

IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 25(47) 32275–32730 (2023)



Cover

See Gaige Zheng *et al.*, pp. 32336–32344. Image reproduced by permission of Gaige Zheng from *Phys. Chem. Chem. Phys.*, 2023, 25, 32336.



Inside cover

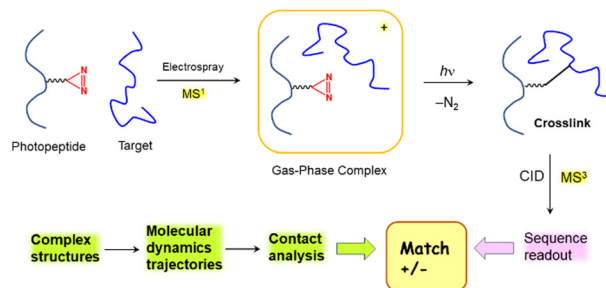
See Hamilton Varela *et al.*, pp. 32345–32355. Image reproduced by permission of Hamilton Varela from *Phys. Chem. Chem. Phys.*, 2023, 25, 32345.

PERSPECTIVES

32292

Covalent crosslinking in gas-phase biomolecular ions. An account and perspective

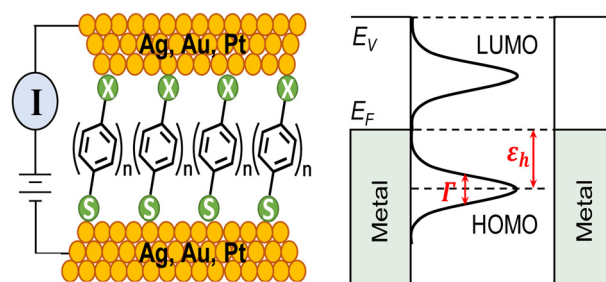
František Tureček



32305

Deciphering I – V characteristics in molecular electronics with the benefit of an analytical model

Davood Taherinia and C. Daniel Frisbie*



Editorial Staff

Executive Editor

Michael A. Rowan

Deputy Editor

Vikki Pritchard

Development Editors

Bee Hockin, Andrea Carolina Ojeda Porras

Editorial Production Manager

Gisela Scott

Senior Publishing Editor

Robin Brabham

Publisher

Jeanne Andres

Publishing Editors

Catherine Au, Isobel Darlington, Konoya Das, Alexandre Dumon, Amy Lucas, Kieran Nicholson, Rini Prakash, Charlotte Pugsley, Hugh Ryan

Publishing Assistant

Robert Griffiths

Editorial Assistant

Daphne Houston

For queries about submitted papers, please contact Gisela Scott, Editorial Production Manager, in the first instance. E-mail: pccp@rsc.org

For pre-submission queries, please contact Michael A. Rowan, Executive Editor. Email: pccp-rsc@rsc.org

PCCP (electronic ISSN 1463-9084) is published 48 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK.

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: £4448; US\$7835. 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

PCCP

Physical Chemistry Chemical Physics – An international journal

rsc.li/pccp

PCCP is an international journal for the publication of original research papers, Communications and Perspective articles in the areas of physical chemistry, chemical physics and biophysical chemistry.

Owner Societies

Canadian Society for Chemistry
Deutsche Bunsen-Gesellschaft für
Physikalische Chemie
Institute of Chemistry of Ireland
Israel Chemical Society
Kemisk Forenin
Koninklijke Nederlandse Chemische
Vereniging

Korean Chemical Society
New Zealand Institute of Chemistry
Norsk Kjemisk Selskap
Österreichische Physikalische Gesellschaft
Polskie Towarzystwo Chemiczne
Real Sociedad Española de Química
Royal Australian Chemical Institute
Incorporated

Royal Society of Chemistry
Società Chimica Italiana
Suomen Kemian Seura – Kemiska Sällskapet
I Finland
Svenska Kemisamfundet
Swiss Chemical Society
Türkiye Kimya Derneği

Honorary Board

G Ertl, Berlin, Germany
B Feringa, University of Groningen,
Netherlands
S W Hell, Max Planck Institute for Biophysical
Chemistry, Germany
J Jortner, Tel Aviv, Israel
M Karplus, Harvard University, USA

K Kohse-Hoeinghaus, Universitaet Bielefeld,
Germany
Y T Lee, Academia Sinica, Taiwan
S Matsika, Temple University, USA
E Neher, Max Planck Institute for Biophysical
Chemistry, Germany
J Polanyi, Toronto, Canada

H Schwarz, Technische Universität Berlin,
Germany
J P Simons, University of Oxford, UK
G A Somorjai, University of California,
Berkeley, USA
J Troe, GWDG, Germany
R N Zare, Stanford, USA

Editorial Board

B Albinsson, Chalmers University of
Technology, Sweden
L Bañares, Universidad Complutense de
Madrid, Spain
M Curri, University of Bari, Italy
C Daniel, Institute of Chemistry, University of
Strasbourg, France
L Goerigk, The University of Melbourne,
Australia
K Gordon, University of Otago, New Zealand

H Kondoh, Keio University, Japan
P Maiti, Indian Institute of Science, India
S Matsika, Temple University, USA
R Naaman, Weizmann Institute of Science,
Israel
A Rijs, Vrije Universiteit Amsterdam,
The Netherlands (Chair)
L Schaefer III, University of Georgia, USA
(Deputy Chair)
I Tamblin, University of Ottawa, Canada

