

## IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 25(23) 15569–16160 (2023)



### Cover

See Hui-wang Ai, Chong Fang *et al.*, pp. 15624–15634. Image reproduced by permission of Chong Fang from *Phys. Chem. Chem. Phys.*, 2023, 25, 15624.



### Inside cover

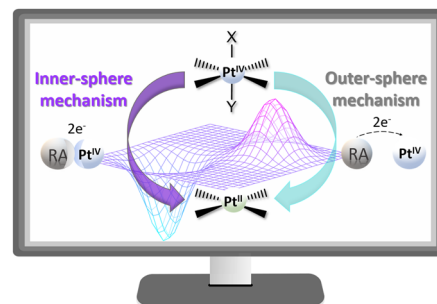
See Dario Barreiro-Lage, Paola Bolognesi *et al.*, pp. 15635–15646. Image reproduced by permission of Paola Bolognesi and Dario Barreiro-Lage from *Phys. Chem. Chem. Phys.*, 2023, 25, 15635. Background image credits: NASA/JPL-Caltech/Potsdam Univ

## PERSPECTIVES

15586

### The current status in computational exploration of Pt(IV) prodrug activation by reduction

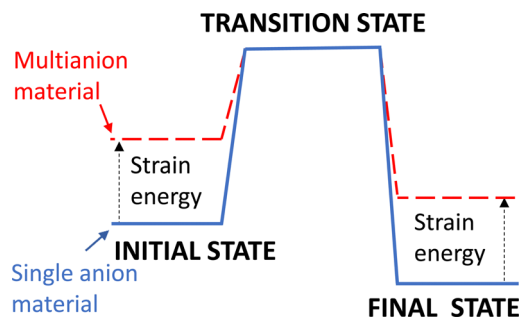
Fortuna Ponte, Stefano Scoditti, Gloria Mazzone\* and Emilia Sicilia\*



15600

### New perspectives on the multianion approach to adapt electrode materials for lithium and post-lithium batteries

Carlos Pérez-Vicente and Ricardo Alcántara\*



## Editorial Staff

### Executive Editor

Michael A. Rowan

### Deputy Editor

Vikki Pritchard

### Development Editors

Bee Hockin, Andrea Carolina Ojeda Porras

### Editorial Production Manager

Gisela Scott

### Senior Publishing Editor

Robin Brabham

### Publisher

Jeanne Andres

### Publishing Editors

Catherine Au, Isobel Darlington, Konoya Das, Alexandre Dumon, Amy Lucas, Kieran Nicholson, 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 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](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

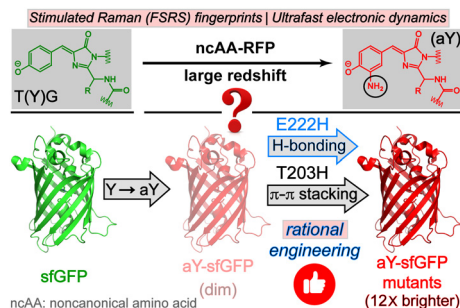


## RESEARCH PAPERS

15624

### Structural origin and rational development of bright red noncanonical variants of green fluorescent protein

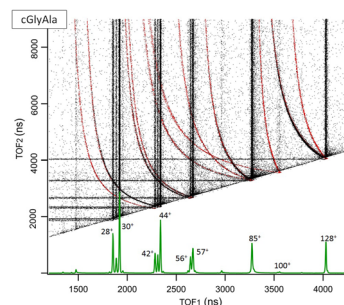
Cheng Chen, Hao Zhang, Jing Zhang, Hui-wang Ai\* and Chong Fang\*



15635

### Photofragmentation specificity of photoionized cyclic amino acids (diketopiperazines) as precursors of peptide building blocks

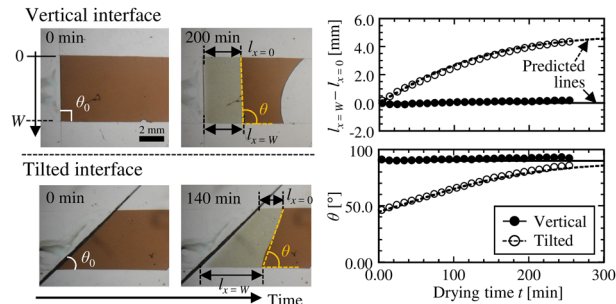
Dario Barreiro-Lage,\* Jacopo Chiarinelli, Paola Bolognesi,\* Robert Richter, Henning Zettergren, Mark H. Stockett, Sergio Díaz-Tendero and Lorenzo Avaldi



