

IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 25(12) 8223–8970 (2023)



Cover
See Panpan Wang et al., pp. 8341–8354. Image reproduced by permission of Panpan Wang from *Phys. Chem. Chem. Phys.*, 2023, 25, 8341.



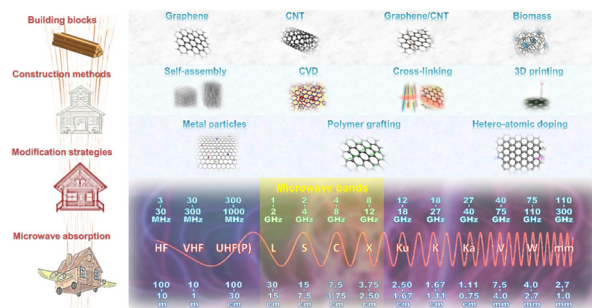
Inside cover
See David A. Dixon et al., pp. 8355–8368. Image reproduced by permission of David A. Dixon from *Phys. Chem. Chem. Phys.*, 2023, 25, 8355.

REVIEWS

8244

Construction and application of carbon aerogels in microwave absorption

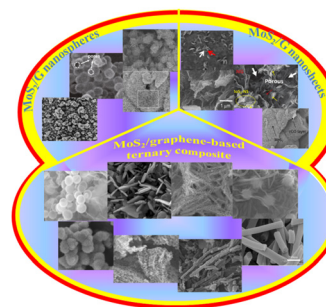
Yifan Guo, Junhua Su, Tongxin Bian, Jing Yan, Longkun Que, Hunan Jiang, Jinlong Xie, Ying Li, Yong Wang and Zuowan Zhou*



8263

Recent advances in hierarchical MoS₂/graphene-based materials for supercapacitor applications

Ying Ma, Jinchuan Liu, Yinhe Lin* and Yulong Jia*



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, Hugh Ryan, Wing So

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-Hoinghaus, Universitaet Bielefeld, Germany
Y T Lee, Academia Sinica, Taiwan
W H Miller, Berkeley, 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
I Bañares, Universidad Complutense de Madrid, Spain
M Curri, University of Bari, Italy
C Daniel, Institute of Chemistry, University of Strasbourg, France
K Gordon, University of Otago, New Zealand

J Janek, Justus Liebig University Giessen, Germany
H Kondoh, Keio University, Japan
A Krylov, University of Southern California, USA
P Maiti, Indian Institute of Science, India
R Naaman, Weizmann Institute of Science, Israel

A Rijs, Vrije Universiteit Amsterdam, The Netherlands (Chair)
H 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 Pyykkö, 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 Weckhuyzen, 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

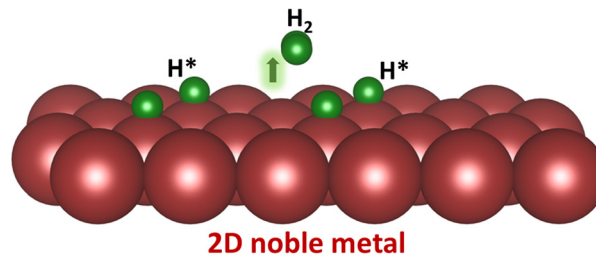


PERSPECTIVES

8281

2D noble metals: growth peculiarities and prospects for hydrogen evolution reaction catalysis

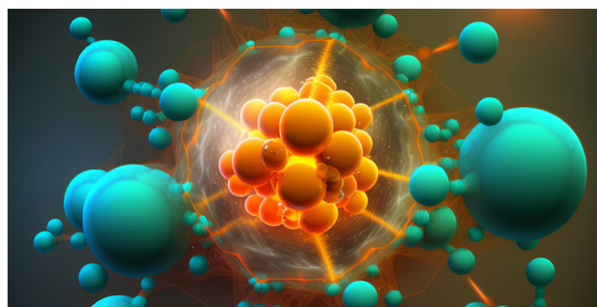
Ivan Shteplyuk



8293

Surface hopping modeling of charge and energy transfer in active environments

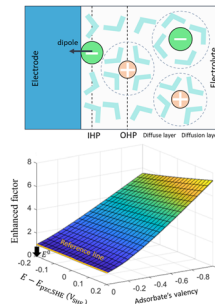
Josene M. Toldo,* Mariana T. do Casal, Elizete Ventura, Silmar A. do Monte* and Mario Barbatti*



8317

The electrostatic effect and its role in promoting electrocatalytic reactions by specifically adsorbed anions

Wei Chen, Lu-Lu Zhang, Zhen Wei, Meng-Ke Zhang, Jun Cai* and Yan-Xia Chen*

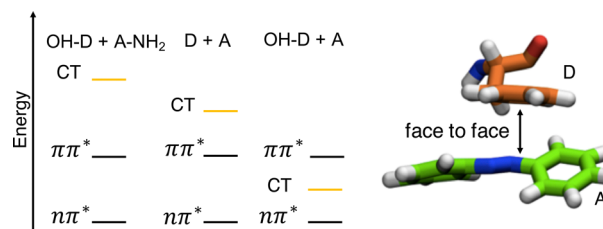


COMMUNICATIONS

8331

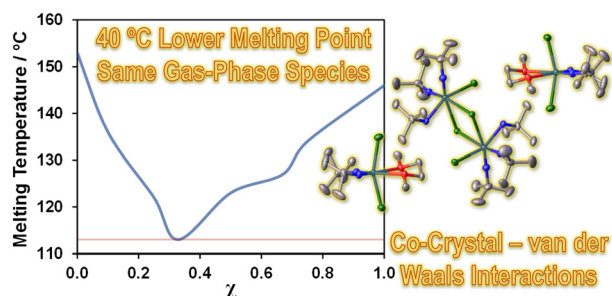
Effect of stacking interactions on charge transfer states in photoswitches interacting with ion channels

Vito F. Palmisano, Shirin Faraji* and Juan J. Nogueira*



COMMUNICATIONS

8336

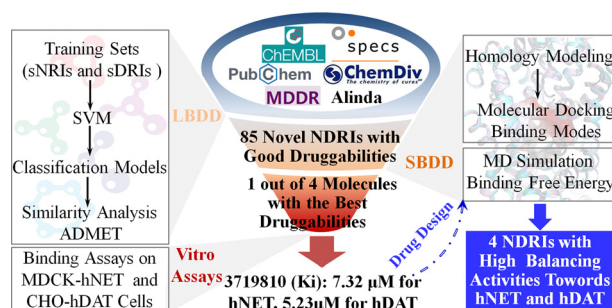


Disturbance of intermolecular forces: eutectics as a new tool for the preparation of vapor-phase deposition precursors

