

# PCCP

Physical Chemistry Chemical Physics – An international journal

[rsc.li/pccp](https://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

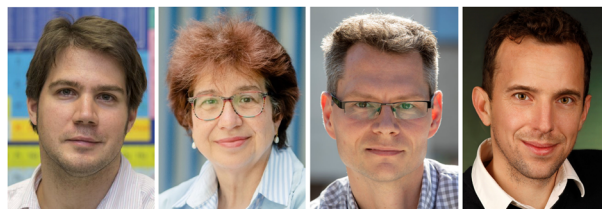
See Prasad Ramesh Joshi, Masashi Tsuge, Yuan-Pern Lee *et al.*, pp. 11934–11950. Image reproduced by permission of Yuan-Pern Lee from *Phys. Chem. Chem. Phys.*, 2023, 25, 11934. Background Image credit: X-ray: NASA/CXC/Penn State Univ./L. Townsley *et al.*; IR: NASA/ESA/CSA/STScI/JWST ERO Production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

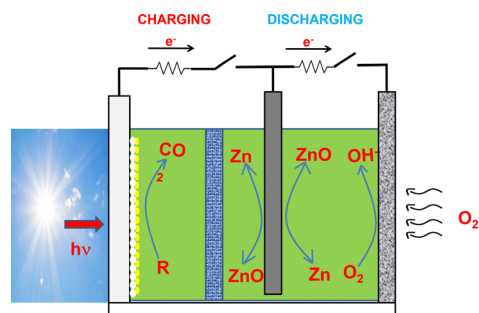


## REVIEWS

11883

### A brief review on solar charging of Zn–air batteries

Panagiotis Lianos



## 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](mailto:pccp@rsc.org)

For pre-submission queries, please contact

Michael A. Rowan, Executive Editor.

Email: [pccp-rsc@rsc.org](mailto: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](mailto: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](http://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](mailto:advertising@rsc.org)

For marketing opportunities relating to this journal, contact [marketing@rsc.org](mailto:marketing@rsc.org)

# PCCP

Physical Chemistry Chemical Physics – An international journal

[rsc.li/pccp](http://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  
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 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 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 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](http://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

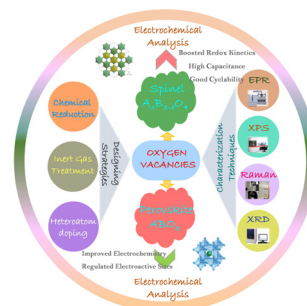


## REVIEWS

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\*

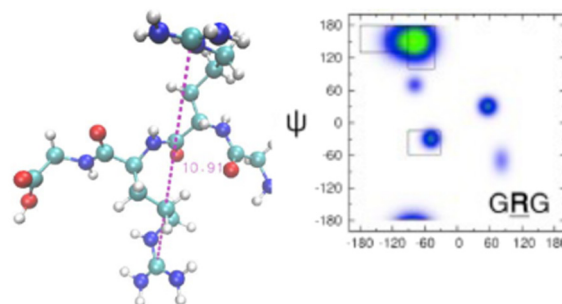


## PERSPECTIVE

11908

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

Reinhard Schweitzer-Stenner

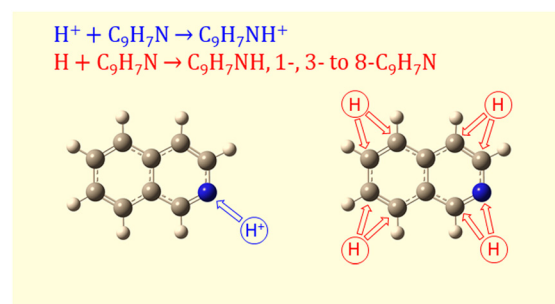


## RESEARCH PAPERS

11934

## Infrared spectra of isoquinolinium (iso-C<sub>9</sub>H<sub>7</sub>NH<sup>+</sup>) and isoquinolinyl radicals (iso-C<sub>9</sub>H<sub>7</sub>NH and 1-, 3-, 4-, 5-, 6-, 7- and 8-iso-HC<sub>9</sub>H<sub>7</sub>N) isolated in solid *para*-hydrogen

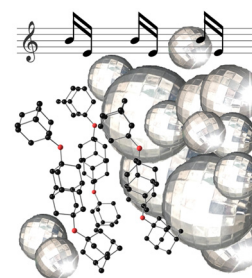
Prasad Ramesh Joshi,\* Masashi Tsuge,\* Chih-Yu Tseng and Yuan-Pern Lee\*



