Open Access Article. Published on 03 May 2023. Downloaded on 7/24/2025 11:00:25 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

PCCP

Physical Chemistry Chemical Physics – An international journal

rsc.li/pccp

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 1463–9076 CODEN PPCPFQ 25(17) 11861–12534 (2023)

Cover
See Prasad Ramesh Joshi, Masashi Tsuge, Yuan-Pern Lee *et al.*, pp. 11934–11950. Image reproduced by permission of Yuan-Pern Lee from *Phys. Chem. Chem. Phys.*, 2023, **25**, 11934. Background Image credit: X-ray: NASA/CXC/Penn State Univ./L. Townsley *et al.*; IR: NASA/ESA/CSA/STScI/JWST ERO Production Team.

EDITORIAL

11880

Festschrift for Wolfgang E. Ernst – electronic and nuclear dynamics and their interplay in molecules, clusters and on surfaces

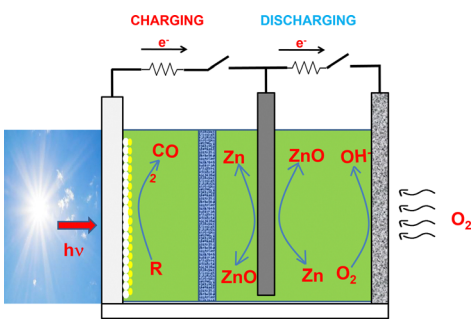
Andreas W. Hauser, Martina Havenith, Markus Koch and Martin Sterrer

REVIEWS

11883

A brief review on solar charging of Zn–air batteries

Panagiotis Lianos



Open Access Article. Published on 03 May 2023. Downloaded on 7/24/2025 11:00:25 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

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.

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, 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**

ROYAL SOCIETY OF 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
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
L 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 Tamblyn, 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 Neumark, 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 Pumera, 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 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

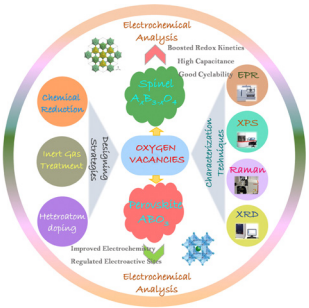
Open Access Article. Published on 03 May 2023. Downloaded on 7/24/2025 11:00:25 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

REVIEWS

11892

Overview of the oxygen vacancy effect in bimetallic spinel and perovskite oxide electrode materials for high-performance supercapacitors

Sk. Khaja Hussain and Jin Ho Bang*

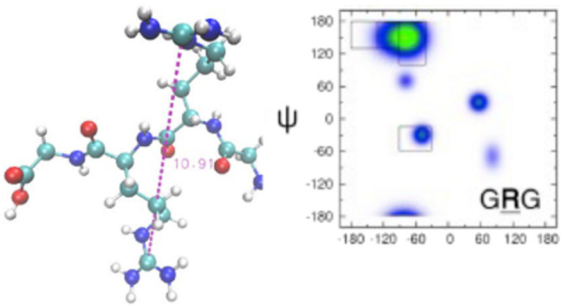


PERSPECTIVE

11908

The relevance of short peptides for an understanding of unfolded and intrinsically disordered proteins

Reinhard Schweitzer-Stenner

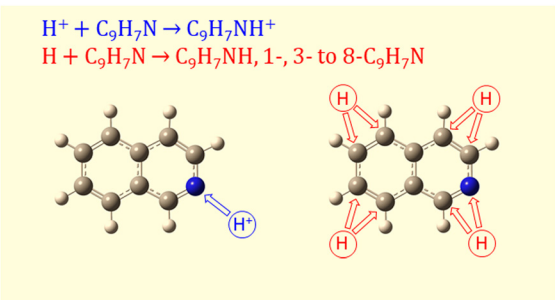


RESEARCH PAPERS

11934

Infrared spectra of isoquinolinium (iso-$C_9H_7NH^+$) and isoquinolinyl radicals (iso-C_9H_7NH and 1-, 3-, 4-, 5-, 6-, 7- and 8-iso-HC_9H_7N) isolated in solid *para*-hydrogen

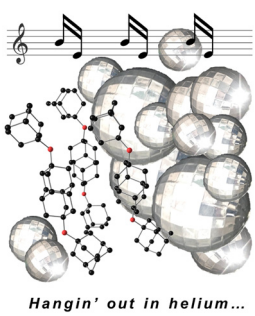
Prasad Ramesh Joshi,* Masashi Tsuge,* Chih-Yu Tseng and Yuan-Pern Lee*



11951

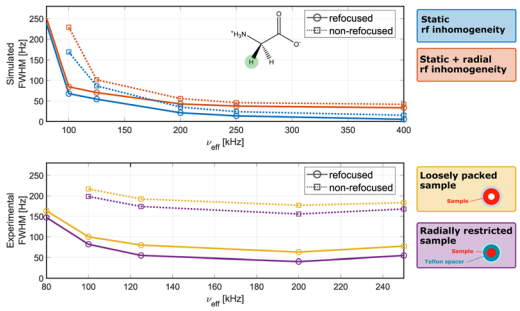
Diamondoid ether clusters in helium nanodroplets

Jasna Alić, Roman Messner, Marija Alešković, Florian Küstner, Mirta Rubčić, Florian Lackner,* Wolfgang E. Ernst* and Marina Šekutor*



Open Access Article. Published on 03 May 2023. Downloaded on 7/24/2025 11:00:25 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

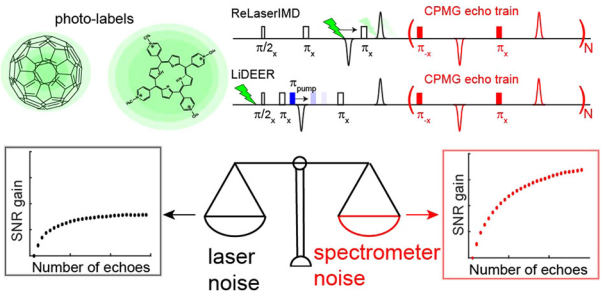
11959



Residual proton line width under refocused frequency-switched Lee-Goldburg decoupling in MAS NMR