Michael A. Land,* Katherine N. Robertson,
Jason A. C. Clyburne and Seán T. Barry

RESEARCH PAPERS

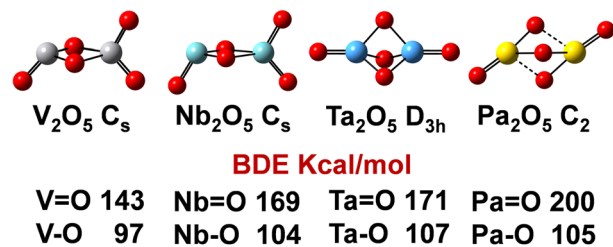
8341



A multiple-step screening protocol to identify norepinephrine and dopamine reuptake inhibitors for depression

Panpan Wang,* Fengmei Yan, Jianghong Dong,
Shengqiang Wang, Yu Shi, Mengdan Zhu, Yuting Zuo,
Hui Ma, Ruirui Xue, Dingjie Zhai and Xiaoyu Song

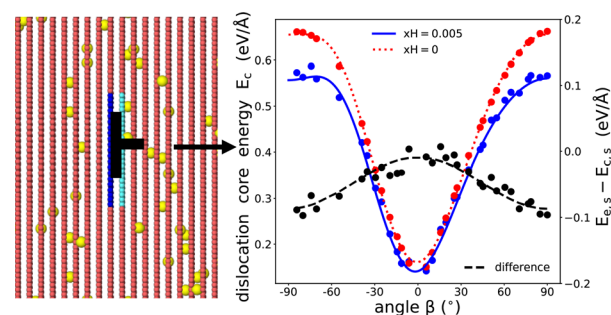
8355



Prediction of the structures and heats of formation of MO_2 , MO_3 , and M_2O_5 for $M = V, Nb, Ta, Pa$

Eddy Lontchi, Marcos M. Mason, Monica Vasiliu and
David A. Dixon*

8369



An interplay between a hydrogen atmosphere and dislocation characteristics in BCC Fe from time-averaged molecular dynamics

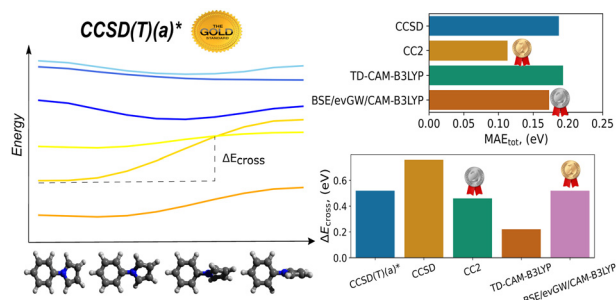
C. Nowak and X. W. Zhou*



8376

Excited state potential energy surfaces of *N*-phenylpyrrole upon twisting: reference values and comparison between BSE/GW and TD-DFT

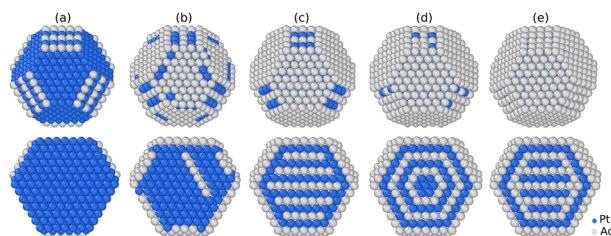
Iryna Knysh, Kelvine Letellier, Ivan Duchemin, Xavier Blase* and Denis Jacquemin*



8386

Composition-dependent chemical ordering predicted in Pt–Ag nanoalloys

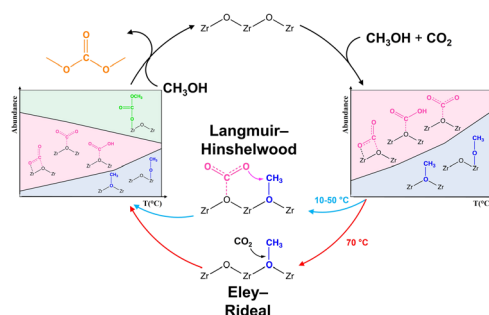
Alexis Front and Christine Mottet



8392

Surface species in direct liquid phase synthesis of dimethyl carbonate from methanol and CO₂: an MCR-ALS augmented ATR-IR study

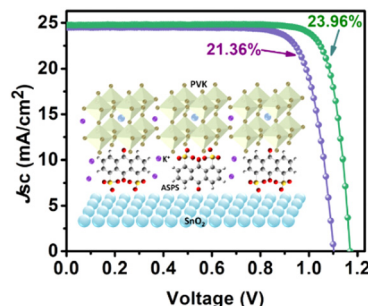
Matteo Signorile,* Davide Salusso, Valentina Crocellà, Maria Cristina Paganini, Silvia Bordiga, Francesca Bonino and Davide Ferri



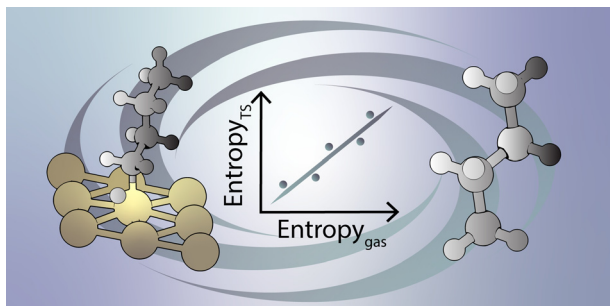
8403

Multifunctional anthraquinone-sulfonic potassium salts passivate the buried interface for efficient and stable planar perovskite solar cells

Yanqiang Hu, Zong Xu, Zhi Wang, Yifan Zhou, Wenwu Song, Yushuang Gao, Guangping Sun, Tongming Sun, Shufang Zhang* and Yanfeng Tang*



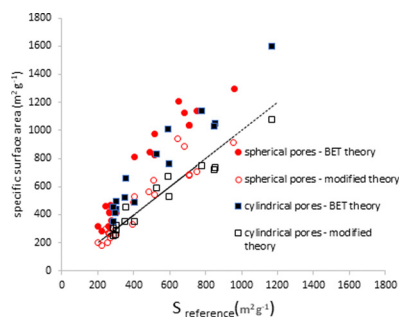
8412



Transition-state correlations for predicting thermochemistry of adsorbates and surface reactions