Y Xu, University of Alberta, Canada
J Zhang, New York University Shanghai, China

Advisory Board

C Adamo, ENSCP - Chimie ParisTech, France
H Ågren, KTH Royal Institute of Technology,
Sweden
K Ariga, National Institute for Materials
Science, Japan
P Ayers, McMaster University, Canada
A Ajayaghosh, CSIR-National Institute for
Interdisciplinary Science and Technology
(NIIST), India
P Baglioni, University of Florence, Italy
V Barone, Scuola Normale Superiore di Pisa,
Italy
M Biczysko, Shanghai University, China
E Bieske, University of Melbourne, Australia
J Biteen, University of Michigan, USA
D Casanova, Donostia International Physics
Center, Spain
P Casavecchia, University of Perugia, Italy
O Christiansen, University of Aarhus, Denmark
G A Cisneros, University of North Texas, USA
S Coriani, Technical University of Denmark,
Denmark
M DeVries, University of California Santa
Barbara, USA
C Diaz, Universidad Complutense de Madrid,
Spain
J Dupont, University of Nottingham, UK
S Faraji, University of Groningen, Netherlands
D Frenkel, University of Cambridge, UK
A Fujii, Tohoku University, Japan

S George, Jawaharlal Nehru Centre for
Advanced Scientific Research (JNCASR), India
R B Gerber, Hebrew University Jerusalem,
Israel
D Ghosh, Indian Association for the
Cultivation of Science, India
D Goldfarb, Weizmann Institute of Science,
Israel
S Grimme, University of Bonn, Germany
M Havenith, Ruhr-University Bochum,
Germany
K Holmberg, Chalmers University of
Technology, Sweden
Y Iwasawa, University of Tokyo, Japan
D Jacquemin, Université de Nantes, France
T Jagau, KU Leuven, Belgium
E Johnson, Dalhousie University, Canada
J MacPherson, University of Warwick, UK
S.Matsika, Temple University, USA
H Mattoussi, Florida State University, USA
G Meijer, Fritz-Haber-Institut der Max-Planck-
Gesellschaft, Germany
F Neese, Max Planck Institute for Chemical
Energy Conversion, Germany
D Nesbitt, University of Colorado, USA
D Neumaier, University of California, Berkeley,
USA
M Orozco, IRB Barcelona - Parc Científic de
Barcelona, Spain
K Pas, Monash University, Australia

G Patwari, Indian Institute of Technology
Bombay, India
M-P Pileni, Université Pierre et Marie Curie,
France
M Pummer, Nanyang Technological University,
Singapore
P Pykkö, University of Helsinki, Finland
M Rodgers, Wayne State University, USA
S Sampath, Indian Institute of Science
Bangalore, India
R Signorell, ETH Zurich, Switzerland
T Schmidt, University of New South Wales,
Australia
M Suhm, University of Göttingen, Germany
A Suits, University of Missouri, USA
D Sundholm, University of Helsinki, Finland
T Suzuki, Kyoto University, Japan
A Troisi, University of Warwick, UK
S Vega, Weizmann Institute of Science, Israel
D Waldeck, University of Pittsburgh, USA
L J Wan, Institute of Chemistry, Chinese
Academy of Sciences, China
B Weckhuysen, Utrecht University,
The Netherlands
X Yang, Dalian Institute of Chemical Physics,
Chinese Academy of Sciences, China
A Zehnacker-Rentien, Université Paris, France

Information for Authors

Full details on how to submit material for publication in PCCP 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/pccp

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 Owner Societies.

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

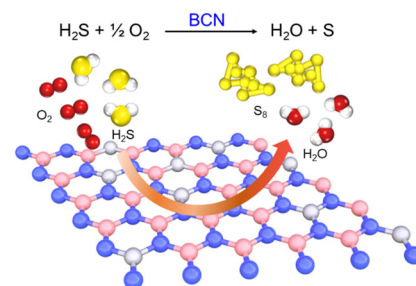


COMMUNICATIONS

32317

Carbon-doped boron nitride nanosheets as an efficient metal-free catalyst for the selective oxidation of H₂S

Ganchang Lei, Sihui Qi, Haiyan Li, Yinjiang Xue, Lijuan Shen,* Xiaohai Zheng, Shiping Wang, Yanning Cao and Yingying Zhan*

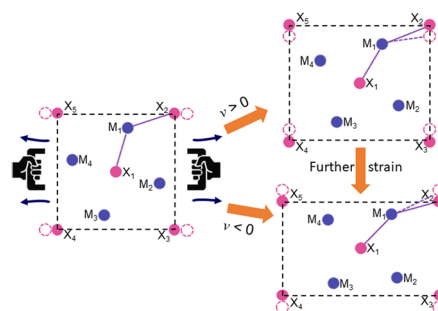


Enhancing sulfur and corrosion resistance performance

32323

Prediction of 2D group-11 chalcogenides: insights into novel auxetic M₂X (M = Cu, Ag, Au; X = S, Se, Te) monolayers

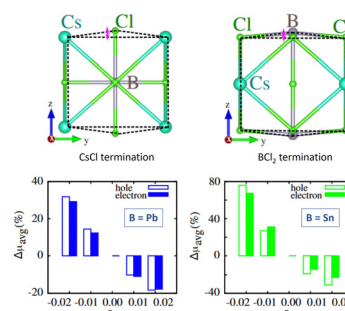
Yufei Xue, Lei Gao,* Weina Ren, Xuxia Shai, Tingting Wei, Chunhua Zeng* and Hua Wang*



32330

Surface termination and strain-induced modulation of the structure and electronic properties in 2D perovskites (Cs₂BCl₄ & CsB₂Cl₅, B = Pb, Sn): a first-principles study