Kathrin Aebischer and Matthias Ernst*

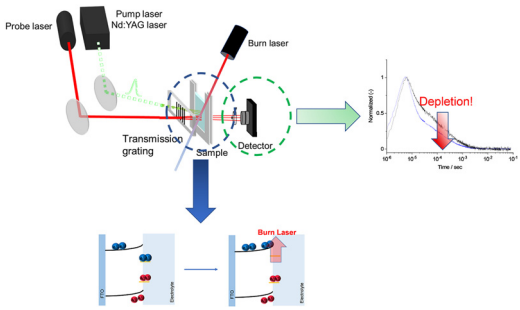
11971



Sensitivity optimization in pulse EPR experiments with photo-labels by multiple-echo-integrated dynamical decoupling

Natalya E. Sannikova, Anatoly R. Melnikov, Sergey L. Veber, Olesya A. Krumkacheva* and Matvey V. Fedin*

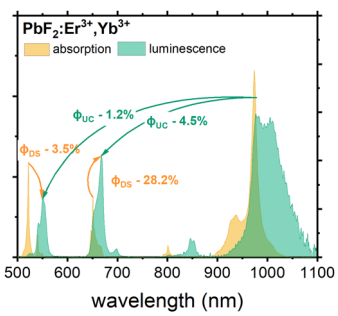
11981



Development of charge carrier-selective heterodyne transient grating spectroscopic technique and its application in the distinction of surface trap states in hematite

Young Hyun Kim, Yu Gyeong Bae and Woon Yong Sohn*

11986



Absolute quantum yield for understanding upconversion and downshift luminescence in $PbF_2:Er^{3+},Yb^{3+}$ crystals

Eduard Madirov, Dmitry Busko, Ian A. Howard, Bryce S. Richards and Andrey Turshatov*

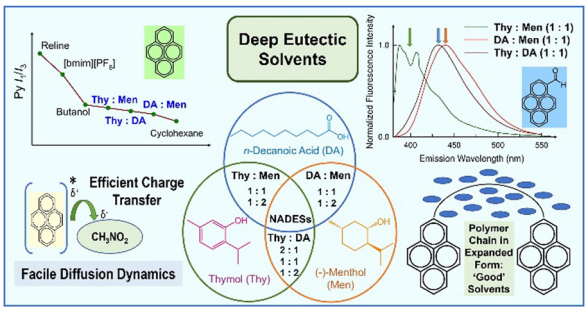
This journal is © the Owner Societies 2023

Open Access Article. Published on 03 May 2023. Downloaded on 7/24/2025 11:00:25 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

11998

Fluorescence of pyrene and its derivatives to reveal constituent and composition dependent solvation within hydrophobic deep eutectic solvents

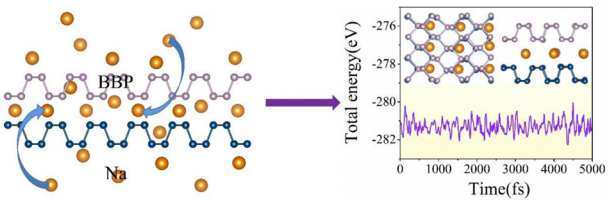
Deepika, Shreya Juneja and Siddharth Pandey*



12013

A first-principles study of bilayered black phosphorene as a potential anode material for sodium-ion batteries

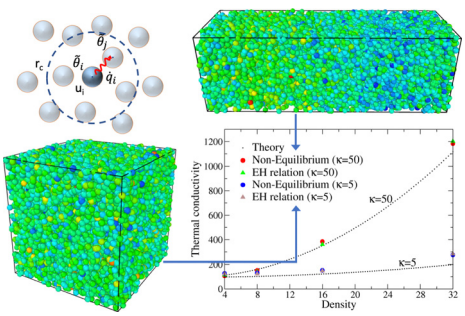
Jiaxin Li, Weiling Chen, Xian Lin, Guigui Xu, Kehua Zhong,* Jian-Min Zhang* and Zhigao Huang*



12025

Transport coefficients from Einstein–Helfand relations using standard and energy-conserving dissipative particle dynamics methods

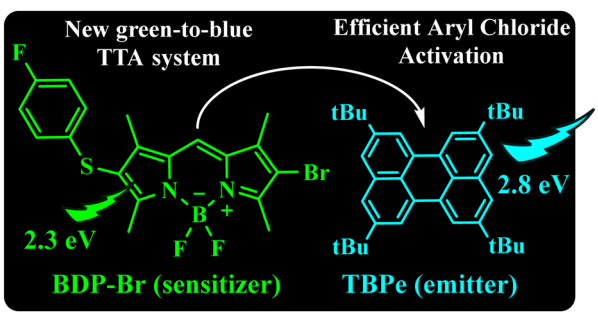
D. C. Malaspina, M. Lísal, J. P. Larentzos, J. K. Brennan, A. D. Mackie and J. Bonet Avalos*



12041

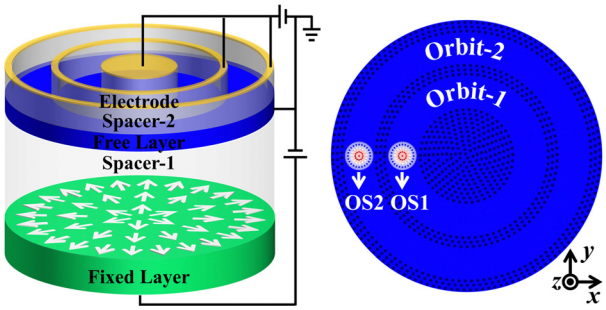
A new green-to-blue upconversion system with efficient photoredox catalytic properties

Jorge Castellanos-Soriano, Till J. B. Zähringer, Jorge C. Herrera-Luna, M. Consuelo Jiménez, Christoph Kerzig* and Raúl Pérez-Ruiz*



Open Access Article. Published on 03 May 2023. Downloaded on 7/24/2025 11:00:25 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