Sophia J. Kurdziel and Dionisios G. Vlachos*

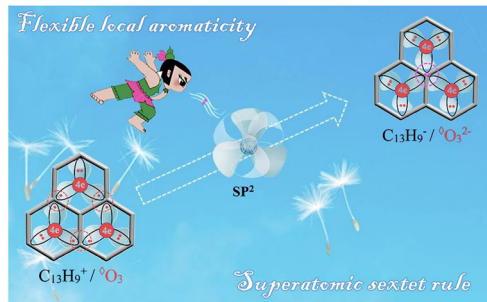
8424



Modified BET theory for actual surfaces: implementation of surface curvature

Behnaz Alinaghypour and Cavus Falamaki*

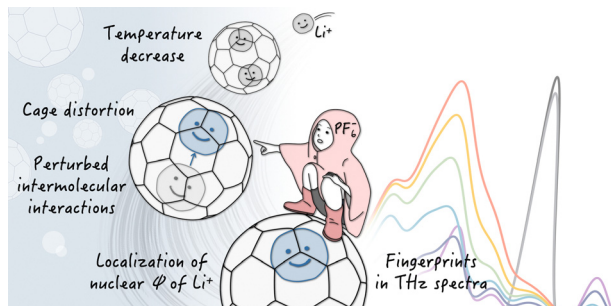
8439



Unraveling the flexible aromaticity of $C_{13}H_9^{+/0/-}$: a 2D superatomic-molecule theory

Dan Li, Chen Yan, Qinqin Yuan,* Lili Shi and Longjiu Cheng*

8446



Localization of nuclear wave functions of lithium in $[Li^+@C_{60}]PF_6^-$: molecular insights into two-site disorder–order transition

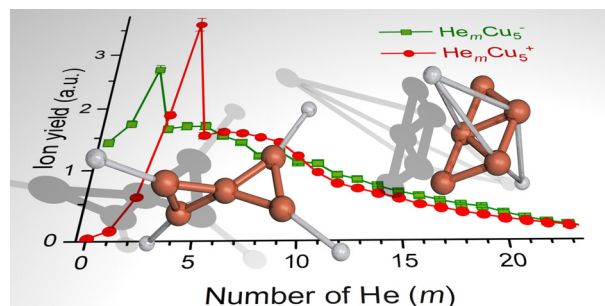
Hideo Ando* and Yoshihide Nakao



8463

Structure and formation of copper cluster ions in multiply charged He nanodroplets

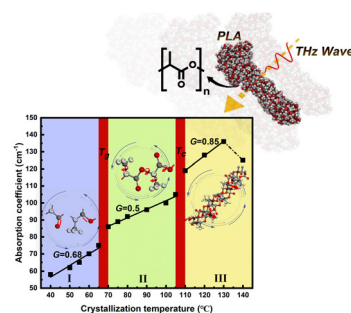
O. V. Lushchikova,* M. Gatchell, J. Reichegger, S. Kollotzek, F. Zappa, M. Mahmoodi-Darian and P. Scheier



8472

Study on the crystallization behavior and conformation adjustment scale of poly(lactic acid) in the terahertz frequency range

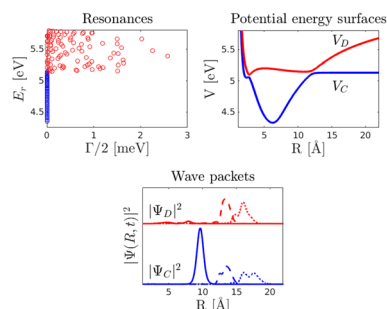
Zhenqi Zhu, Yujing Bian, Xun Zhang, Ruonan Zeng and Bin Yang*



8482

Nonadiabatic wave packet dynamics and predissociation resonances in sodium hydride

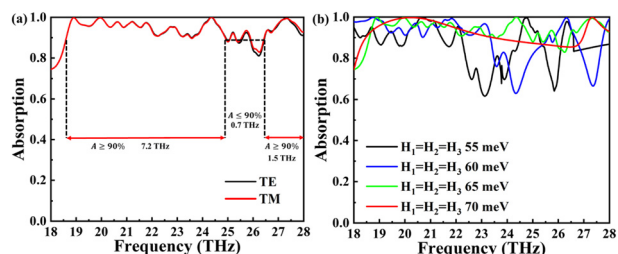
Hans O. Karlsson



8489

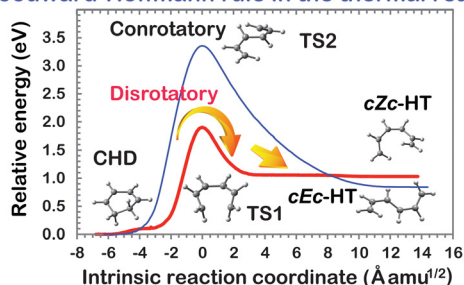
Tunable broadband absorber based on a layered resonant structure with a Dirac semimetal

Wenxin Li, Jing Ma, Huafeng Zhang, Shubo Cheng,* Wenxing Yang,* Zao Yi,* Hua Yang, Jianguo Zhang, Xianwen Wu and Pinghui Wu



8497

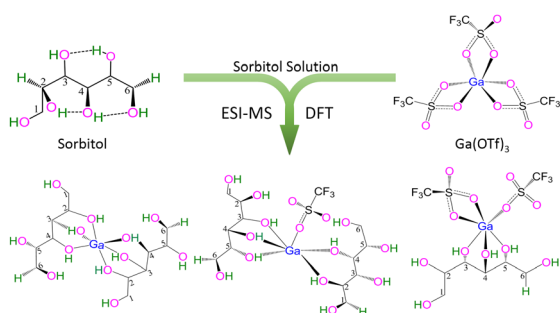
Woodward-Hoffmann rule in the thermal reaction



Real-time observation of the Woodward–Hoffmann rule for 1,3-cyclohexadiene by femtosecond soft X-ray transient absorption

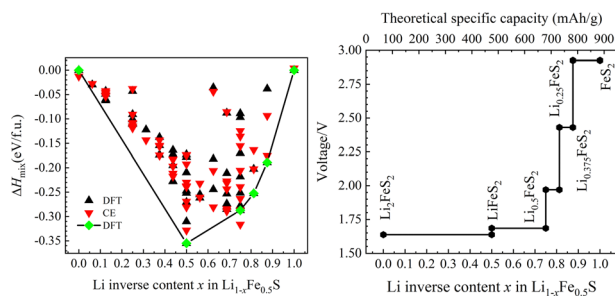
Taro Sekikawa,* Nariyuki Saito, Yutaro Kurimoto, Nobuhisa Ishii, Tomoya Mizuno, Teruto Kanai, Jiro Itatani, Kenichiro Saita and Tetsuya Taketsugu