15647

### Position-dependent rates of film growth in drying colloidal suspensions on tilted air–water interfaces

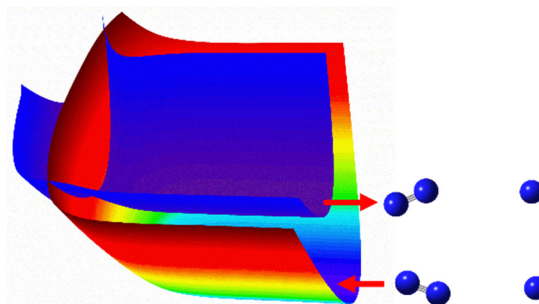
Kohei Abe\* and Susumu Inasawa\*



15656

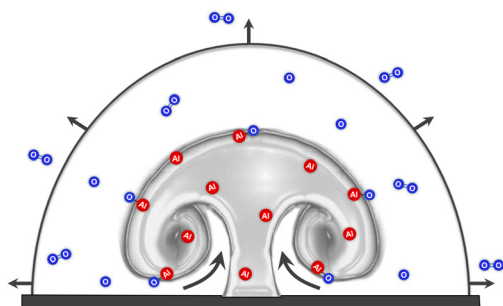
### Quantum and semiclassical studies of nonadiabatic electronic transitions between $N(^4S)$ and $N(^2D)$ by collisions with $N_2$

Dandan Lu, Breno R. L. Galvão, Antonio J. C. Varandas and Hua Guo\*



## RESEARCH PAPERS

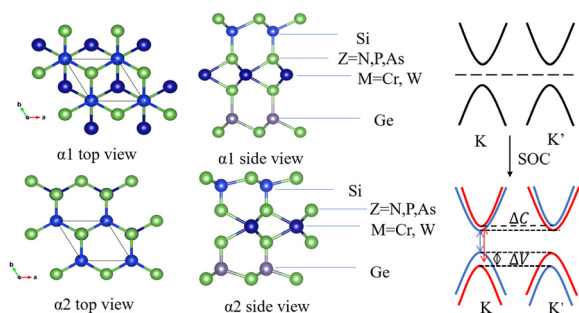
15666



### Experimental and computational investigation into the hydrodynamics and chemical dynamics of laser ablation aluminum plasmas

Emily H. Kwapis,\* Jacob W. Posey, Enrique Medici, Kira Berg, Ryan W. Houim and Kyle C. Hartig

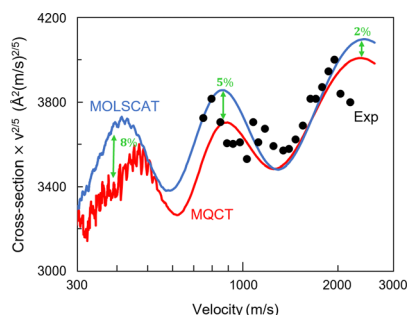
15676



### Theoretical prediction of valley spin splitting in two-dimensional Janus MSiGeZ<sub>4</sub> (M = Cr and W; Z = N, P, and As)

Ying Li, Mengxian Lan, Suen Wang, Tian Huang, Yu Chen, Hong Wu, Feng Li\* and Yong Pu\*

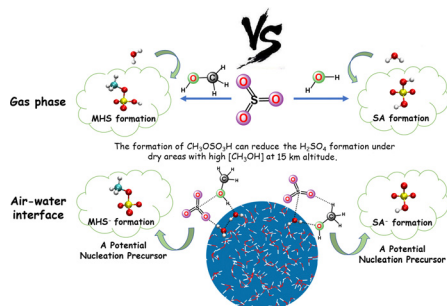
15683



### Description of quantum interference using mixed quantum/classical theory of inelastic scattering

Dulat Bostan, Bikramaditya Mandal, Carolin Joy and Dmitri Babikov\*

15693



### Determination of the influence of water on the SO<sub>3</sub> + CH<sub>3</sub>OH reaction in the gas phase and at the air–water interface

Chao Ding, Yang Cheng, Hui Wang, Jihuan Yang, Zeyao Li, Makroni Lily,\* Rui Wang and Tianlei Zhang\*

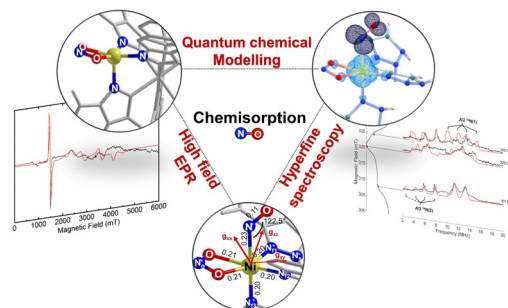


## RESEARCH PAPERS

15702

### Unveiling the atomistic and electronic structure of Ni<sup>II</sup>–NO adduct in a MOF-based catalyst by EPR spectroscopy and quantum chemical modelling