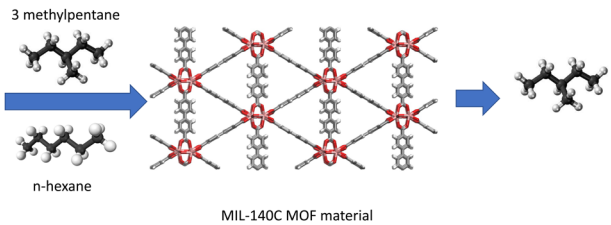
12050



Dynamics of orbital skyrmions in a circular nanodisk

Youhua Feng, Xi Zhang* and Gang Xiang*

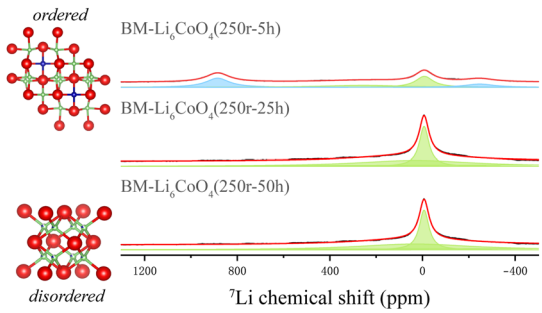
12057



Adsorption and dynamics of linear and mono-branched hexane isomers in MIL-140 metal–organic frameworks

Hengli Zhao, José A. C. Silva, Adriano Henrique, Farid Nouar, Christian Serre, Guillaume Maurin and Aziz Ghoufi*

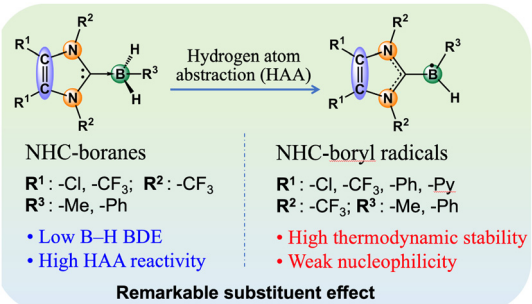
12065



Measuring T_1 relaxation in paramagnetic solids with solid-state NMR: a case study on the milling induced phase transition in Li_6CoO_4

Nianrui Guo, Fushan Geng, Guozhong Lu, Xinbiao Jiang, Chao Li, Bingwen Hu and Ming Shen*

12072



Formation and reactivity of NHC-boryl radicals: insight into substituent effect from theoretical calculations

Lin Zhang and Zexing Cao*

This journal is © the Owner Societies 2023

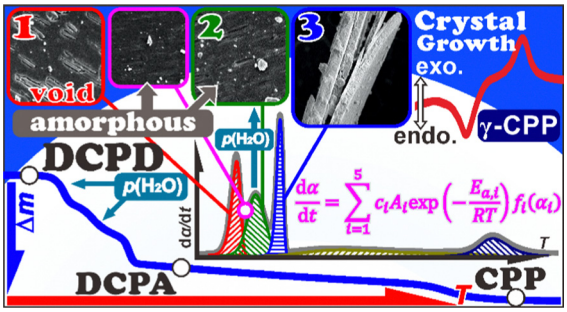
Open Access Article. Published on 03 May 2023. Downloaded on 7/24/2025 11:00:25 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

12081

Physico-geometrical kinetic insight into multistep thermal dehydration of calcium hydrogen phosphate dihydrate

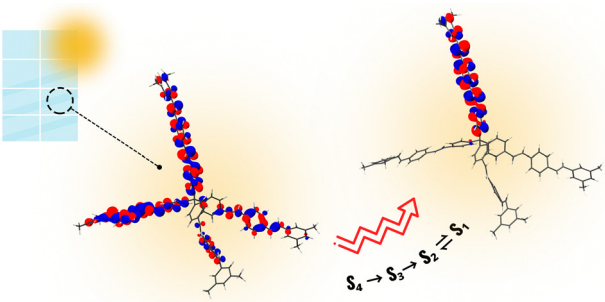
Masami Hara and Nobuyoshi Koga*



12097

Impact of the core on the inter-branch exciton exchange in dendrimers

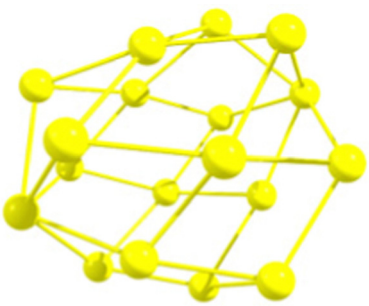
Valeria Bonilla, Victor M. Freixas, Sebastian Fernandez-Alberti and Johan Fabian Galindo*



12107

Engineering magic number Au_{19} and Au_{20} cage structures using electron withdrawing atoms

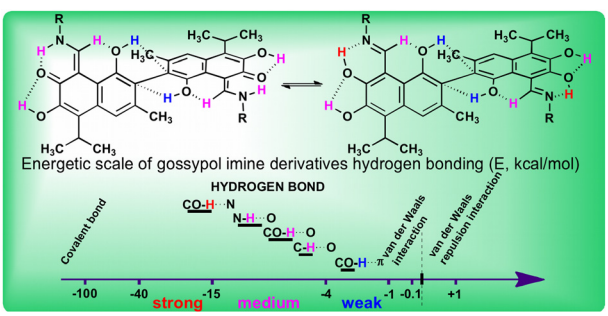
Heather M. Gaebler, Julianna R. Castiglione and Ian P. Hamilton*



12113

Intramolecular hydrogen bonds of gossypol imine derivatives

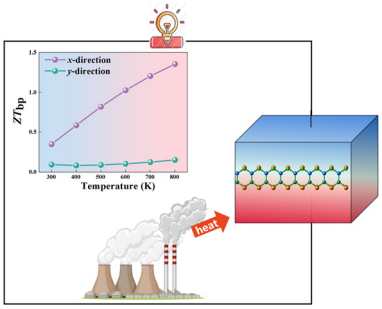
Oleksii M. Dykun,* Viktor M. Anishchenko, Andrii M. Redko and Volodymyr I. Rybachenko



Open Access Article. Published on 03 May 2023. Downloaded on 7/24/2025 11:00:25 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

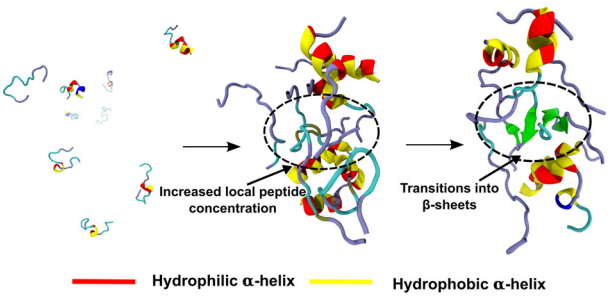
12125



Electron–phonon coupling, bipolar effects, and thermoelectric performance of the $CuSbS_2$ monolayer