8507

Coordination of sorbitol to Ga(OTf)₃ in the liquid phase: an experimental and theoretical study

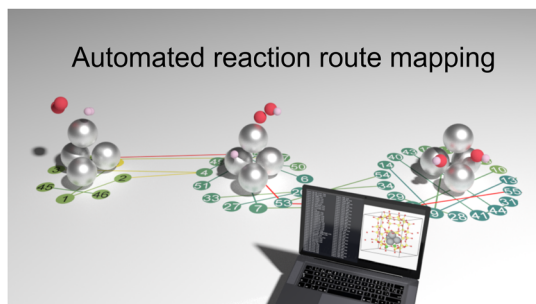
Mei Li, Jin-Shan Xiong, Han-Yun Min, Ye-Xin Hu, Liang-Fang Zhu, Chang-Wei Hu and Hua-Qing Yang*

8515

Insights into the electrochemical properties of Li₂FeS₂ after FeS₂ discharging

Cheng-dong Wei, Hong-tao Xue, Xu-dong Zhao and Fu-ling Tang*

8524

An automated reaction route mapping for the reaction of NO and active species on Ag₄ clusters in zeolites

Shunsaku Yasumura, Taisetsu Kato, Takashi Toyao, Zen Maeno and Ken-ichi Shimizu*

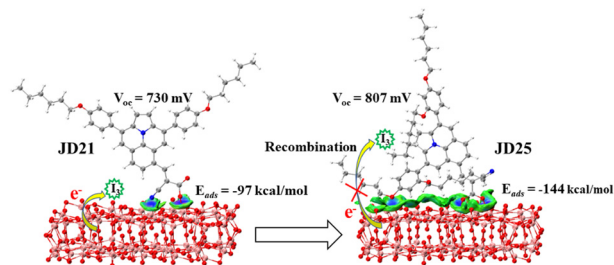


RESEARCH PAPERS

8532

New insights into the alkoxy effects on auxiliary adsorption and inhibiting charge recombination in dye-sensitized solar cells with high open circuit voltage: a theoretical investigation

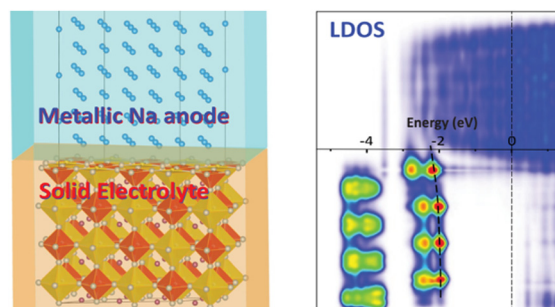
Zi-Han Xu, Chang-Yan Zhu, Xiao-Fei Zhu, Yu-Juan Zhai, Ji Zhang* and Han-Cheng Zhu*



8544

Insight into the structural and electrochemical properties of the interface between a Na_6SOI_2 solid electrolyte and a metallic Na anode

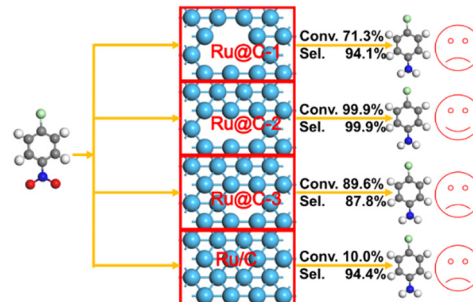
Song-Hyok Choe,* Won-Hyok Hong, Kum-Chol Kim and Chol-Jun Yu*



8556

A well-fabricated Ru@C material derived from Ru/Zn-MOF with high activity and stability in the hydrogenation of 4-chloronitrobenzene

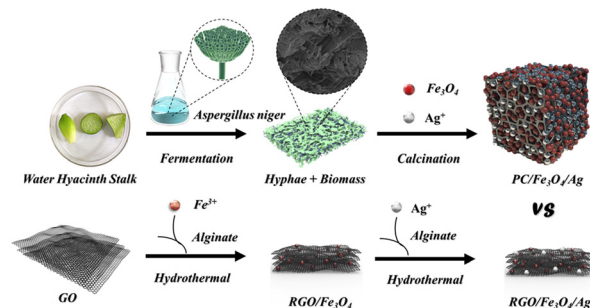
Zijian Wang, Jiaxin Zhang, Lele Yan, Bo Zhao, Lin Zheng, Haoran Guo, Yuxue Yue, Deman Han, Xianlang Chen* and Rongrong Li*



8564

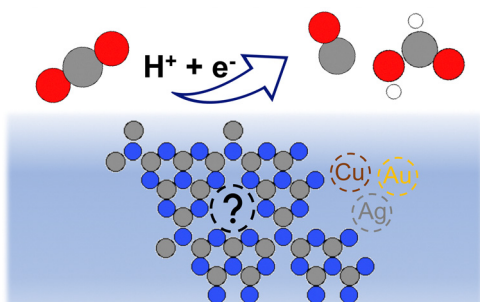
Fungi-enabled pore channel regulation and defect engineering of a novel micro-reactor for treating complex effluents

Xiaoying Jiang, Yan Zhang, Feiyang Zhang, Jiashuo Tian, Liuping Zhang, Xinrui Zhao and Fengling Cui*



RESEARCH PAPERS

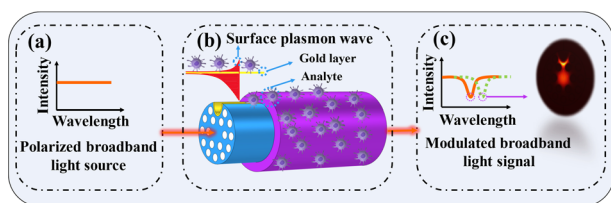
8574



2D carbon nitride as a support with single Cu, Ag, and Au atoms for carbon dioxide reduction reaction