11951

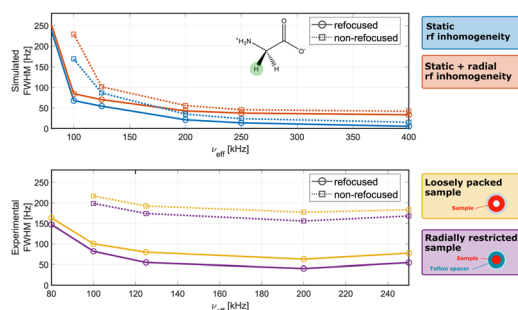
## Diamondoid ether clusters in helium nanodroplets

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

*Hangin' out in helium...*

## RESEARCH PAPERS

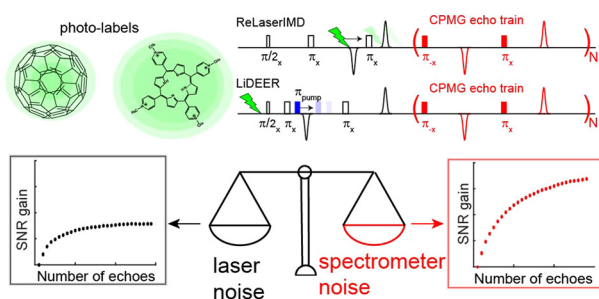
11959



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

Kathrin Aebischer and Matthias Ernst\*

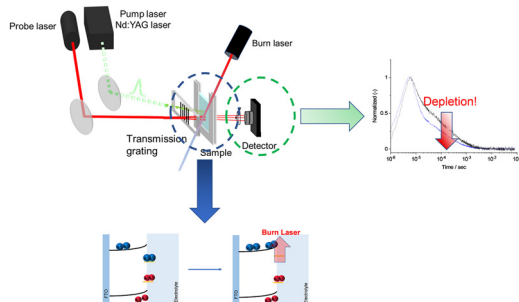
11971



## 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\*

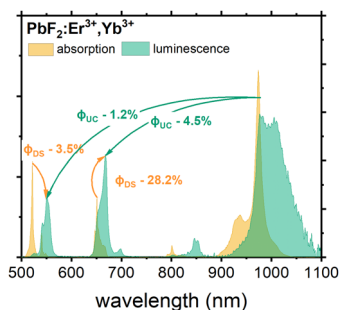
11981



## 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 $\text{PbF}_2:\text{Er}^{3+}, \text{Yb}^{3+}$ crystals

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

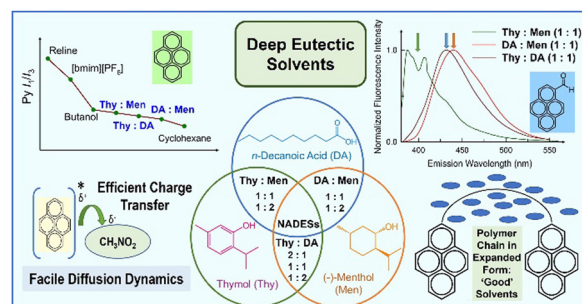


## RESEARCH PAPERS

11998

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

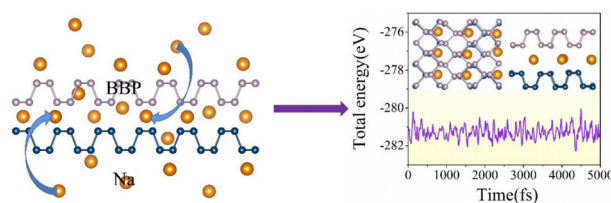
Deepika, Shreya Juneja and Siddharth Pandey\*



12013

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

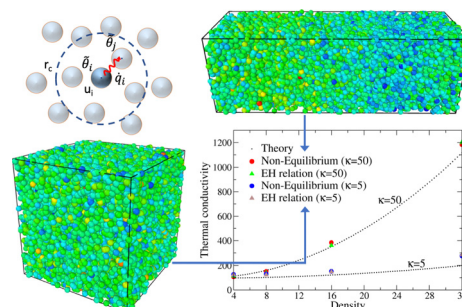
Jiaxin Li, Weiling Chen, Xian Lin, Guigui Xu, Kehua Zhong,\* Jian-Min Zhang\* and Zhigao Huang\*



12025

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

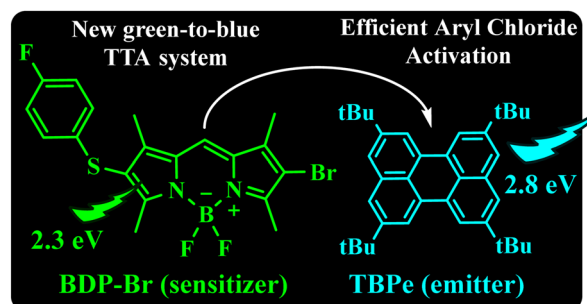
D. C. Malaspina, M. Lisal, J. P. Larentzos, J. K. Brennan, A. D. Mackie and J. Bonet Avalos\*