Ao-Dong Chen, Chuan-Lu Yang,* Mei-Shan Wang and Xiao-Guang Ma

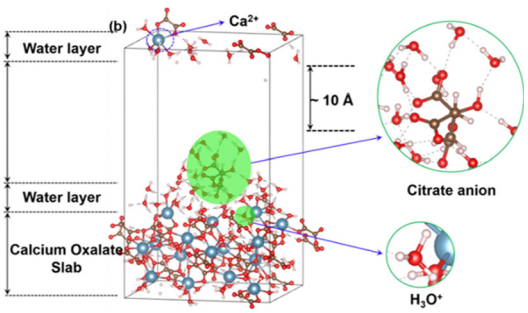
12134



Helical intermediate formation and its role in amyloids of an amphibian antimicrobial peptide

Anup Kumar Prasad, Lisandra L. Martin and Ajay S. Panwar*

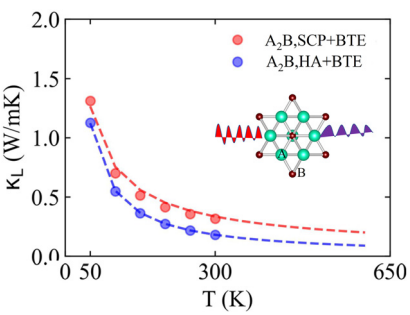
12148



A molecular understanding of citrate adsorption on calcium oxalate polyhydrates

Yangyang Su, Jelle Vekeman, Flavio Siro Brigiano, Etienne Paul Hessou, Yuheng Zhao, Diane Sorgeloos, Marc Raes, Tom Hauffman, Kehzi Li and Frederik Tielens*

12157



Ultralow lattice thermal conductivity of binary compounds A_2B (A = Cs, Rb & B = Se, Te) with higher-order anharmonicity correction

Shuming Zeng,* Lei Fang, Yusong Tu, M. Zulfiqar* and Geng Li*

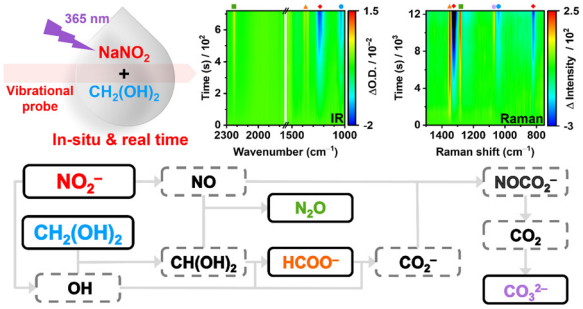
This journal is © the Owner Societies 2023

Open Access Article. Published on 03 May 2023. Downloaded on 7/24/2025 11:00:25 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

12165

***In situ* and real-time vibrational spectroscopic characterizations of the photodegradation of nitrite in the presence of methanediol**

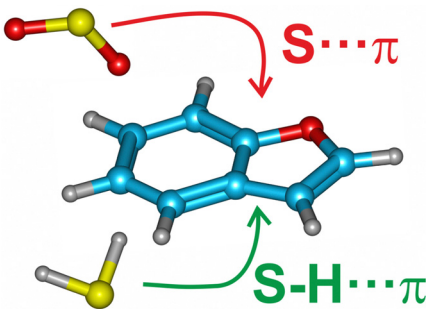
Chiao-Mi Cheng, Cheng-Zong Lu, Chun-Yao Hou, Yuan-Jyun Jhao, Yi-Fen Lai, I-Chia Chen, Yi-Hsueh Chuang and Li-Kang Chu*



12174

Sulfur–arene interactions: the S···π and S–H···π interactions in the dimers of benzofuran···sulfur dioxide and benzofuran···hydrogen sulfide

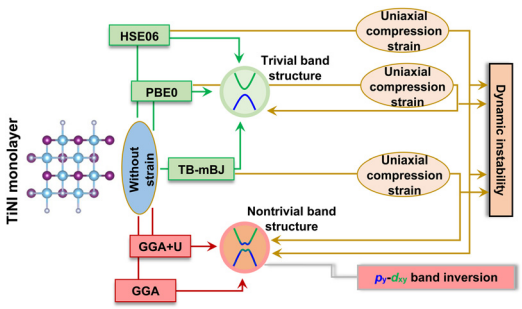
Yan Jin, Wenqin Li, Rizalina Tama Saragi, Marcos Juanes, Cristóbal Pérez, Alberto Lesarri* and Gang Feng*



12182

New insights into band inversion and topological phase of TiNI monolayer

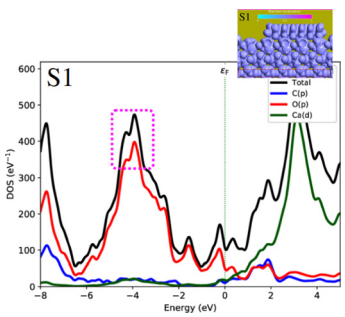
Shahram Yalameha, Zahra Nourbakhsh, Mohammad Saeed Bahramy and Daryoosh Vashaee*



12192

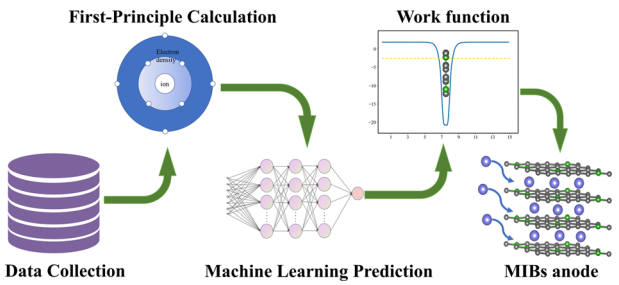
Unravelling the impact of oily alkane molecules on the optical properties of the calcite(10.4) surface

Junais Habeeb Mokkath



Open Access Article. Published on 03 May 2023. Downloaded on 7/24/2025 11:00:25 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