Sergio Posada-Pérez,* Anna Vidal-López, Miquel Solà and Albert Poater*

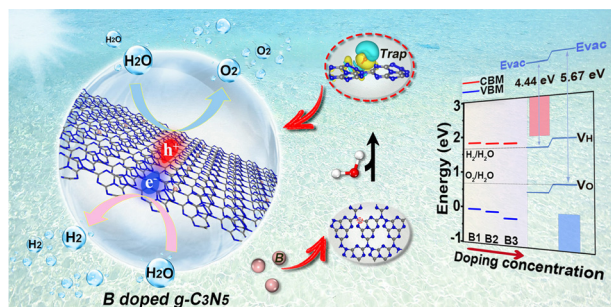
8583



High confidence plasmonic sensor based on photonic crystal fibers with a U-shaped detection channel

Wanlai Zhu, Yingting Yi, Zao Yi,* Liang Bian, Hua Yang, Jianguo Zhang, Yang Yu, Chao Liu, Gongfa Li and Xianwen Wu

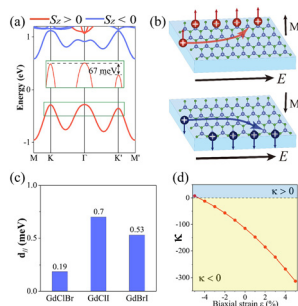
8592



The regulating effect of boron doping and its concentration on the photocatalytic overall water splitting of a polarized g-C₃N₅ material

Xianghong Niu,* Xuemei Zhang, Anqi Shi, Dazhong Sun, Dingbang Chen, Lu Zhang, Jialin Huang, Liqing Liu, Bing Wang* and Xiuyun Zhang*

8600



Combined piezoelectricity, valley splitting and Dzyaloshinskii–Moriya interaction in Janus GdXY (X, Y = Cl, Br, I) magnetic semiconductors

Dehe Zhang, Aolin Li, Bei Zhang, Wenzhe Zhou,* Haiming Duan* and Fangping Ouyang*

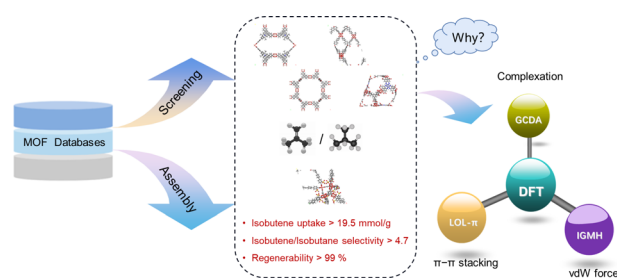


RESEARCH PAPERS

8608

Accelerated screening and assembly of promising MOFs with open Cu sites for isobutene/isobutane separation using a data-driven approach

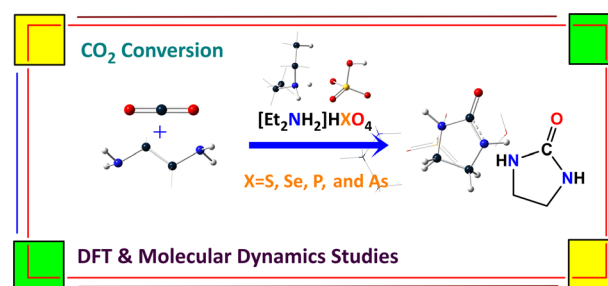
Xi Sun, Wangqiang Lin, Kun Jiang, Heng Liang and Guanghui Chen*



8624

Computational predictions on Brønsted acidic ionic liquid-catalyzed carbon dioxide conversion to five-membered heterocyclic carbonyl derivatives

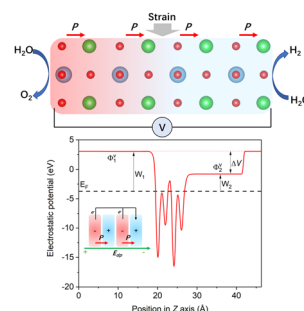
Yusif Abdullayev,* Nazani Karimova, Leonardo A. Schenberg, Lucas C. Ducati and Jochen Autschbach



8631

Understanding the piezocatalytic properties of the BaTiO₃(001) surface via density functional theory

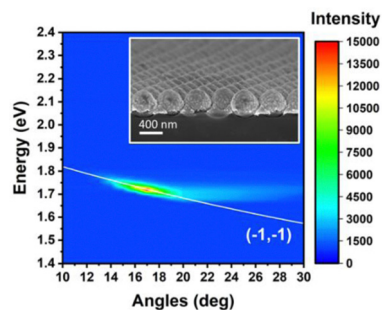
Zeying Zhou, Cheng Zhan* and Erjun Kan



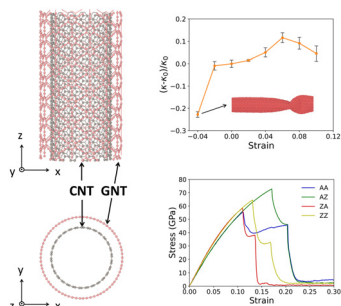
8641

Polarized coherent emission outside high-symmetry points of dye-coupled plasmonic lattices

Diego Piccotti, Mirko Trevisani, Giuseppe Pirruccio, Boris Kalinic, Tiziana Cesca* and Giovanni Mattei



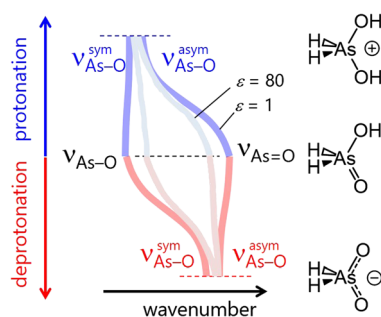
8651



Mechanical and thermal properties of graphyne-coated carbon nanotubes: a molecular dynamics simulation on one-dimensional all-carbon van der Waals heterostructures

Jian Li, Penghua Ying, Ting Liang, Yao Du, Jianli Zhou and Jin Zhang*

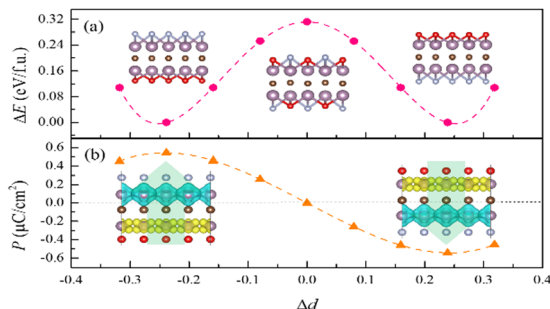
8664



Evolution of vibrational bands upon gradual protonation/deprotonation of arsenic acid $H_2As(O)OH$ in media of different polarity

Elena Yu. Tupikina,* Vladislav O. Korostelev, Danil V. Krutin and Peter M. Tolstoy*