12041

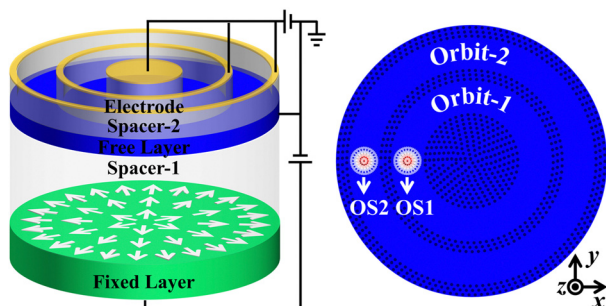
### A new green-to-blue upconversion system with efficient photoredox catalytic properties

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



## RESEARCH PAPERS

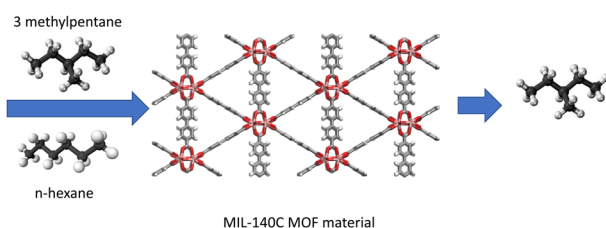
12050



## Dynamics of orbital skyrmions in a circular nanodisk

Youhua Feng, Xi Zhang\* and Gang Xiang\*

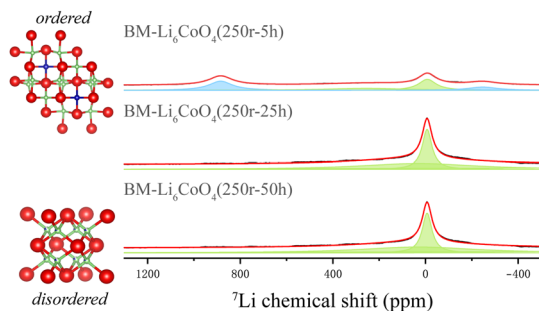
12057



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

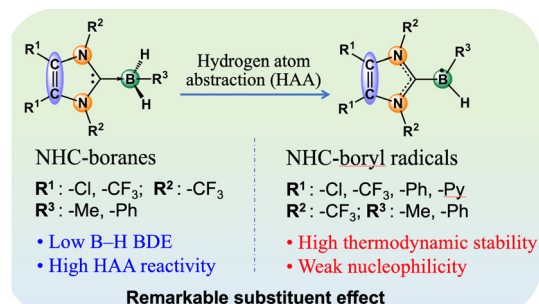
Hengli Zhao, José A. C. Silva, Adriano Henrique, Farid Nouar, Christian Serre, Guillaume Maurin and Aziz Ghoufi\*

12065

Measuring  $T_1$  relaxation in paramagnetic solids with solid-state NMR: a case study on the milling induced phase transition in  $\text{Li}_6\text{CoO}_4$ 

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\*

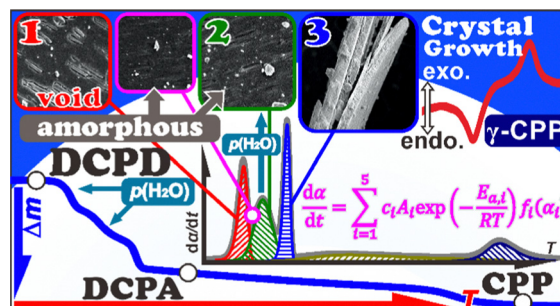


## RESEARCH PAPERS

12081

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

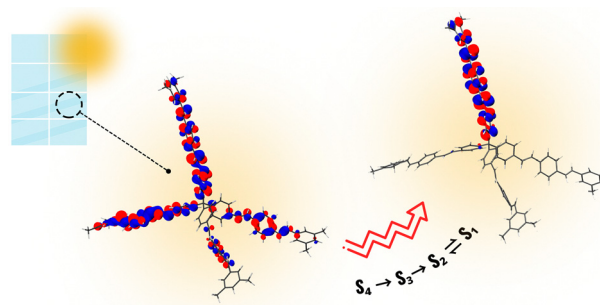
Masami Hara and Nobuyoshi Koga\*



12097

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

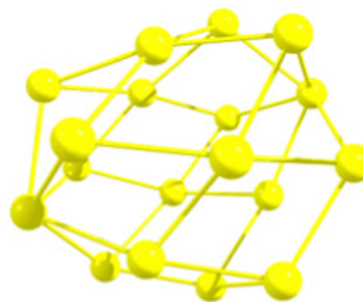
Valeria Bonilla, Victor M. Freixas, Sebastian Fernandez-Alberti and Johan Fabian Galindo\*



