cambridge

Robin Rogers, McGill University

Paolo Samori, University of Strasbourg

Ellen Sletten, University of California, Los

Angeles

David Smith, University of York

Mizuki Tada, Nagoya University

Christine Thomas, Ohio State University

Zhong-Qun Tian, Xiamen University

Tomas Torres, Autonomous University of

Madrid

Helma Wennemers, ETH Zurich

Judy Wu, University of Houston

Yi Xie, University of Science and Technology

of China

Xianran Xing, University of Science and

Technology Beijing

Shuli Yu, Shanghai Institute of Organic

Chemistry, Chinese Academy of Sciences

Atsuo Yamada, University of Tokyo

Qiang Zhang, Tsinghua University

Xi Zhang, Tsinghua University

Wenwan Zhong, University of California,

Riverside

Eli Zysman-Colman, University of St. Andrews

Information for Authors

Full details on how to submit material for publication in Chemical Communications 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/chemcomm

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.

© The paper used in this publication meets the requirements of ANSI/NISO Z39.48-1992 (Permanence of Paper).

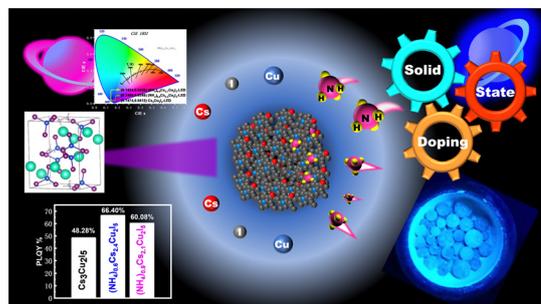
Registered charity number: 207890



5677

Deciphering the roles of ammonium doping for lead-free $(\text{NH}_4)_x\text{Cs}_{3-x}\text{Cu}_2\text{I}_5$ perovskites to regulate the photoelectronic properties

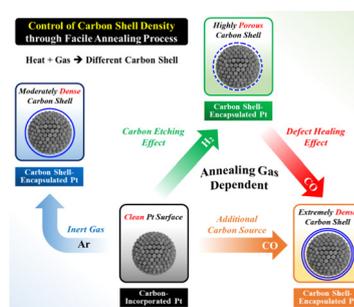
Zeyao Xu, Linqin Jiang,* Hao Xiong, Jiansen Wen, Ping Li, Lingyan Lin, Bo Wu, Aijun Yang and Yu Qiu*



5681

Fine-tuning of ultrathin carbon shells coated on metal nanoparticles: carbon etching and defect healing effects

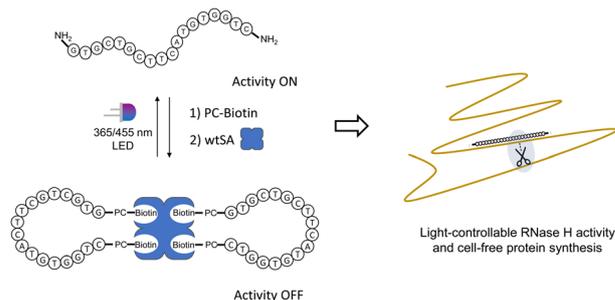
Jiho Min, Keonwoo Ko, Yunjin Kim, Sreya Roy Chowdhury, A. Anto Jeffery, Sourabh S. Chougule and Namgee Jung*