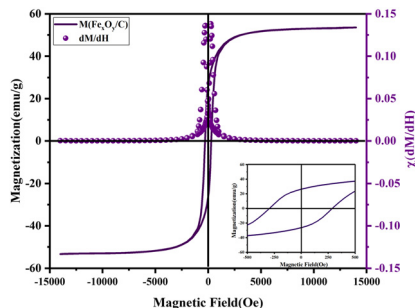
8676



Asymmetric Janus functionalization induced magnetization and switchable out-of-plane polarization in 2D MXene Mo_2CXX'

Chao Xin,* Zhen Fan, Zhixin Sun, Hui Li, Guangyong Jin, Feng Pan* and Yu Sui*

8684



Preparation and characterization study of γ - Fe_2O_3 /carbon composite nanofibers: electrospinning of composite fibers using PVP and iron nitrate as precursors

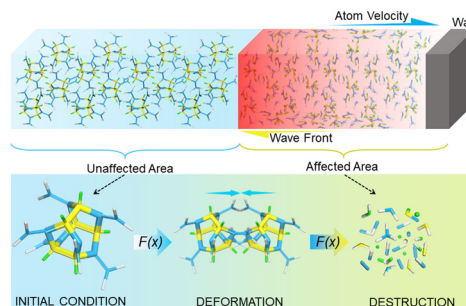
Roya Shokrani Havigh and Hossein Mahmoudi Chenari*



8692

Machine learning quantitatively characterizes the deformation and destruction of explosive molecules

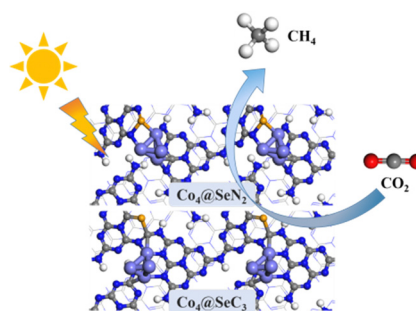
Kaining Zhang, Lang Chen,* Teng Zhang, Jianying Lu, Danyang Liu and Junying Wu



8705

Mechanism of CO₂ photoreduction by selenium-doped carbon nitride with cobalt clusters as cocatalysts

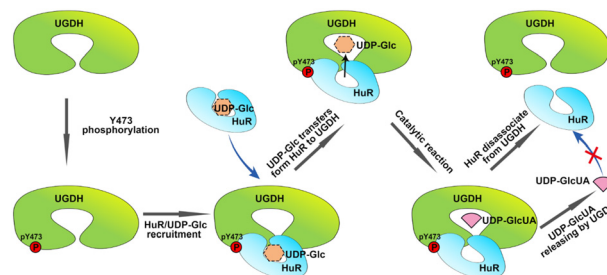
Yuanyuan Hu, Ting Wu, Yi Li, Yongfan Zhang* and Wei Lin*



8714

The molecular mechanism of Y473 phosphorylation of UGDH relieves the inhibition effect of UDP-glucose on HuR

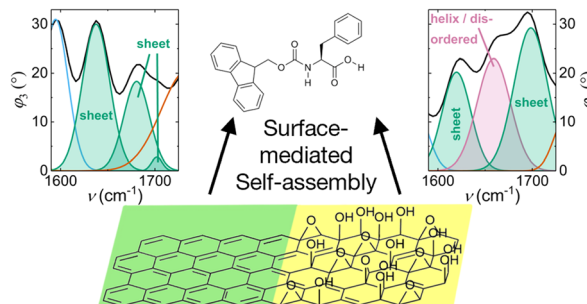
Ye Liu, Yan Li, Guohui Li* and Huiying Chu*



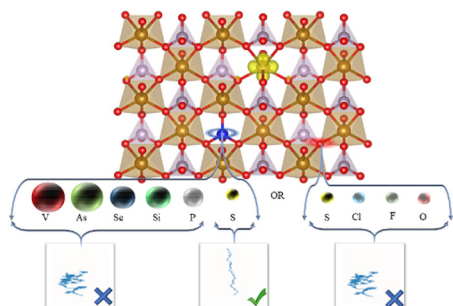
8725

Diversity at the nanoscale: laser-oxidation of single-layer graphene affects Fmoc-phenylalanine surface-mediated self-assembly

Johanna Schirmer, Romain Chevigny, Aleksei Emelianov, Eero Hulkko, Andreas Johansson, Pasi Myllyperkiö, Efstratios D. Sitsanidis,* Maija Nissinen* and Mika Pettersson*



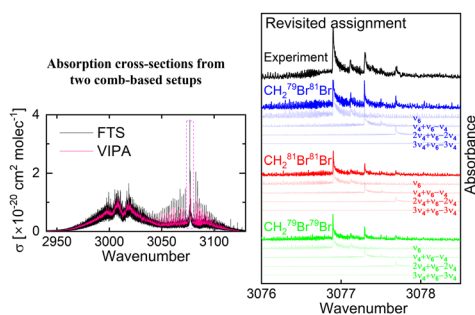
8734



Tuning a small electron polaron in FePO₄ by P-site or O-site doping based on DFT+*U* and KMC simulation

Taowen Chen, Yaokun Ye,* Ying Wang, Chi Fang, Weicheng Lin, Yao Jiang, Bo Xu, Chuying Ouyang* and Jiaxin Zheng*

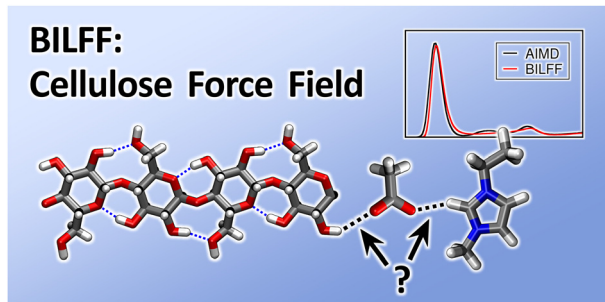
8743



Optical frequency comb-based measurements and the revisited assignment of high-resolution spectra of CH₂Br₂ in the 2960 to 3120 cm⁻¹ region

Ibrahim Sadiek,* Adrian Hjältén, Frances C. Roberts, Julia H. Lehman and Aleksandra Foltynowicz