Kiran Yadav and Nirat Ray*

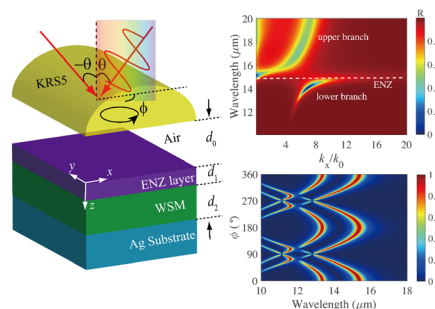


RESEARCH PAPERS

32336

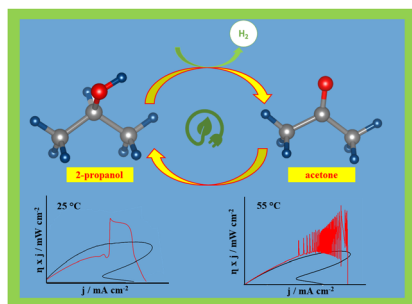
Weyl semimetal mediated epsilon-near-zero hybrid polaritons and the induced nonreciprocal radiation

Sicheng Xu, Liming Qian, Mengran Sun and Gaige Zheng*



RESEARCH PAPERS

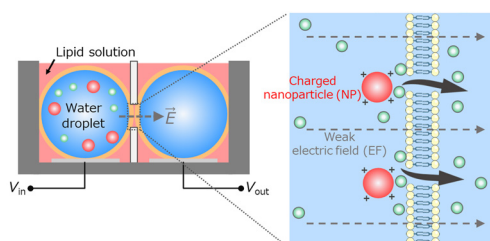
32345



The oscillatory electro-oxidation of 2-propanol on platinum: the effect of temperature and addition of methanol

Gianluca Ragassi, André H. B. Dourado and Hamilton Varela*

32356

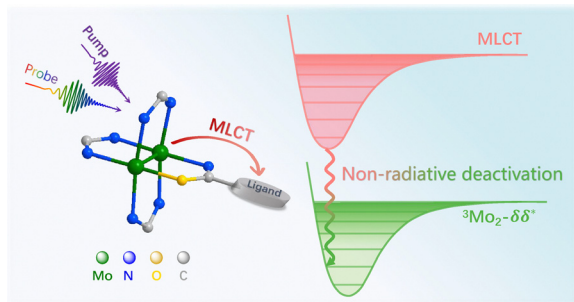


Charged NP + Weak EF = Cell-membrane-crossing of compounds without membrane breakdown

Enhancement of cell membrane permeability by using charged nanoparticles and a weak external electric field

Hideya Nakamura,* Takumi Okamura, Masaya Tajima, Ryuji Kawano, Misa Yamaji, Shuji Ohsaki and Satoru Watano

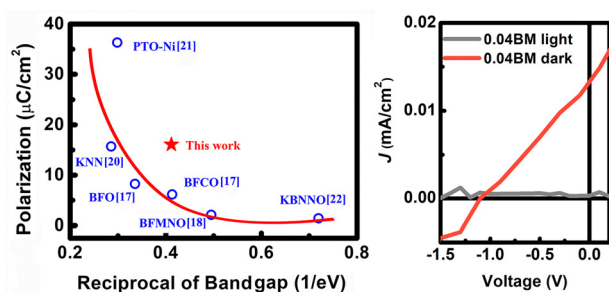
32364



Influence of ligand variation on the deactivation process of metal-to-ligand charge transfer excited states in quadruply bonded dimolybdenum complexes

Yuqing Shi, Juanjuan Li, Can Cui, Guanzhi Wu* and Tao Cheng*

32372



Simultaneous improvement of polarization and bandgap by finite solid solution engineering

Fei Guo,* Rui Liu, Siyuan Guo, Yaping Liu, Lei Gao and Shifeng Zhao*

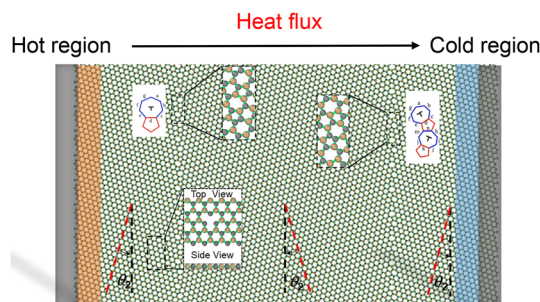


RESEARCH PAPERS

32378

Impacts of defects on the mechanical and thermal properties of SiC and GeC monolayers

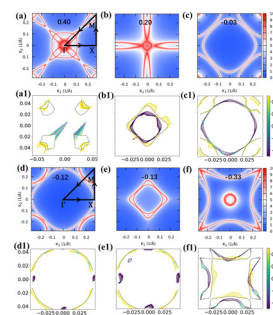
Kai Ren, Lei Huang, Huabing Shu, Guoqiang Zhang, Weihua Mu,* Huanping Zhang, Huasong Qin* and Gang Zhang*



32387

Ab initio study of the topological itinerant transport properties observed between excited edge states in a 2D compound with the $\text{Mn}_{15}\text{B}_{16}\text{Ni}$ composition

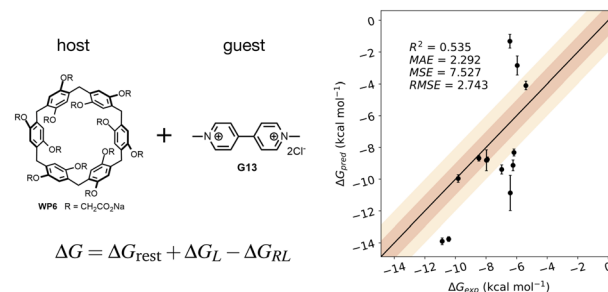
Wuyue Xu, Zhengxin Yan,* Kezhao Xiong, Juntao Kong, Wei Song, Dongxin Li, Qian Cheng, Zehua Zhao and Xingkun Liang