5685

Handcuffed antisense oligonucleotides for light-controlled cell-free expression

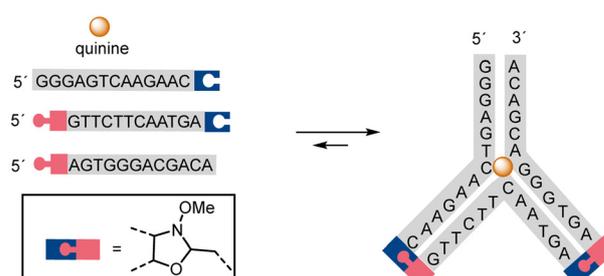
Denis Hartmann and Michael J. Booth*



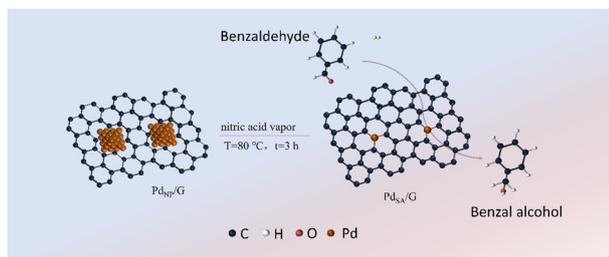
5689

Assembly of split aptamers by dynamic pH-responsive covalent ligation

Aapo Aho and Pasi Virta*



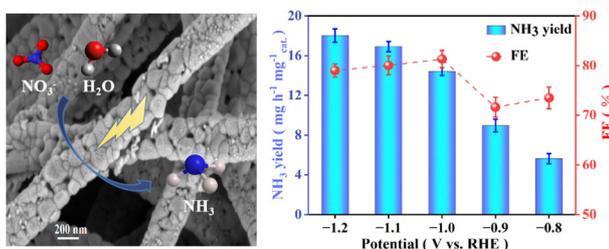
5693



Palladium single-atom catalysts synthesized by a gas-assisted redispersion strategy for efficient benzaldehyde hydrogenation

Lini Yang, Ling Li, Shuai Qin, Jingwang Zhang, Yue Wang, Xuetao Qin, Xiangbin Cai, Jiangyong Diao and Hongyang Liu*

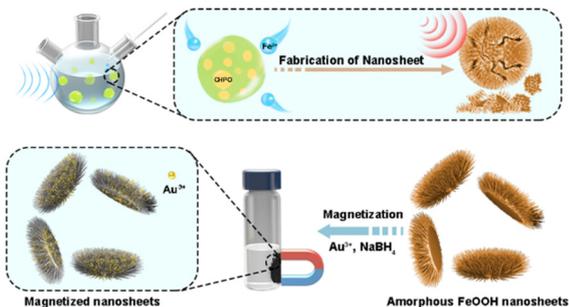
5697



Efficient electrocatalytic reduction of nitrate to ammonia over fibrous SmCoO₃ under ambient conditions

Peiji Hu, Songjie Hu, Hongting Du, Qian Liu, Haoran Guo,* Ke Ma* and Tingshuai Li*

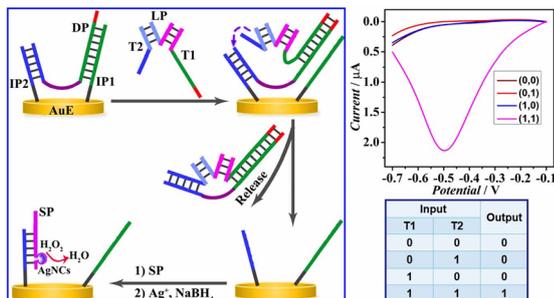
5701



Magnetization of amorphous FeOOH chrysanthemum-like nanosheets under ambient conditions

Yan Si, Siyu Shi, Jingyun Jing, Yun Bai and Qian Wang*

5705



An amplified logic gate driven by *in situ* synthesis of silver nanoclusters for identification of biomarkers

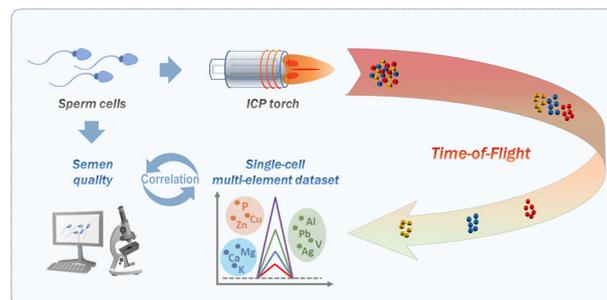
Hui Shen, Zhimin Li, Baoting Dou,* Qiumei Feng and Po Wang*



5709

Single-cell multi-element analysis reveals element distribution pattern in human sperm