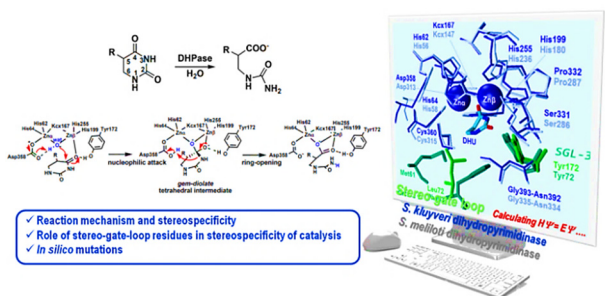
8755



A force field for bio-polymers in ionic liquids (BILFF) – part 2: cellulose in [EMIm][OAc]/water mixtures

Eliane Roos, Daniel Sebastiani and Martin Brehm*

8767



A computational study of the reaction mechanism and stereospecificity of dihydropyrimidinase

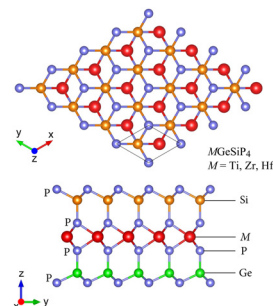
Wijitra Meelua, Tanchanok Wanjai, Natechanok Thinkumrob, Julianna Oláh, James R. Ketudat Cairns, Supa Hannongbua, Ulf Ryde and Jitrayut Jitnonom*



8779

Two-dimensional Janus MGeSiP₄ (M = Ti, Zr, and Hf) with an indirect band gap and high carrier mobilities: first-principles calculations

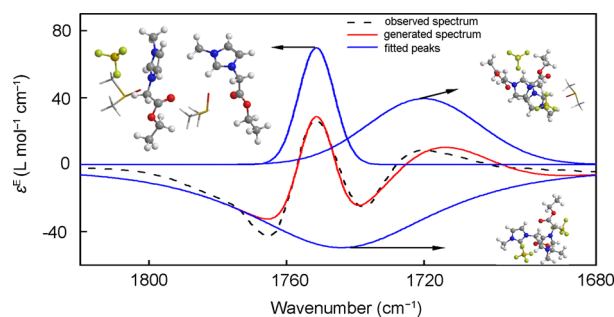
Nguyen T. Hiep, Nguyen P. Q. Anh, Huynh V. Phuc, Cuong Q. Nguyen, Nguyen N. Hieu and Vo T. T. Vi*



8789

Comparative study of the hydrogen bonding interactions between ester-functionalized/non-functionalized imidazolium-based ionic liquids and DMSO

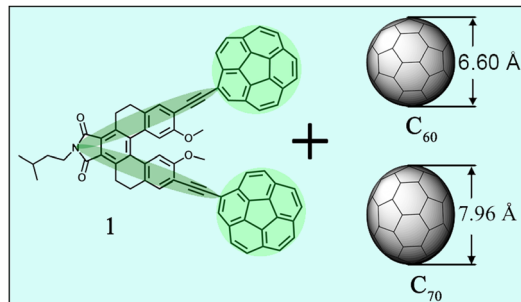
Yuxin Jiang, Xianzhen Xu, Mingzhu Wang, Yu Zhou* and Zonghua Wang*



8799

Effect of intermolecular interaction of the charge-transfer complex between molecular "tweezers" and C₆₀/C₇₀ on second-order nonlinear optical properties

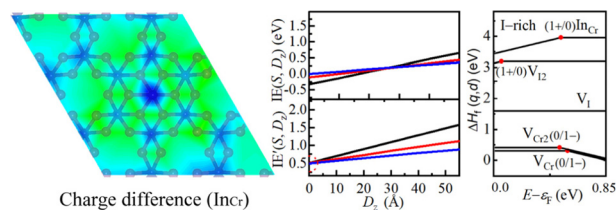
Li Wang,* Yan-Li Liu, Quan-Jiang Li, Di He, Sheng-Hui Chen and Mei-Shan Wang*



8809

Electronic and magnetic properties of charged point defects in monolayer CrI₃

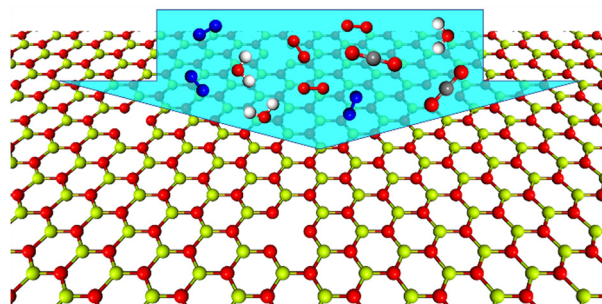
Rongrong Ma, Yun Sun, Mei Ge, Chenrui Ma and Junfeng Zhang*



8853

Robust electronic properties of monolayer BeO against molecule adsorption

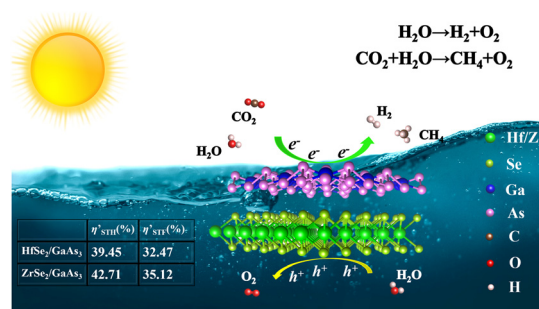
Hongsheng Liu, Vitaly Ksenevich, Jijun Zhao and Junfeng Gao*



8861

Efficient photocatalytic hydrogen evolution and CO₂ reduction by HfSe₂/GaAs₃ and ZrSe₂/GaAs₃ heterostructures with direct Z-schemes

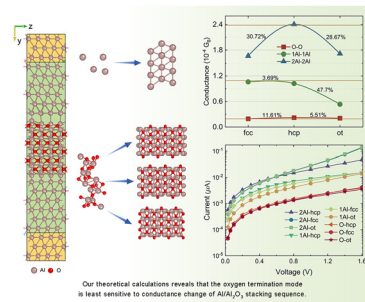
Xue-Qing Wan, Chuan-Lu Yang,* Mei-Shan Wang and Xiao-Guang Ma



8871

Effect of the Al/AlO_x interfacial stacking sequence on the transport properties of alumina tunnel junctions

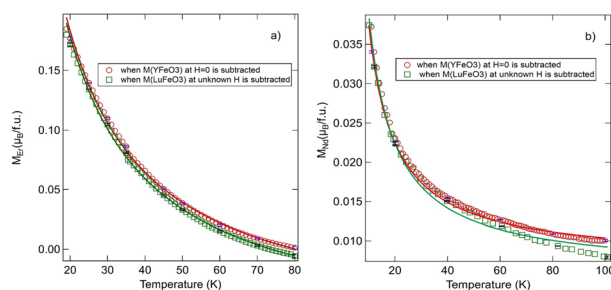
Zheng Shan, Xuelian Gou, Huihui Sun,* Fudong Liu, Lin Han and Jiandong Shang