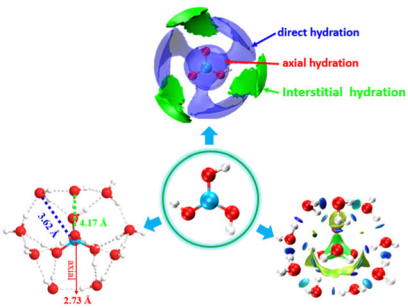
12200



Machine-learning-assisted discovery of boron-doped graphene with high work function as an anode material for Li/Na/K-ion batteries

Yi Luo, Haiyuan Chen,* Jianwei Wang and Xiaobin Niu

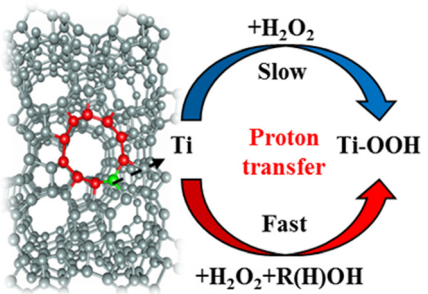
12207



Structural analysis of potassium borate solutions

Fayan Zhu, Daniel T. Bowron, Sabrina Gärtner, Chunhui Fang, Yongquan Zhou, Hongyan Liu and Alex C. Hannon*

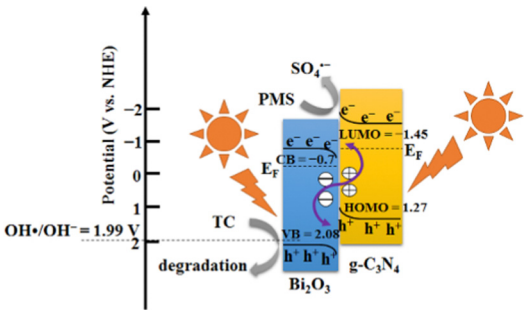
12220



Evidence of solvent-mediated proton transfer during H_2O_2 activation in titanosilicate-catalyzed oxidation systems

Yunkai Yu, Jianhao Wang, Nan Fang, Zhen Chen, Dongxu Liu, Yueming Liu* and Mingyuan He

12231



A 1D/2D Bi_2O_3/g-C_3N_4 step-scheme photocatalyst to activate peroxymonosulfate for the removal of tetracycline hydrochloride: insight into the mechanism, reactive sites, degradation pathway and ecotoxicity

Mingyang Long, Di Li,* Qianqian Zhao, Hongmiao Li, Qi Wen, Li Wang, Lei Wu, Fang Song and Jun Zhou

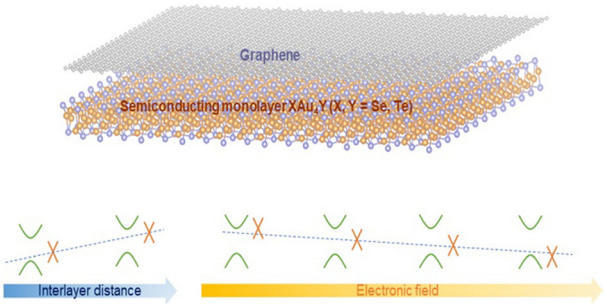
This journal is © the Owner Societies 2023

Open Access Article. Published on 03 May 2023. Downloaded on 7/24/2025 11:00:25 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

12245

Tunable Schottky contacts in graphene/XAu_4Y (X, Y = Se, Te) heterostructures

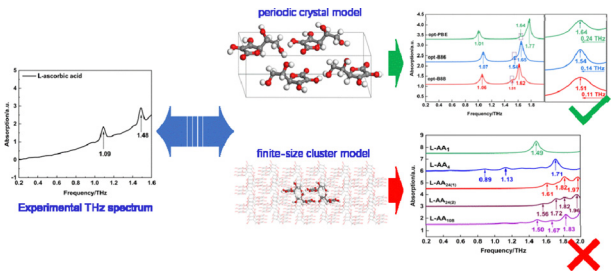
Yufei Xue, Lei Gao,* Weina Ren, Xuxia Shai, Tingting Wei, Chunhua Zeng* and Hua Wang*



12252

First principles terahertz spectroscopy of molecular crystals: the crucial role of periodic boundary conditions benchmarked with experimental L-ascorbic acid spectra

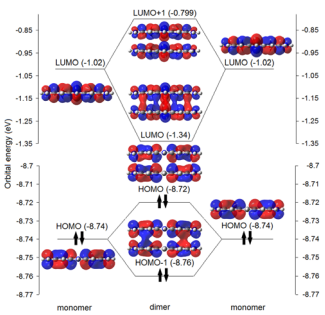
Ying Wang, Huifang Ma, Yanzhao Yang, Jiantao Qi, Guiming Zhang, Hao Ren* and Wenyue Guo*



12259

Theoretical study of the excitation of proflavine H-dimers in an aqueous solution: the effect of functionals and dispersion corrections

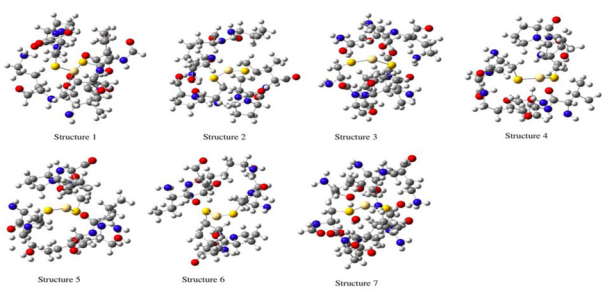
Evgeniy S. Savenko and Victor V. Kostjukov*



12277

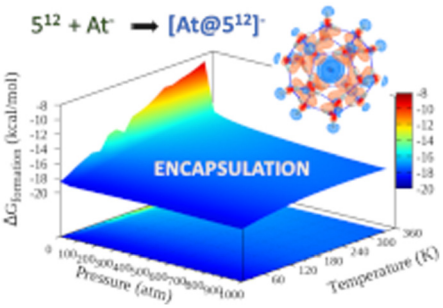
Calculation of electric field gradients in Cd(II) model complexes of the CueR protein metal site

Catriona A. O'Shea, Rasmus Fromsejer, Stephan P. A. Sauer, Kurt V. Mikkelsen* and Lars Hemmingsen*



Open Access Article. Published on 03 May 2023. Downloaded on 7/24/2025 11:00:25 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