12107

### Engineering magic number Au<sub>19</sub> and Au<sub>20</sub> cage structures using electron withdrawing atoms

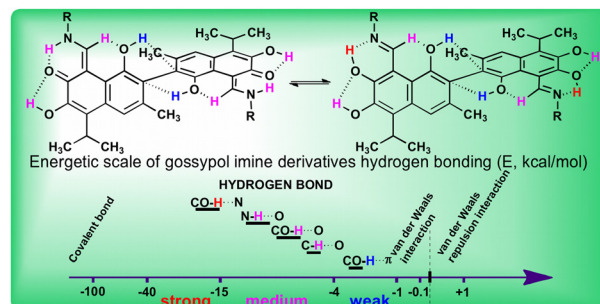
Heather M. Gaebler, Julianna R. Castiglione and Ian P. Hamilton\*



12113

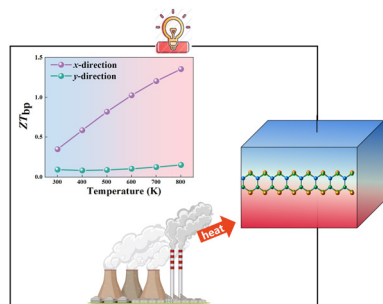
### Intramolecular hydrogen bonds of gossypol imine derivatives

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



## RESEARCH PAPERS

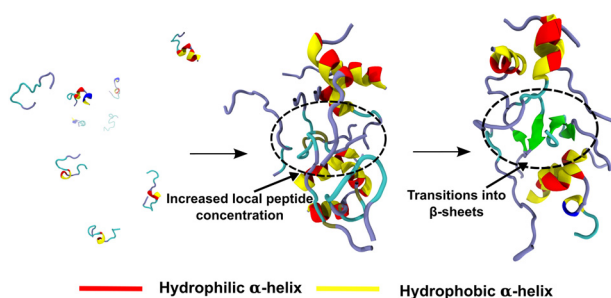
12125



### Electron–phonon coupling, bipolar effects, and thermoelectric performance of the $\text{CuSbS}_2$ monolayer

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

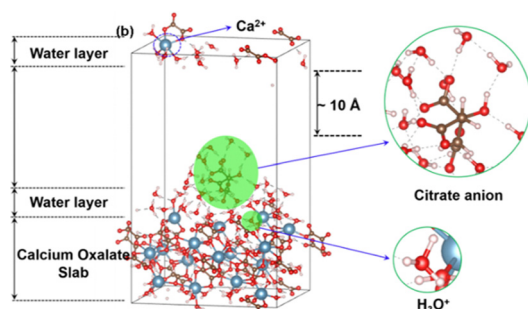
12134



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

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

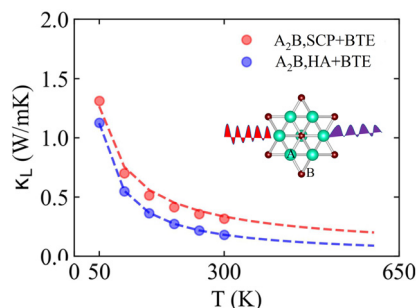
12148



### 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 $\text{A}_2\text{B}$ ( $\text{A} = \text{Cs, Rb}$ & $\text{B} = \text{Se, Te}$ ) with higher-order anharmonicity correction

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

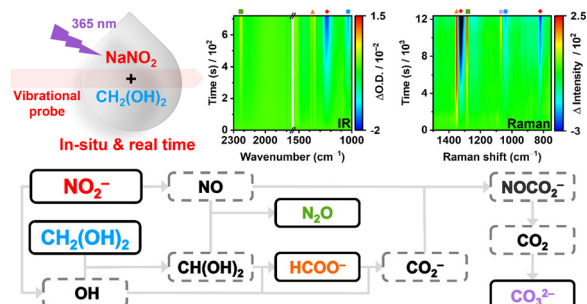


## RESEARCH PAPERS

12165

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

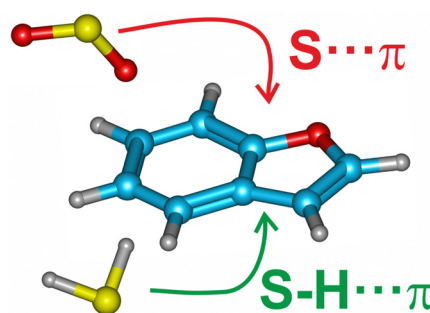
Chiao-Mi Cheng, Cheng-Zong Lu, Chun-Yao Hou, Yuan-Jyun Jhao, Yi-Fen Lai, I-Chia Chen, Yi-Hsueh Chuang and Li-Kang Chu\*