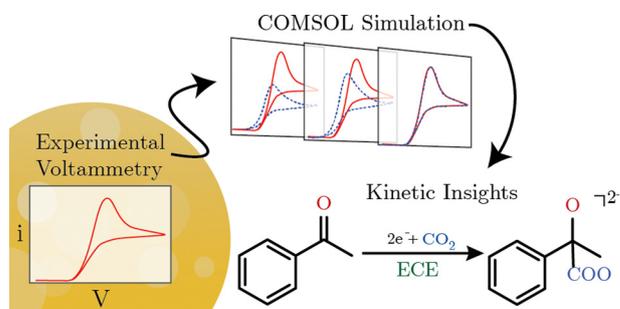
Xiangwei Tian, Xun Li, Nian Liu, Wenbin Cui, Lingna Zheng, Yingying Guo, Yanwei Liu, Ligang Hu, Meng Wang,* Yong Liang, Yongguang Yin,* Yong Cai, Guibin Jiang and Lei Jin*



5713

Distinguishing the mechanism of electrochemical carboxylation in CO₂ expanded Electrolytes

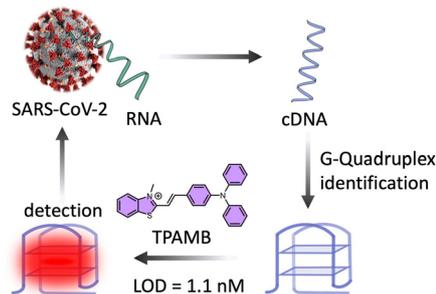
Matthew A. Stalcup, Christian K. Nilles, Bala Subramaniam,* James D. Blakemore* and Kevin C. Leonard*



5717

Coronavirus genomic cDNA derived G-quadruplex as a selective target for fluorometric detection

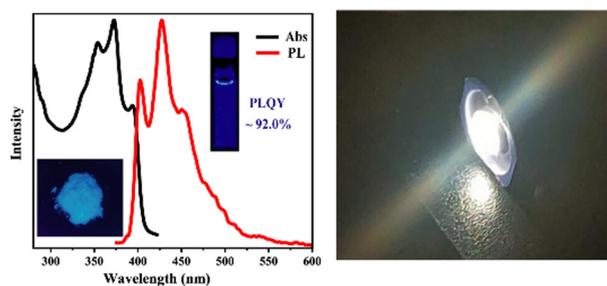
Sumon Pratihar, Mohamed Nabeel Mattath and Thimmaiah Govindaraju*



5721

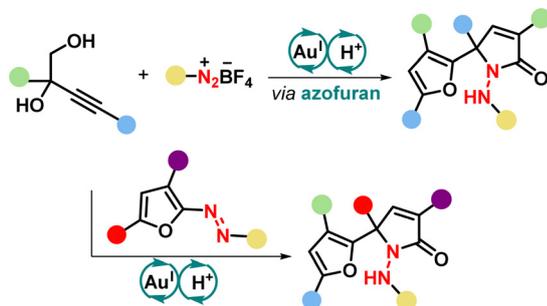
Ultrabright blue-light-emitting cesium bromide quantum dots for white LEDs

Tianfeng Li, Mengdi Qiao, Xingyi He, Rui Zhu, Xia Ran, Xiaojuan Wang,* Yu Jia and Lijun Guo*



COMMUNICATIONS

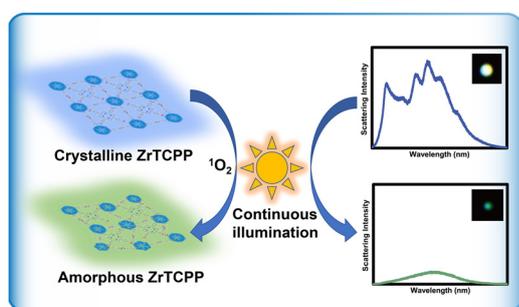
5725



Azofuran activation for annulative rearrangement enabled by gold(I)/Brønsted acid relay catalysis

Qian Rao, Yin Zhang, Yin-Ping Liu, Bo Jiang,*
Xiang Wang, Shu-Jiang Tu* and Wen-Juan Hao*

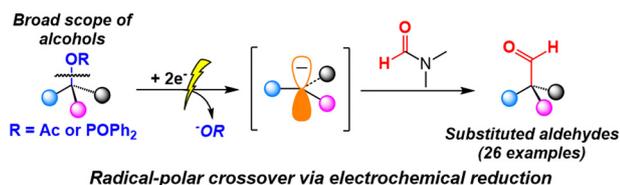
5729



Visual identification of $^1\text{O}_2$ -induced crystal structure transformation of single Zr-MOF by dark-field microscopy