32393

Expanded ensemble predictions of absolute binding free energies in the SAMPL9 host–guest challenge

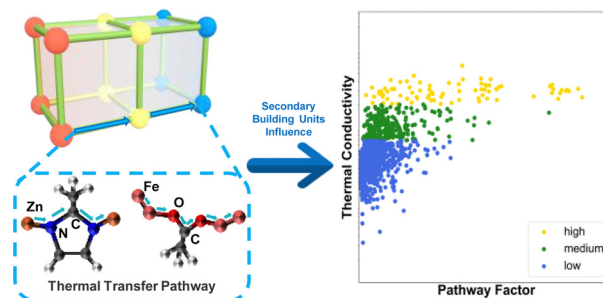
Matthew F. D. Hurley, Robert M. Raddi, Jason G. Pattis and Vincent A. Voelz*



32407

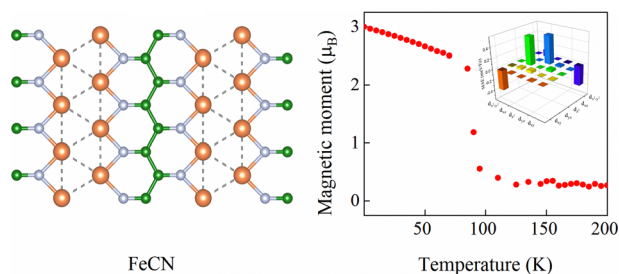
Understanding the influence of secondary building units on the thermal conductivity of metal–organic frameworks via high-throughput computational screening

Yuanchuang Lin, Ruihuan Cheng, Tiangui Liang, Weixiong Wu, Song Li* and Wei Li*



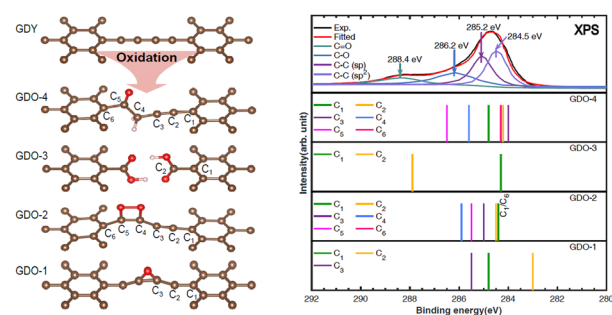
RESEARCH PAPERS

32416

**2D antiferromagnetic semiconducting FeCN with interesting properties**

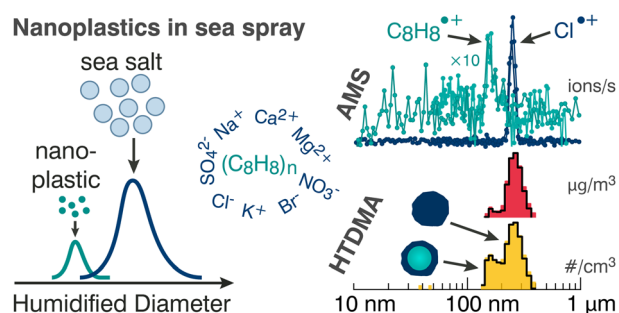
Zhicui Wang, Huan Lou, Xu Yan, Yong Liu* and Guochun Yang*

32421

**First-principles simulation of X-ray spectra of graphdiyne and graphdiyne oxides at the carbon K-edge**

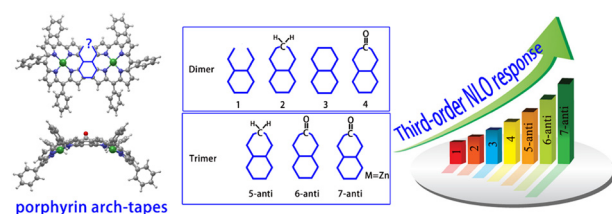
Jing Ming, Jun-Rong Zhang, Xiu-Neng Song, Xin Li, Weijie Hua* and Yong Ma*

32430

**Morphology and hygroscopicity of nanoplastics in sea spray**

Sarah Suda Petters,* Eva Rosendal Kjærgaard, Freja Hasager, Andreas Massling, Marianne Glasius and Merete Bilde*

32443

**Theoretical study on porphyrin arch-tapes of carbonyl-inserted seven-membered rings with high nonlinear optical properties**

Jin-Ting Ye,* Li-Hui Wang and Jia-Qi Yu*

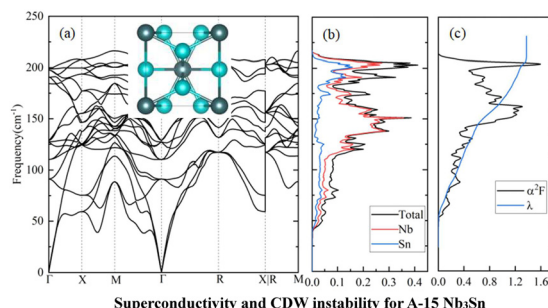


RESEARCH PAPERS

32452

Coexistence of superconductivity and charge density wave instability in A15-Nb₃Sn