12174

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

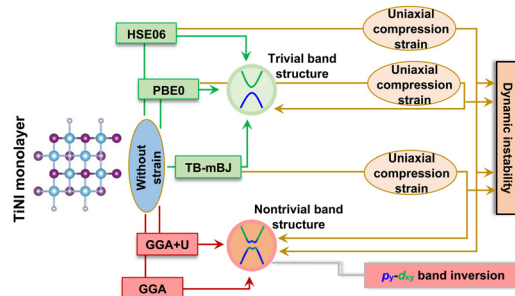
Yan Jin, Wenqin Li, Rizalina Tama Saragi, Marcos Juanes, Cristóbal Pérez, Alberto Lesarri\* and Gang Feng\*



12182

**New insights into band inversion and topological phase of TiNI monolayer**

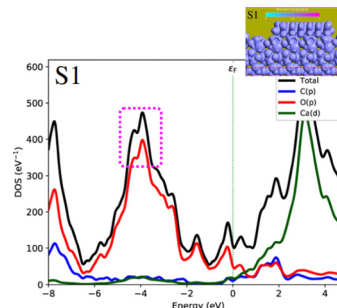
Shahram Yalameha, Zahra Nourbakhsh, Mohammad Saeed Bahramy and Daryoosh Vashaee\*



12192

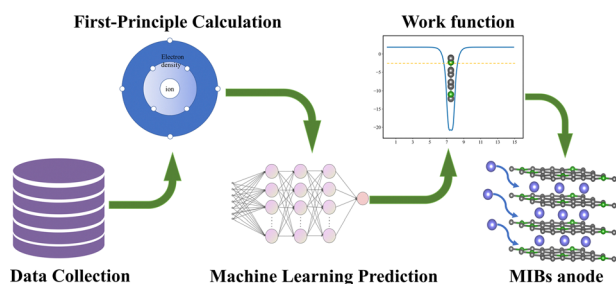
**Unravelling the impact of oily alkane molecules on the optical properties of the calcite(10.4) surface**

Junais Habeeb Mokkaht



## RESEARCH PAPERS

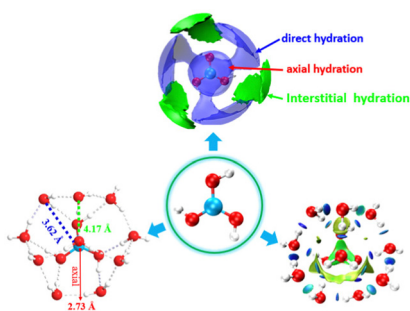
12200



### 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

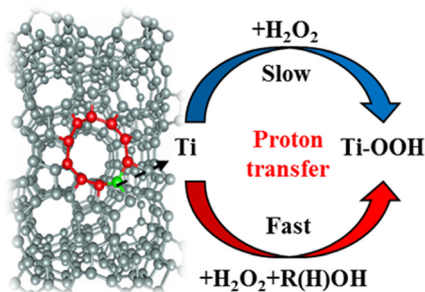
12207



### Structural analysis of potassium borate solutions

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

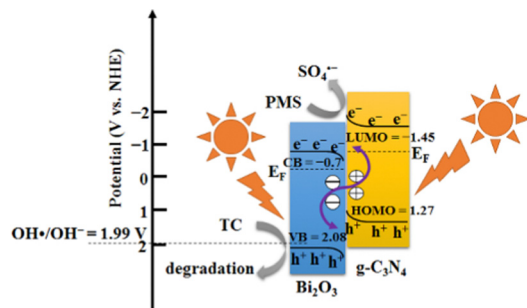
12220



### Evidence of solvent-mediated proton transfer during H<sub>2</sub>O<sub>2</sub> activation in titanasilicate-catalyzed oxidation systems

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

12231



### A 1D/2D Bi<sub>2</sub>O<sub>3</sub>/g-C<sub>3</sub>N<sub>4</sub> step-scheme photocatalyst to activate peroxymonosulfate for the removal of tetracycline hydrochloride: insight into the mechanism, reactive sites, degradation pathway and ecotoxicity

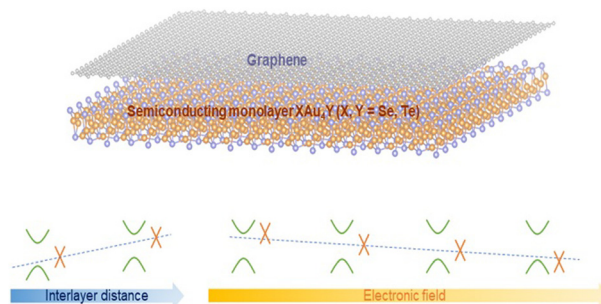
Mingyang Long, Di Li,\* Qianqian Zhao, Hongmiao Li, Qi Wen, Li Wang, Lei Wu, Fang Song and Jun Zhou