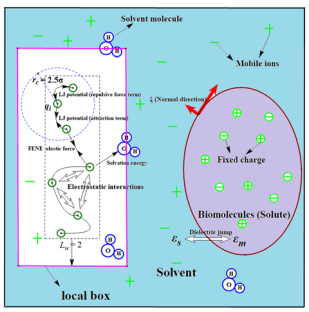
12284



Encapsulation of Astatide by a water cage

Sara Gómez,* Elizabeth Flórez, Nancy Acelas, Cacier Hadad and Albeiro Restrepo*

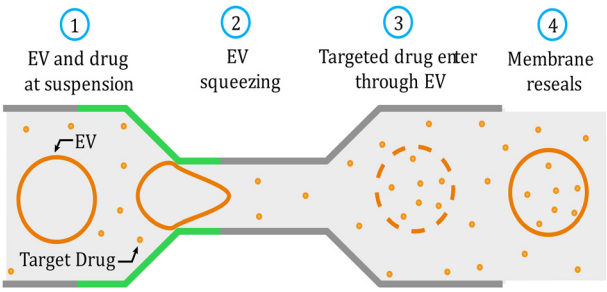
12290



An energy minimization strategy based on an improved nonlinear conjugate gradient method for accelerating the charged polymer dynamics simulation

Hao Lin, Yiwei Shi, Enlong Shang and Shuyang Dai*

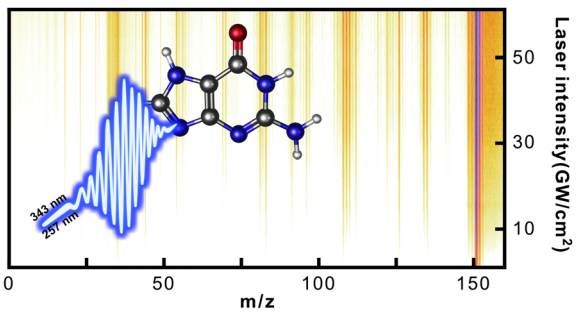
12308



Coarse-grained molecular simulation of extracellular vesicle squeezing for drug loading

Khayrul Islam, Meghdad Razizadeh and Yaling Liu*

12322



High-throughput UV-photofragmentation studies of thymine and guanine

Siwen Wang, Yerbolat Dauletyarov, Peter Krüger and Daniel A. Horke*

This journal is © the Owner Societies 2023

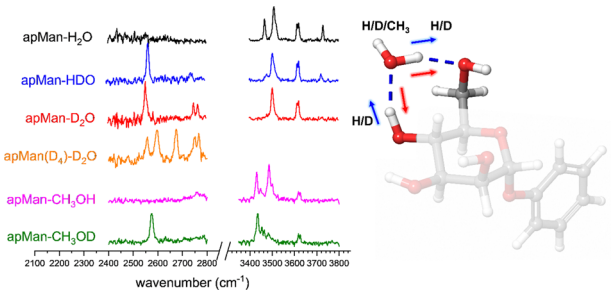
Open Access Article. Published on 03 May 2023. Downloaded on 7/24/2025 11:00:25 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

12331

Isotopic dependence of intramolecular and intermolecular vibrational couplings in cooperative hydrogen bond networks: singly hydrated phenyl-α-D-mannopyranoside as a case study

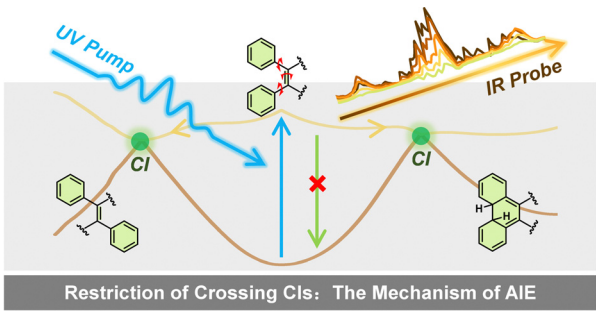
Ander Camiruaga, Gildas Goldsztejn and Pierre Çarçabal*



12342

Restriction of crossing conical intersections: the intrinsic mechanism of aggregation-induced emission

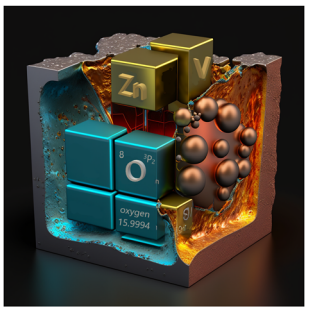
Jie Peng, Xin He, Yao Li, Jianxin Guan, Baihua Wu, Xinmao Li, Zhihao Yu, Jian Liu* and Junrong Zheng*



12352

First principles calculation of the ZnV_2O_6(001) surface terminations: the thermodynamic stability and electronic structure study

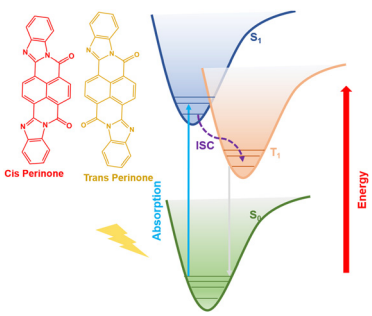
Anqi Yang, Jiaolian Luo,* Zhenyu Xie, Qian Chen* and Quan Xie



12363

Probing the excited state dynamics in perinone molecules for photovoltaic applications using transient absorption spectroscopy

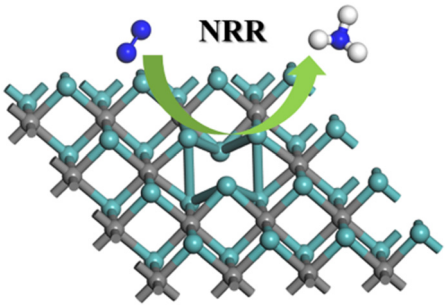
Suman Dhami, Yogesh Kumar, Chaitrali Sengupta and Ravindra Pandey*



Open Access Article. Published on 03 May 2023. Downloaded on 7/24/2025 11:00:25 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