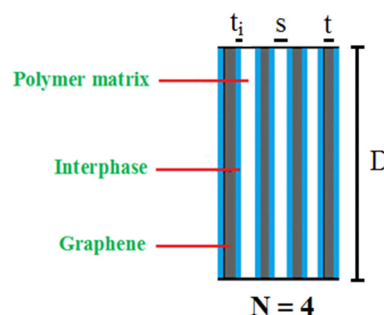
Li-Na Wu, Si-Tong Yang, Jin-Ke Shen, Jian-Sheng Zhang and Fei-Hu Liu*



32460

Percolation onset and conductivity of nanocomposites assuming an incomplete dispersion of graphene nanosheets in a polymer matrix

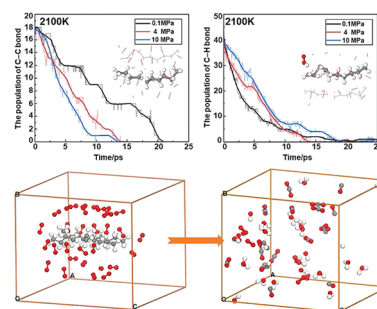
Yasser Zare,* Muhammad Tajammal Munir and Kyong Yop Rhee*



32471

Oxidation kinetic mechanism of *n*-decane under high temperature and pressure: a first-principles molecular dynamics study

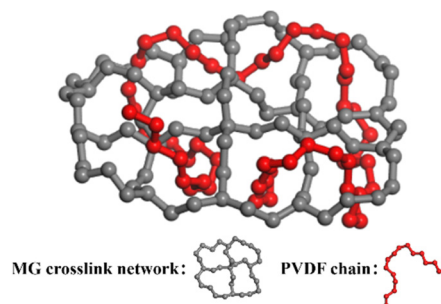
Teng Zhang, Wenbo Xia, Wei Fan,* Lang Chen* and Jun Chen*



32482

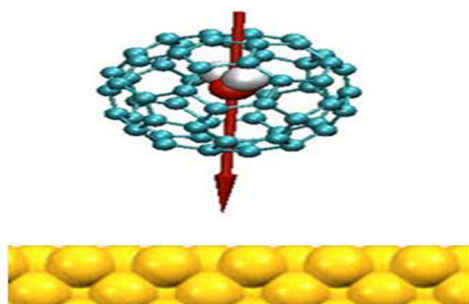
Crosslinking modification and hydrogen bonding synergy to achieve high breakdown strength and energy density of PMMA-co-GMA/PVDF dielectric composite films

Shuo Zheng, Xuanchen Zhao, Junhao Xie and Shulin Sun*



RESEARCH PAPERS

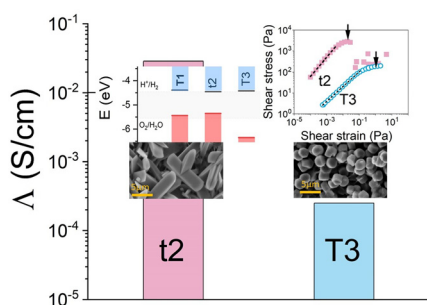
32493



Fullerenes containing water molecules: a study of reactive molecular dynamics simulations

Masumeh Foroutan,* Ahmad Boudaghi and Mahtab Alibalazadeh

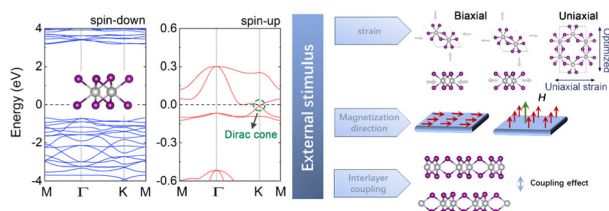
32503



Morphological control for high proton conduction in robust Co_3O_4 -diethylmethylamine (metal–organic framework) membrane

Gargi Yadav, Pardeep K. Jha, Priyanka A. Jha,* Parvin K. Singh, Suman Roy Choudhary and Prabhakar Singh*

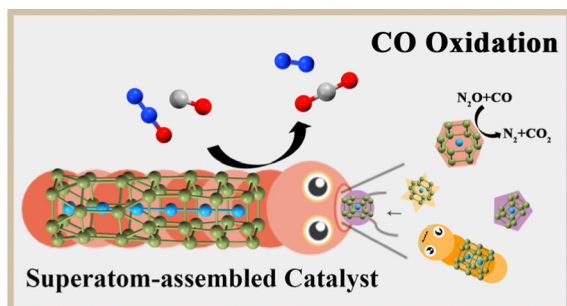
32515



Tunable electronic band structure and magnetic anisotropy in two-dimensional Dirac half-metal MnBr_3 by external stimulus: strain, magnetization direction, and interlayer coupling

Fangyuan Xie, Zhengyu Yin, Baozeng Zhou* and Yanhong Ding*

32525



Theoretical prediction of superatom WSi_{12} -based catalysts for CO oxidation by N_2O

Ya-Ling Ye, Zhi-Chao Zhang, Bi-Lian Ni, Dan Yu, Jing-Hua Chen and Wei-Ming Sun*

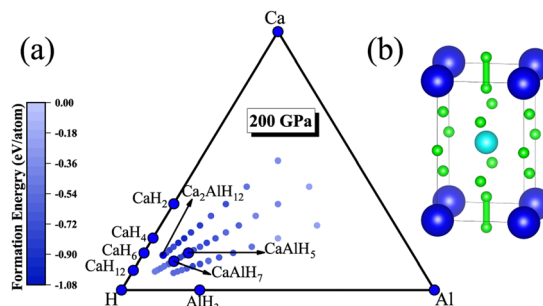


RESEARCH PAPERS

32534

Phase diagrams and superconductivity of ternary Ca–Al–H compounds under high pressure