12245

### Tunable Schottky contacts in graphene/XAu<sub>4</sub>Y (X, Y = Se, Te) heterostructures

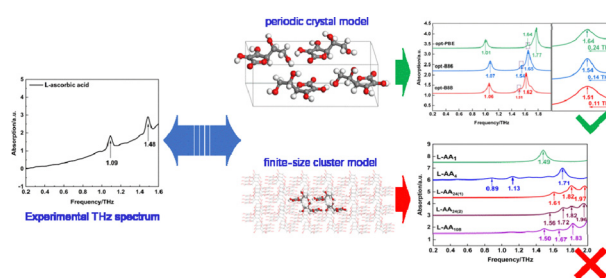
Yufei Xue, Lei Gao,\* Weina Ren, Xuxia Shai, Tingting Wei, Chunhua Zeng\* and Hua Wang\*



12252

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

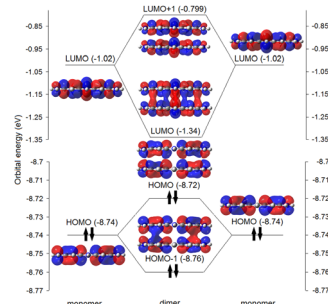
Ying Wang, Huifang Ma, Yanzhao Yang, Jiantao Qi, Guiming Zhang, Hao Ren\* and Wenyue Guo\*



12259

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

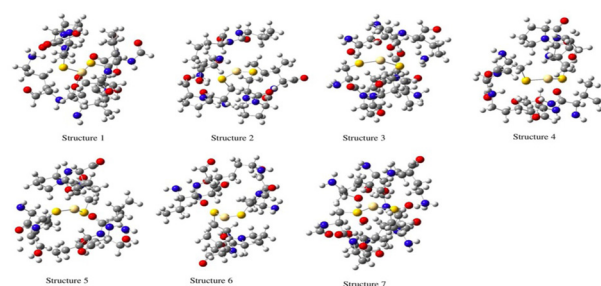
Evgeniy S. Savenko and Victor V. Kostjukov\*



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\*



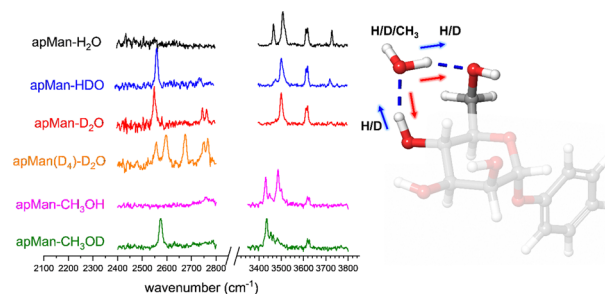


## RESEARCH PAPERS

12331

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

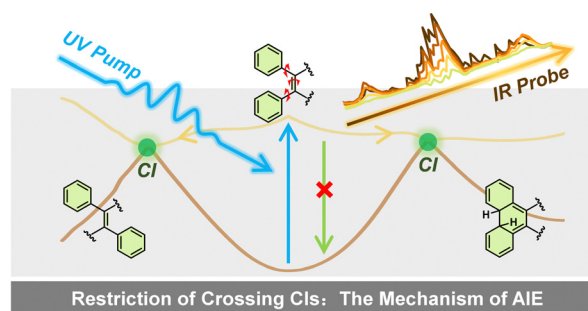
Ander Camiruaga, Gildas Goldsztejn and Pierre Çarçabal\*



12342

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

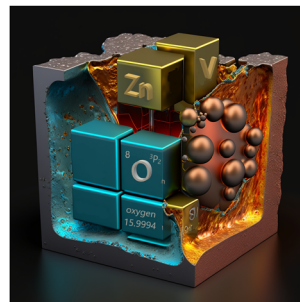
Jie Peng, Xin He, Yao Li, Jianxin Guan, Baihua Wu, Xinmao Li, Zhihao Yu, Jian Liu\* and Junrong Zheng\*



12352

### First principles calculation of the ZnV<sub>2</sub>O<sub>6</sub>(001) surface terminations: the thermodynamic stability and electronic structure study

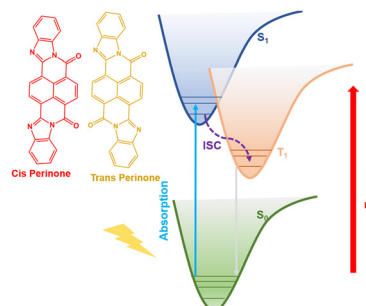
Anqi Yang, Jiaolian Luo,\* Zhenyu Xie, Qian Chen\* and Quan Xie