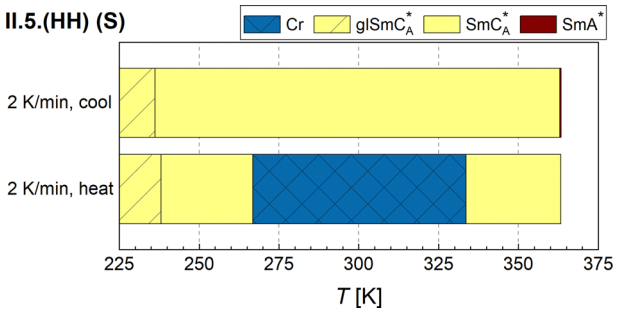
12371



Defective Mo_2C as a promising electrocatalyst for the nitrogen reduction reaction

Xuanyue Zhang, Tingting Zhao, Likai Yan* and Zhongmin Su

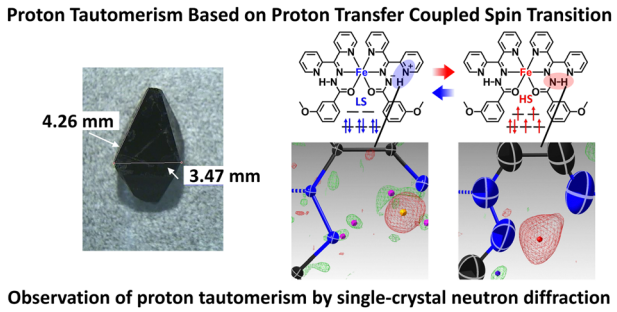
12379



Vitrification of the smectic C_A* phase and kinetics of cold crystallization investigated for a fluorinated compound with a chiral centre based on (*S*)-(+)-3-octanol

Aleksandra Deptuch,* Artur Lelito, Ewa Juszyńska-Gałązka, Małgorzata Jasiurkowska-Delaporte and Magdalena Urbańska

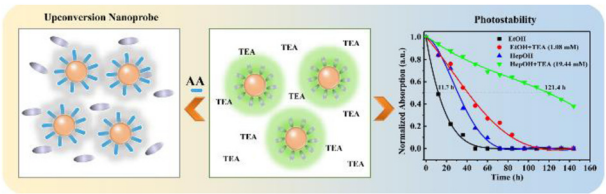
12394



Observation of proton-transfer-coupled spin transition by single-crystal neutron-diffraction measurement

Takumi Nakanishi, Yuta Hori, Yasuteru Shigeta, Hiroyasu Sato, Shu-Qi Wu, Ryoji Kiyanagi, Koji Munakata, Takashi Ohhara and Osamu Sato*

12401



The effect of triethylamine on dye-sensitized upconversion luminescence and its application in nanoprobes and photostability

Xiao-Bo Zhang, Zuo-Qin Liang,* Xu Yan, Mao-Mao Li, Chang-Qing Ye, Xiao-Mei Wang and Xu-Tang Tao

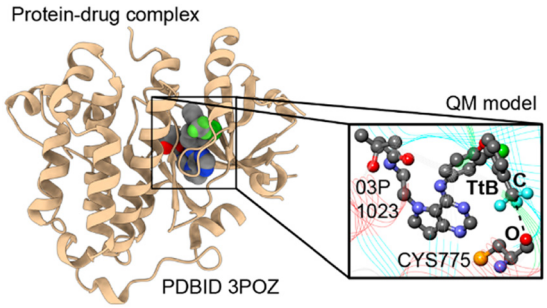
This journal is © the Owner Societies 2023

Open Access Article. Published on 03 May 2023. Downloaded on 7/24/2025 11:00:25 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

12409

Tetrel bonds involving a CF_3 group participate in protein–drug recognition: a combined crystallographic and computational study

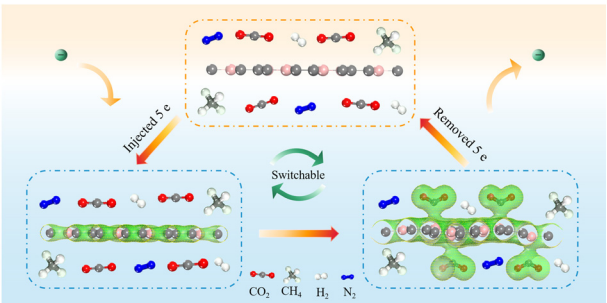
María de las Nieves Piña, Akshay Kumar Sahu, Antonio Frontera, Himansu S. Biswal* and Antonio Bauzá*



12420

Charge-controlled switchable CO_2 capture and gas separation using BC_3 nanosheets

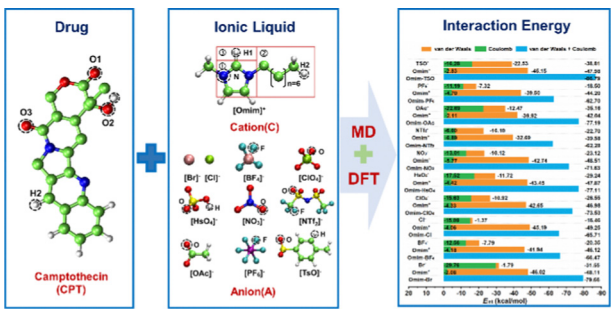
Yiqun Guo, Xuxin Kang, Shan Gao* and Xiangmei Duan*



12426

Theoretical study on the solvation mechanism of camptothecin in ionic liquids

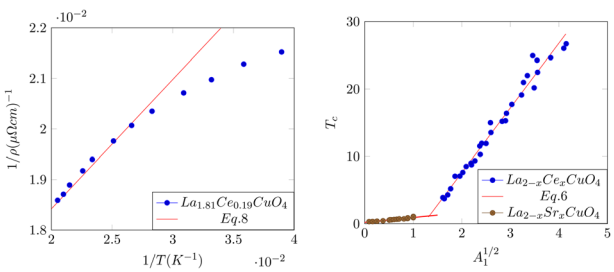
Xiaotong Zhu, Yiping Huang and Yuanhui Ji*



12443

Universal correlation of the superconducting transition temperature with the linear-in-T coefficient, electron packing parameter, and the numbers of valence and conduction electrons

Tian Hao

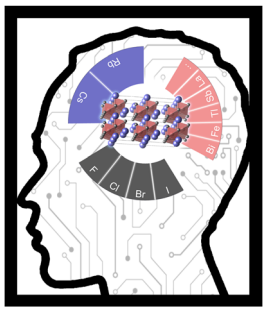


(a) Data fitted with Eq. 8 (b) Data fitted with Eq. 6

Open Access Article. Published on 03 May 2023. Downloaded on 7/24/2025 11:00:25 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