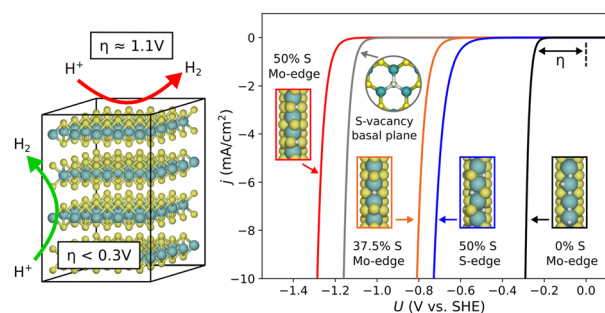
Ming Xu, Defang Duan, Mingyang Du, Wendi Zhao, Decheng An, Hao Song* and Tian Cui*



32541

Sulfur-deficient edges as active sites for hydrogen evolution on MoS₂

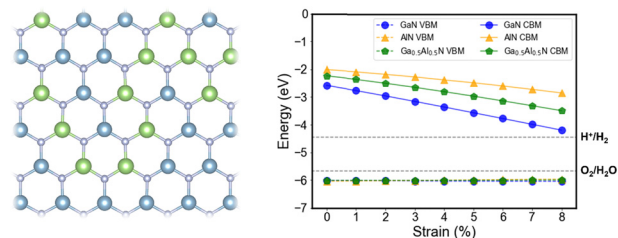
Sander Ø. Hanslin, Hannes Jónsson and Jaakko Akola*



32549

Two-dimensional III-nitride alloys: electronic and chemical properties of monolayer Ga_(1-x)Al_xN

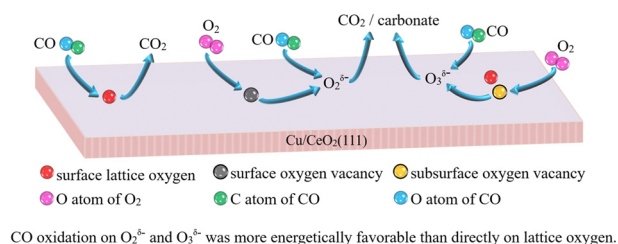
Yiqing Chen, Ying Zhao, Pengfei Ou* and Jun Song*



32557

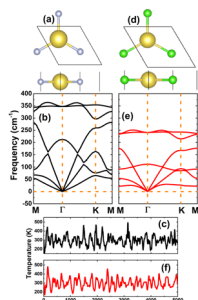
Formation of superoxide and ozone-like species on Cu doped CeO₂(111) and their CO oxidation reactivity: a DFT study

Hao Wang, Yuan Li, Jiao Han, Caishun Zhang, Honghao Wang, Daosheng Liu, Xiaoning Hou, Lei Zhang* and Zhixian Gao*



RESEARCH PAPERS

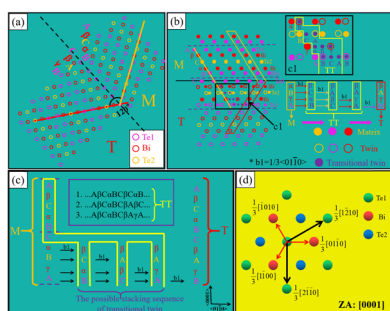
32569



Doping-mediated electronic and magnetic properties of graphene-like ionic NaX (X = F and Cl) monolayers

Bich Ngoc Nguyen Thi, Chu Viet Ha, Nghiem Thi Ha Lien, J. Guerrero-Sanchez and D. M. Hoat*

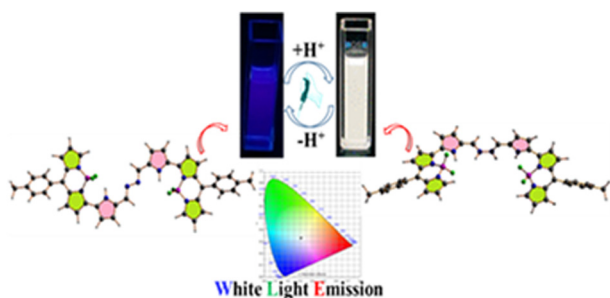
32578



Transitional structure of {0001} twin in a deformed p-type (Bi,Sb)₂Te₃ alloy: a direct experimental basis for understanding the twinning mechanism

Jie Ren, Wenbin Guo, Fuzhou Han,* Qichen Wang, Yi Cao, Songbin Li, Geping Li,* Muhammad Ali, Jianan Hu, Fusen Yuan and Yingdong Zhang

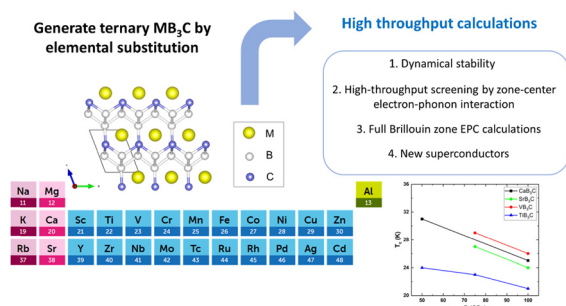
32584



A white light emitting single halochromic hydrazine bridged bis(3-pyrrolyl BODIPY) fluorophore

Kanhu Charan Behera and Mangalampalli Ravikanth*

32594



Prediction of superconductivity in metallic boron-carbon compounds from 0 to 100 GPa by high-throughput screening

Feng Zheng, Yang Sun,* Renhai Wang, Yimei Fang, Feng Zhang, Shunqing Wu,* Qiubao Lin,* Cai-Zhuang Wang, Vladimir Antropov and Kai-Ming Ho