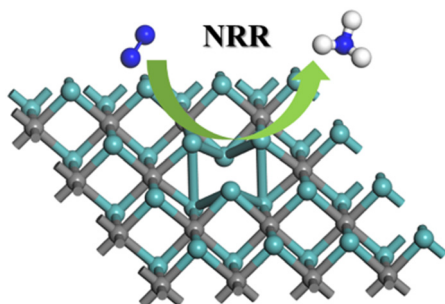
12363

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

Suman Dhama, Yogesh Kumar, Chaitrali Sengupta and Ravindra Pandey\*



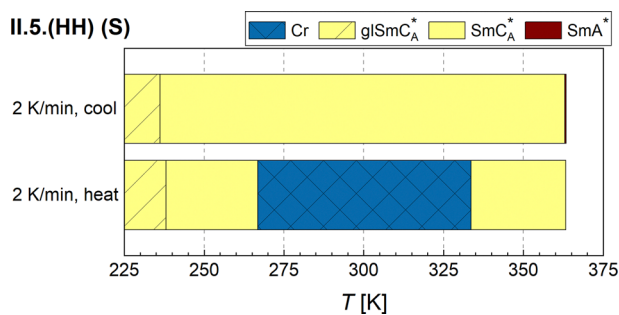
12371



### Defective Mo<sub>2</sub>C as a promising electrocatalyst for the nitrogen reduction reaction

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

12379

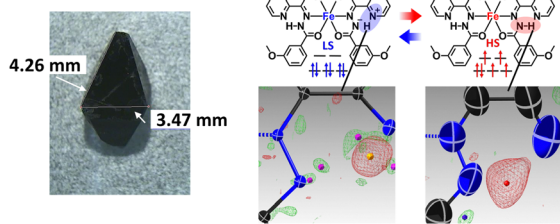


### Vitrification of the smectic C<sub>A</sub>\* phase and kinetics of cold crystallization investigated for a fluorinated compound with a chiral centre based on (S)-(+)-3-octanol

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

12394

### Proton Tautomerism Based on Proton Transfer Coupled Spin Transition

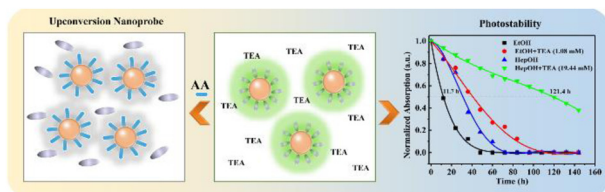


Observation of proton tautomerism by single-crystal neutron diffraction

### 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 Kiyonagi, 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

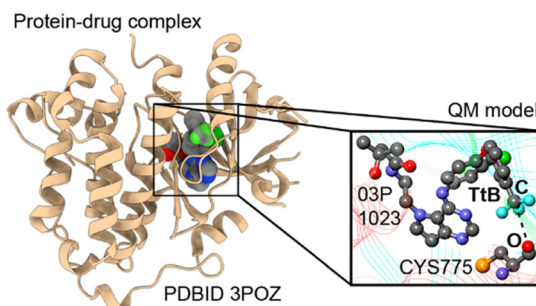


## RESEARCH PAPERS

12409

Tetrel bonds involving a  $\text{CF}_3$  group participate in protein–drug recognition: a combined crystallographic and computational study

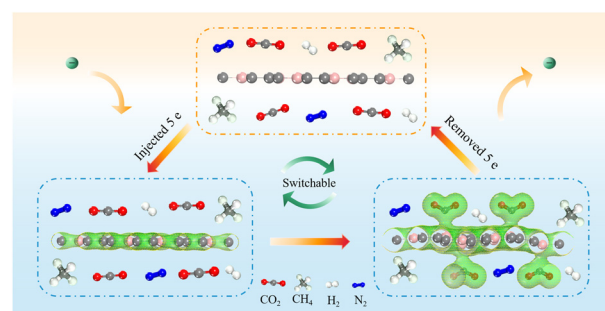
María de las Nieves Piña, Akshay Kumar Sahu, Antonio Frontera, Himansu S. Biswal\* and Antonio Bauzá\*



12420

Charge-controlled switchable  $\text{CO}_2$  capture and gas separation using  $\text{BC}_3$  nanosheets

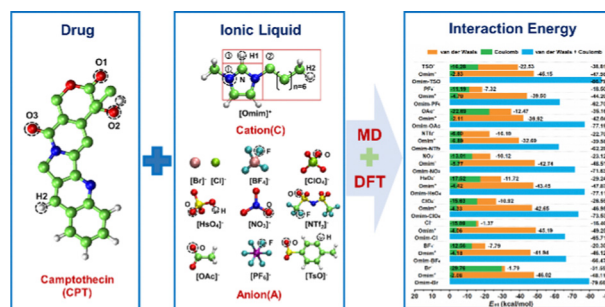
Yiqun Guo, Xuxin Kang, Shan Gao\* and Xiangmei Duan\*