Yue Xu, Qian Li, Wei He, Chang Ping Yang,
Peng Fei Gao,* Yuan Fang Li* and Cheng Zhi Huang*

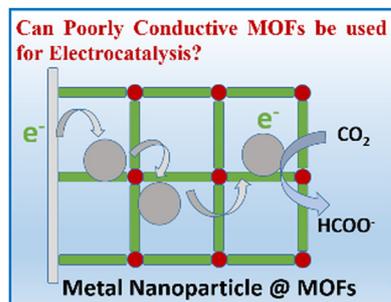
5733



Electroreductive formylation of activated alcohols via radical-polar crossover

Jungtaek Kang, Heyjin Cho and Hyunwoo Kim*

5737



Why can poorly conductive Bi@UiO-MOF catalyze CO_2 electroreduction?

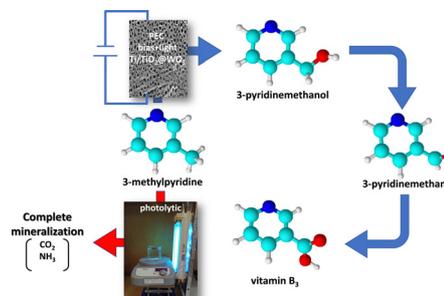
Xinru He, Ying Guo, Jingzheng Zhang, Shuangli Yang,
Jiawei Chen, Shurong Li, Shunji Xie, Ye Wang and
Cheng Wang*



5741

Selective photoelectrocatalytic oxidation of 3-methylpyridine to vitamin B₃ by WO₃ decorated nanotube-structured TiO₂

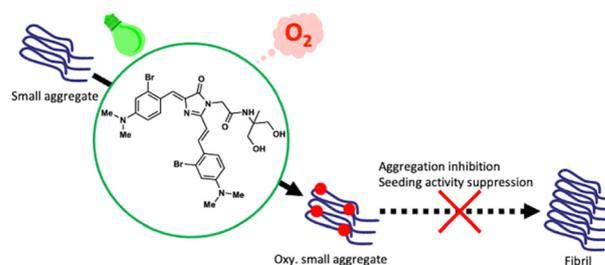
Sıdıka Çetinkaya, Levent Özcan, Oğuzhan Alagöz, Leonardo Palmisano and Sedat Yurdakal*



5745

Attenuation of α -synuclein aggregation by catalytic photo-oxygenation

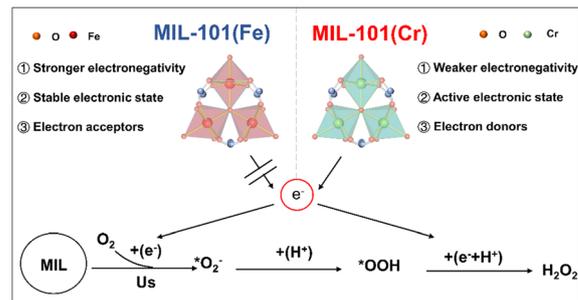
Atsushi Iwai, Reito Nakamura, Ikumi Tomizawa, Harunobu Mitsunuma, Yukiko Hori, Taisuke Tomita, Youhei Sohma* and Motomu Kanai*



5749

Modulating the metal center in MIL-101 for the piezoelectric catalytic synthesis of hydrogen peroxide

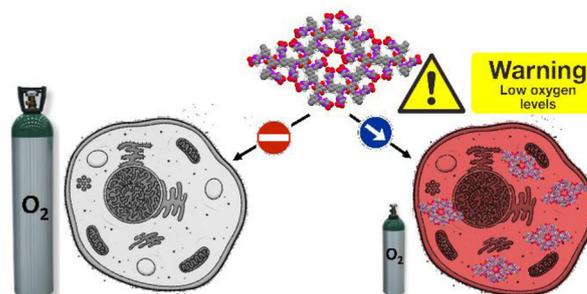
Yatai Li, Zhi Li, Xuecong Lin, Hao Lv and Mingshan Zhu*