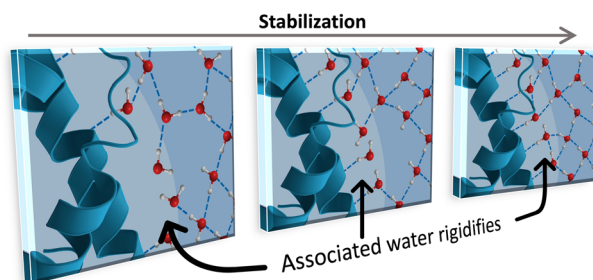


RESEARCH PAPERS

32602

Osmolyte induced protein stabilization: modulation of associated water dynamics might be a key factor

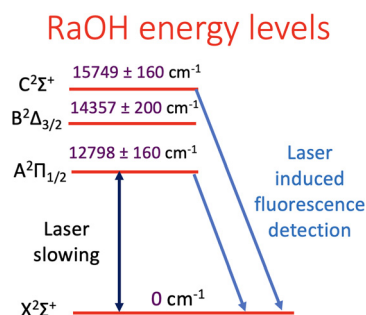
Kuldeep Singh Negi, Nilimesh Das, Tanmoy Khan and Pratik Sen*



32613

Relativistic coupled-cluster calculations of RaOH pertinent to spectroscopic detection and laser cooling

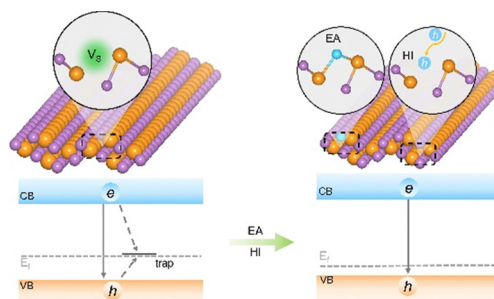
Chaoqun Zhang, Phelan Yu, Chandler J. Conn, Nicholas R. Hutzler* and Lan Cheng*



32622

Blocking recombination centers by controlling the charge density of a sulfur vacancy in antimony trisulfide

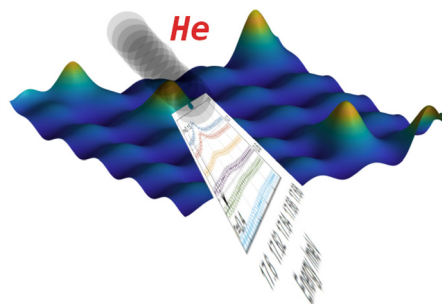
Xiao Han, Qi Zhao, Xiaodan Yan, Ting Meng* and Jinlu He*



32632

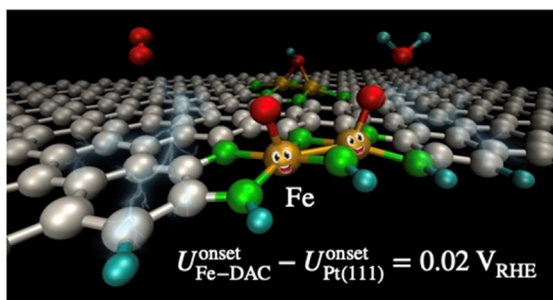
Blue shifts in helium-surface bound-state resonances and quantum effects in cosine-law scattering

Luke Staszewski and Nadav Avidor*



RESEARCH PAPERS

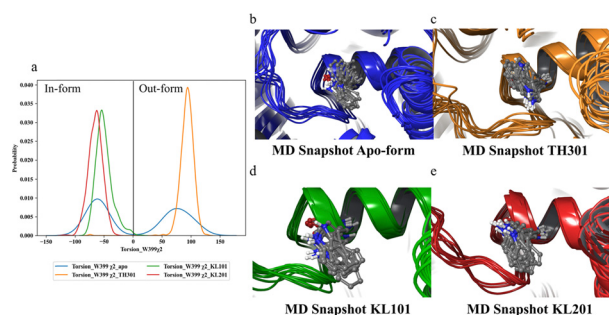
32637



Graphene-edge-supported iron dual-atom for oxygen reduction electrocatalysts

Joel F. Sumbowo, Farhan A. Ihsan, Fadjar Fathurrahman, Nadya Amalia, Fiki T. Akbar, Hadi T. Yudistira, Nadhratun N. Mobarak, Hermawan K. Dipojono, Sasfan A. Wella* and Adhitya G. Saputro*

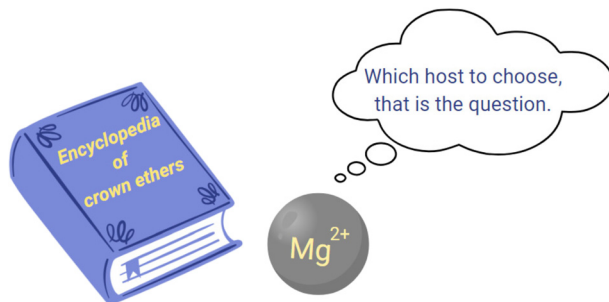
32648



Elucidating TH301's influence on the torsion angle of CRY1 W399 using replica exchange with solute tempering (REST) molecular dynamics (MD) simulations

Yeongrae Cho, Kexin Li, Jin Hyup Lee, Seung Pil Pack and Art E. Cho*

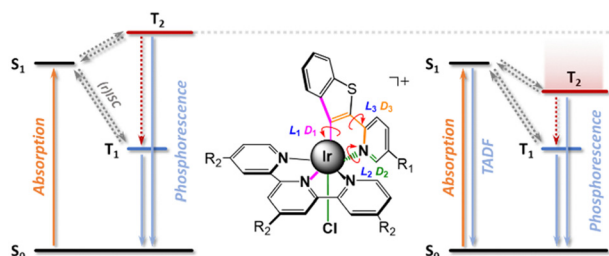
32656



Density functional theory study of crown ether–magnesium complexes: from a solvated ion to an ion trap