8882

Temperature dependence of magnetic moment of rare earth ions in ErFeO₃ and NdFeO₃ single crystals

Mohanad H. Mohammed, Zhenxiang Cheng, Shixun Cao and Joseph Horvat



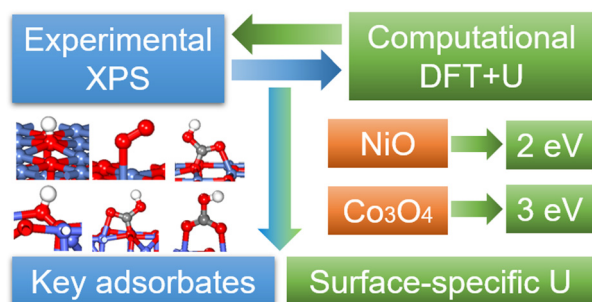
8891



Protonation of serine: conformers, proton affinities and gas-phase basicities at the “gold standard” and beyond

András B. Nacsa,* Máté Kigyósi and Gábor Czakó*

8903

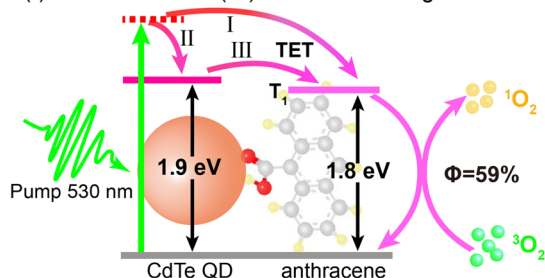


Determining surface-specific Hubbard-*U* corrections and identifying key adsorbates on nickel and cobalt oxide catalyst surfaces

Shang Jiang and Samir H. Mushrif*

8913

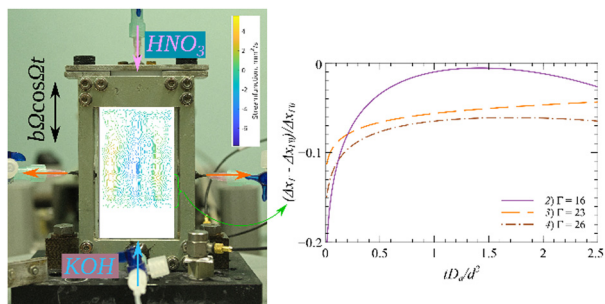
hot (I) and thermalized (III) electron exchange mediated TET



Triplet generation at the CdTe quantum dot/anthracene interface mediated by hot and thermalized electron exchange for enhanced production of singlet oxygen

Zhen Chi, Jia Xu, Shida Luo, Xia Ran, Xiaojuan Wang, Pingan Liu,* Yulu He, Yanmin Kuang and Lijun Guo*

8921



Investigation of chemoconvection in vibration fields

Nikolai Kozlov* and Elena Mosheva

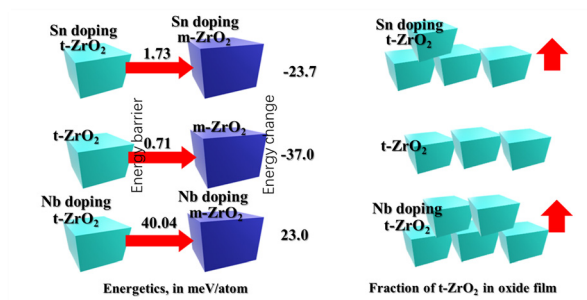


RESEARCH PAPERS

8934

Unraveling different influences of the fraction of the tetragonal phase in oxide films on the corrosion resistance of Zr alloys from the phase transition mechanism

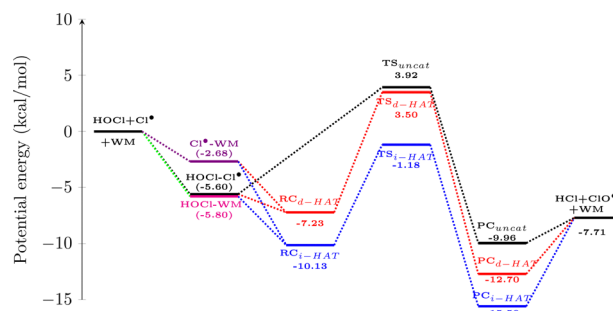
Jiang-Wei Wu, Yao-Ping Xie,* Mei-Yi Yao, Shu-Hui Guan, Yi Zhao, Rong-Jian Pan, Lu Wu and Zhi-Pan Liu



8948

Effect of $(\text{H}_2\text{O})_n$ ($n = 1$ and 2) on HOCl + Cl reaction

Amit Kumar and Pradeep Kumar*

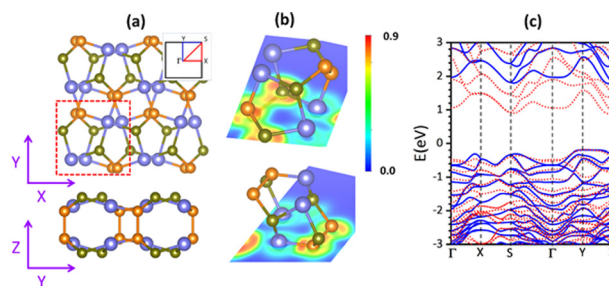


COMMENTS

8961

Comment on "Two-dimensional penta-like PdPse with a puckered pentagonal structure: a first-principles study" by A. Bafekry, M. M. Fadlallah, M. Faraji, A. Shafique, H. R. Jappor, I. Abdolhoseini Sarsari, Y. S. Ang and M. Ghergherehchii, *Phys. Chem. Chem. Phys.*, 2022, 24, 9990

Suman Chowdhury, Fazel Shojaei and Bohayra Mortazavi*



8966

Reply to the 'Comment on "Two-dimensional penta-like PdPse with a puckered pentagonal structure: a first-principles study"' by S. Chowdhury, F. Shojaei and B. Mortazavi, *Phys. Chem. Chem. Phys.*, 2023, 25, DOI: 10.1039/D2CP01587K

Asadollah Bafekry,* Mohamed M. Fadlallah, Mehrdad Faraji, A. Shafique, Hamad R. Jappor, I. Abdolhoseini Sarsari, Yee Sin Ang and Mitra Ghergherehchi