12426

## Theoretical study on the solvation mechanism of camptothecin in ionic liquids

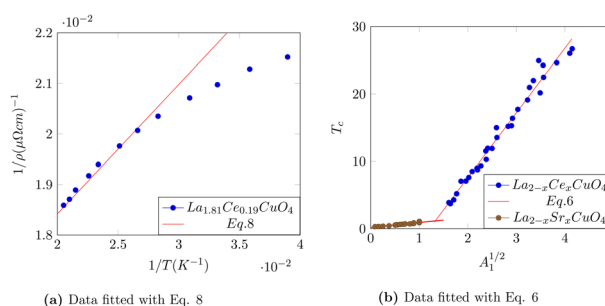
Xiaotong Zhu, Yiping Huang and Yuanhui Ji\*



12443

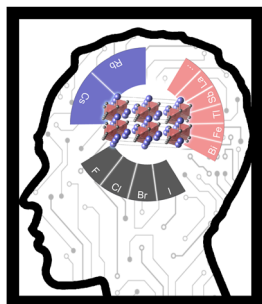
## Universal correlation of the superconducting transition temperature with the linear-in-T coefficient, electron packing parameter, and the numbers of valence and conduction electrons

Tian Hao



## RESEARCH PAPERS

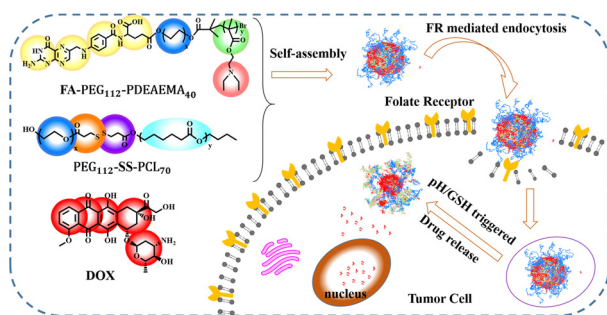
12450



### 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\*

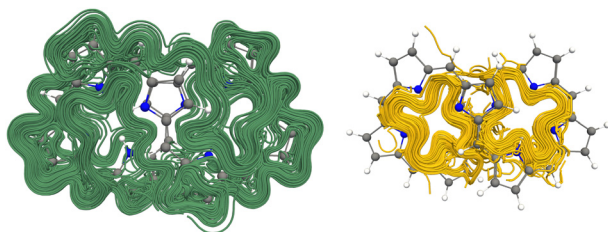
12458



### 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\*

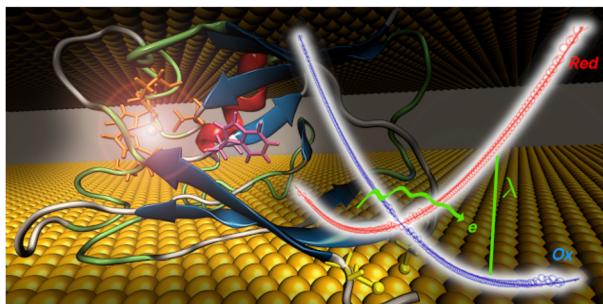
12469



### 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\*

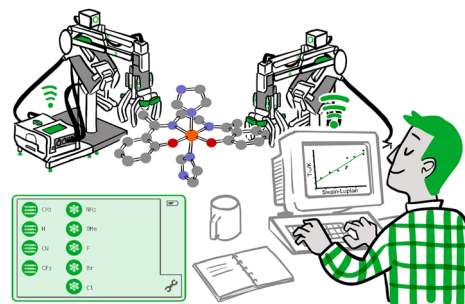


## RESEARCH PAPERS

12490

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

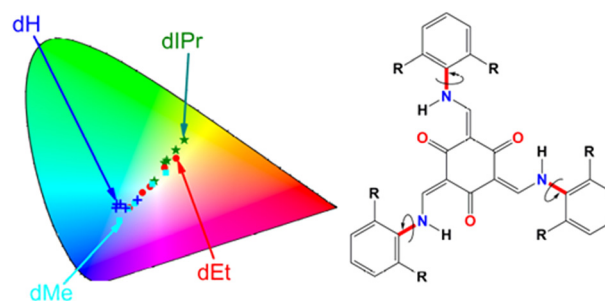
Daniel Vidal, Jordi Cirera\* and Jordi Ribas-Arino\*



12500

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

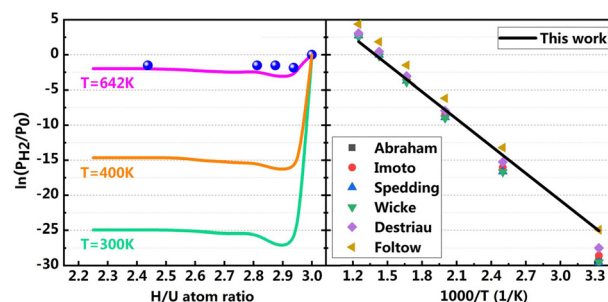
Pawel Gawrys, Olaf Morawski,\* Marzena Banasiewicz and Cristina A. Barboza\*



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\*