5753

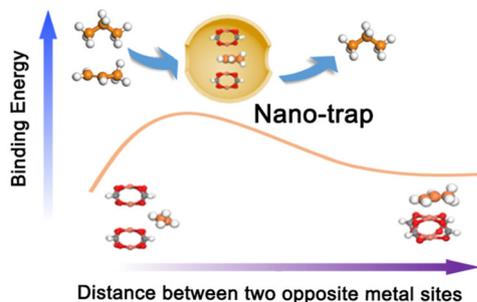
Nitroreductase-sensitive fluorescent covalent organic framework for tumor hypoxia imaging in cells

Tina Skorjanc,* Dinesh Shetty,* Sushil Kumar, Damjan Makuc, Gregor Mali, Janez Volavšek, Martina Bergant Marušič and Matjaz Valant



COMMUNICATIONS

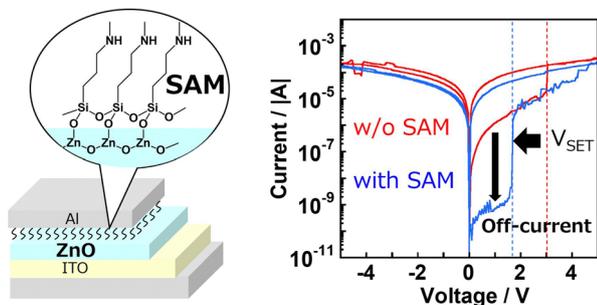
5757



Design of a MOF-based nano-trap for the efficient separation of propane from propylene

Hua Zhu, Yue Wang, Xin Wang, Zi-Wen Fan, Hui-Fang Wang,* Zheng Niu* and Jian-Ping Lang*

5761

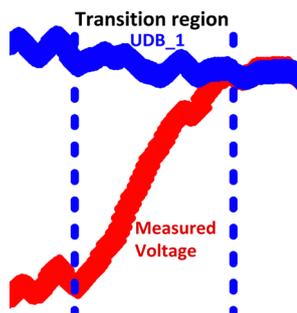


Control of the resistive switching voltage and reduction of the high-resistive-state current of zinc oxide by self-assembled monolayers

Masahiro Nakano,* Hiroki Matsui, Sae Nakagawa, Jiaxun You, Md. Shahiduzzaman, Makoto Karakawa and Tetsuya Taima

COMMENT

5765

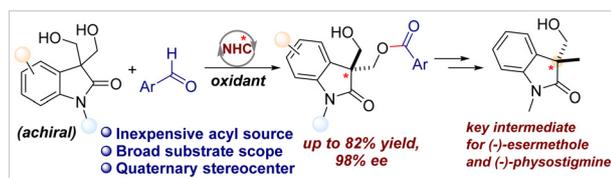


Comment on "Carbon content drives high temperature superconductivity in a carbonaceous sulfur hydride below 100 GPa" by G. A. Smith, I. E. Collings, E. Snider, D. Smith, S. Petitgirard, J. S. Smith, M. White, E. Jones, P. Ellison, K. V. Lawler, R. P. Dias and A. Salamat, *Chem. Commun.*, 2022, 58, 9064

J. E. Hirsch

COMMUNICATIONS

5771



N-Heterocyclic carbene catalyzed desymmetrization of diols: access to enantioenriched oxindoles having a C3-quaternary stereocenter

Sourav Dutta, Arka Porey and Joyram Guin*



5775

Intermolecular proton transfer from flavonol to human serum albumin triggers a red-shifted ratiometric fluorescence response

Zhongyong Xu, Mingyuan Zhang, Zihao Chen, Yutian Zhao, Lei Wang, Xiaoqiang Chen, Bin Liu* and Xiaojun Peng



5779

Intelligent convolution neural network-assisted SERS to realize highly accurate identification of six pathogenic *Vibrio*

Hui Yu, Zhilan Yang, Shiyong Fu, Yuejiao Zhang, Rajapandiyar Panneerselvam, Baoqiang Li, Lin Zhang,* Zehui Chen,* Xin Wang* and Jianfeng Li*