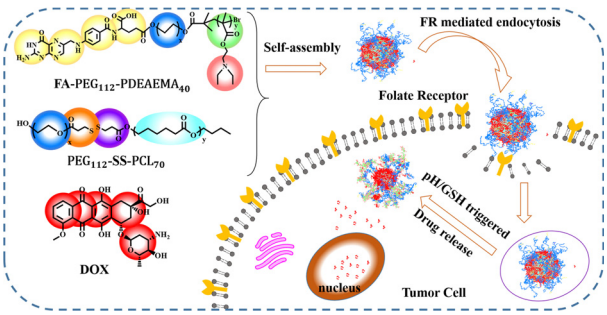
12450



Substitution engineering of lead-free halide perovskites for photocatalytic applications assisted by machine learning

Tao Wang, Shuxin Fan, Hao Jin,* Yunjin Yu and Yadong Wei*

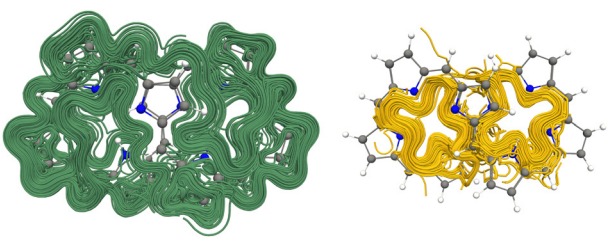
12458



Folate modified dual pH/reduction-responsive mixed micelles assembled using FA-PEG-PDEAEMA and PEG-SS-PCL for doxorubicin delivery

Chufen Yang, Delin Wang, Wenyao Liu, Zexiong Yang, Teng He, Fang Chen and Wenjing Lin*

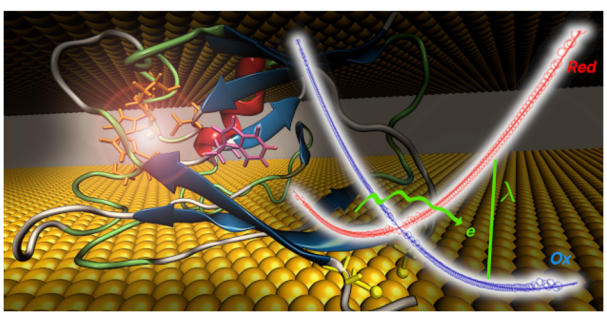
12469



Current-density pathways in figure-eight-shaped octaphyrins

Qian Wang, Jaakko Pyykkö, Maria Dimitrova, Stefan Taubert and Dage Sundholm*

12479



Applicability of perturbed matrix method for charge transfer studies at bio/metallic interfaces: a case of azurin

Outi Vilhelmiina Kontkanen, Denys Biriukov and Zdenek Futera*

This journal is © the Owner Societies 2023

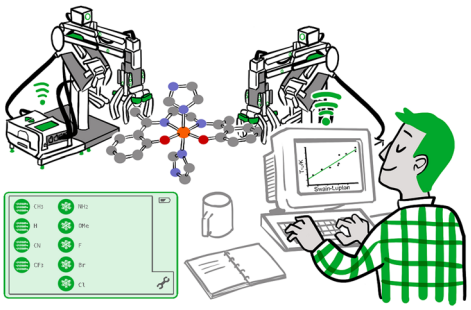
Open Access Article. Published on 03 May 2023. Downloaded on 7/24/2025 11:00:25 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

12490

Fine-tuning of the spin-crossover properties of Fe(III) complexes *via* ligand design

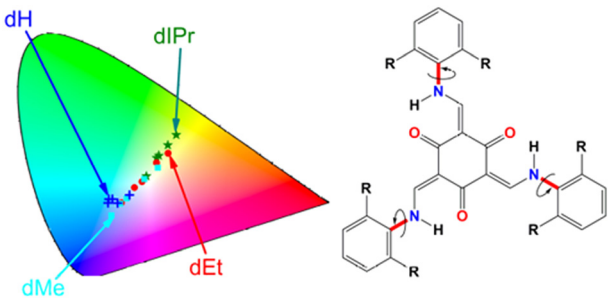
Daniel Vidal, Jordi Cirera* and Jordi Ribas-Arino*



12500

Magnifying the ESIPT process in tris(salicylideneanilines) *via* the steric effect – a pathway to the molecules with panchromatic fluorescence

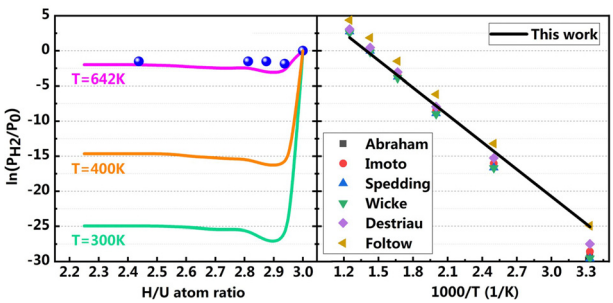
Pawel Gawrys, Olaf Morawski,* Marzena Banasiewicz and Cristina A. Barboza*



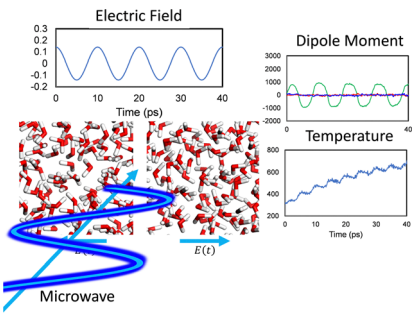
12515

Initial decomposition mechanisms and the inverse effects of temperature and P_{H_2} on the thermodynamic stability of UH_3

Le Zhang, Yanhong Zhao, Hongzhou Song, Xingyu Gao, Qili Zhang, Yu Liu, Bo Sun,* Mingfeng Tian, Haifeng Song and Haifeng Liu*



12522

The selective heating effect of microwave irradiation on a binary mixture of water and polyethylene oxide: a molecular dynamics simulation approach

Junhe Chen, Matthew J. Warner, Benjamin Sikora, Daniel Kiddle, Danielle Coverdell, Omar Allam, Paul A. Kohl and Seung Soon Jang*