Katarina Čeranić, Branislav Milovanović and Milena Petković*

32666



Computational study of the photophysical properties and electronic structure of iridium(III) photosensitizer complexes with electron-withdrawing groups

Yunlong Shang, Zhoujie Zhang, Mengping Huang, Na Shu, Hanyu Luo, Qiyan Cao, Bingbing Fan, Yu Han, Min Fang,* Yong Wu* and Jiawei Xu*

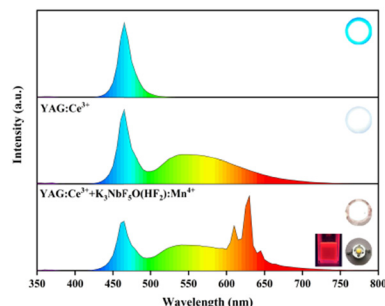


RESEARCH PAPERS

32675

A highly efficient Mn^{4+} activated Nb-based oxyfluoride red fluorescent material with excellent water stability: preparation and performance analysis

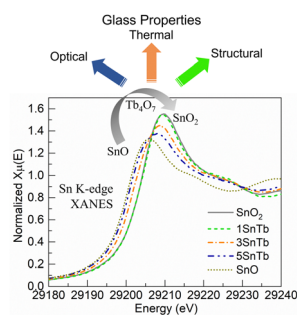
Ruiyang Wang, Hui Zhou, Wenjie Shi, Xiaofang Yu,*
Xiaoyun Mi,* Xiuling Liu and Yanping Wang



32688

XANES analysis of phosphate glasses melted with Tb_4O_7 and SnO : evaluating the impact of valence states on structural, thermal, and luminescent properties

José A. Jiménez,* Dugan Hayes, Cali Antolini and Benjamin J. Reinhart



32699

Styrylpyrimidine chromophores with bulky electron-donating substituents: experimental and theoretical investigation

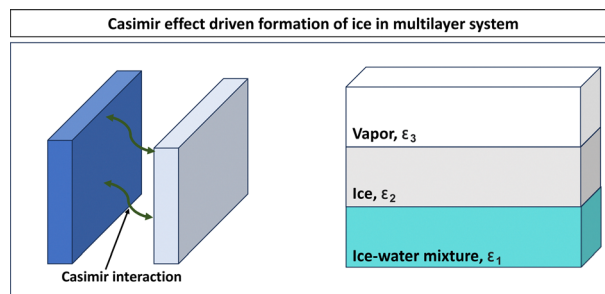
Maxime Hodée, Julien Massue,* Sylvain Achelle,*
Arnaud Fihey,* Denis Tondelier, Gilles Ulrich,
Françoise Robin-le Guen and Claudine Katan



32709

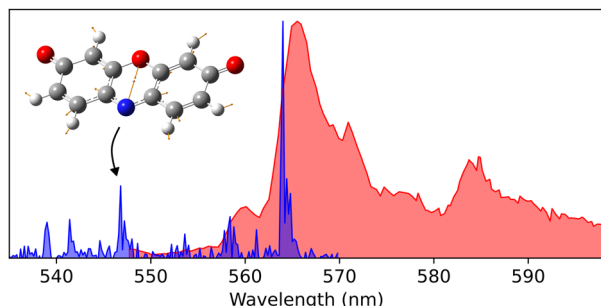
van der Waals induced ice growth on partially melted ice nuclei in mist and fog

M. Boström,* Y. Li,* I. Brevik, C. Persson,
S. Carretero-Palacios and O. I. Malyi*



RESEARCH PAPERS

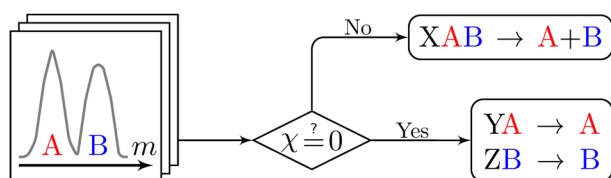
32715

**Cryogenic fluorescence spectroscopy of oxazine ions isolated *in vacuo***

Christina Kjær,* Emil Vogt, Jeppe Langeland, Nanna Falk Christensen, Thomas Toft Lindkvist, Henrik G. Kjaergaard and Steen Brøndsted Nielsen

COMMENT

32723

**Comment on “Cumulant mapping as the basis of multi-dimensional spectrometry” by Leszek J. Frasinski, *Phys. Chem. Chem. Phys.*, 2022, 24, 20776–20787**

Åke Andersson

Original work: $\chi_1, \dots, \chi_6(\dots) = \dots$
 This comment: $\forall n \in \mathbb{N}: \chi_n(\dots) = \dots$

CORRECTIONS

32726

Correction: Cumulant mapping as the basis of multi-dimensional spectrometry

Leszek J. Frasinski

32727

Correction: Understanding the charge transfer dynamics of the Cu₂WS₄–CNT–FeOOH ternary composite for photo-electrochemical studies

Preeti Dagar, Nandan Ghorai, Manisha Bungla, Hirendra N. Ghosh* and Ashok K. Ganguli*



CORRECTIONS

32728

Correction: UV and VUV-induced fragmentation of tin-oxo cage ions

Jarich Haitjema, Lianjia Wu, Alexandre Giuliani, Laurent Nahon, Sonia Castellanos and Albert M. Brouwer*