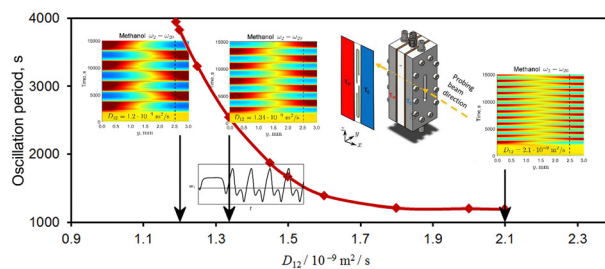
Kavipriya Thangavel, Paolo Cleto Bruzzese, Matthias Mendt, Andrea Folli, Katharina Knippen, Dirk Volkmer, Damien M. Murphy and Andreas Pöpl<sup>\*</sup>



15715

### Cross diffusion governs an oscillatory instability in a ternary mixture with the Soret effect

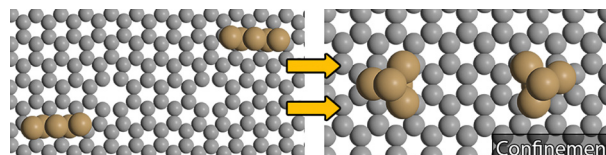
Berin Seta, Ane Errarte, Aliaksandr Mialdun, Ilya I. Ryzhkov, Mounir M. Bou-Ali and Valentina Shevtsova<sup>\*</sup>



15729

### Carbon vacancy-assisted stabilization of individual Cu<sub>5</sub> clusters on graphene. Insights from *ab initio* molecular dynamics

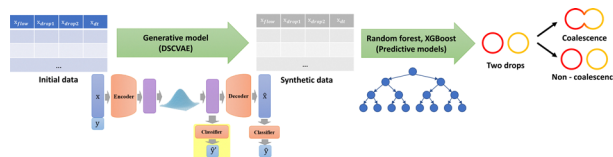
Lenard L. Carroll, Lyudmila V. Moskaleva<sup>\*</sup> and Maria Pilar de Lara-Castells<sup>\*</sup>



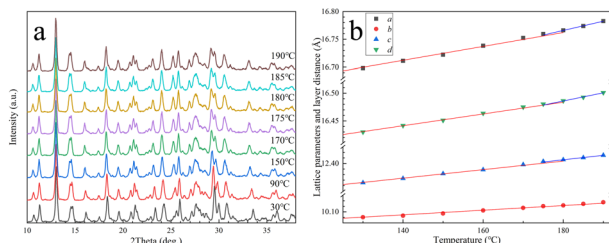
15744

### Analyzing drop coalescence in microfluidic devices with a deep learning generative model

Kewei Zhu, Sib0 Cheng,<sup>\*</sup> Nina Kovalchuk, Mark Simmons, Yi-Ke Guo, Omar K. Matar and Rossella Arcucci



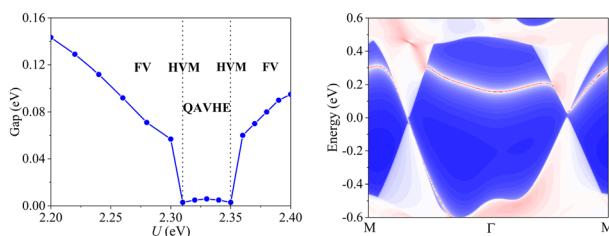
15756



### Isothermal structural evolution of CL-20/HMX cocrystals under slow roasting at 190 °C

Wentao Liang, Xiaoyu Sun, He Wang, Junke Wang, Zhilei Sui, Haichao Ren, Rucheng Dai, Xianxu Zheng, Zhongping Wang,\* Xiaohui Duan\* and Zengming Zhang\*

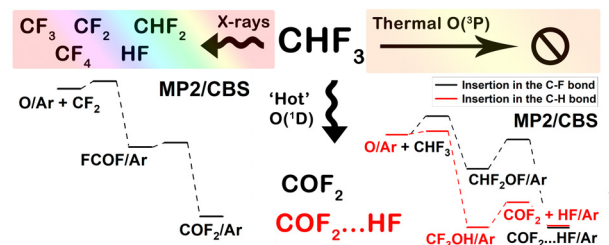
15767



### Electronic-correlation induced sign-reversible Berry phase and quantum anomalous valley Hall effects in Janus monolayer OsClBr

Kang Jia, Xiao-Jing Dong, Sheng-Shi Li, Wei-Xiao Ji and Chang-Wen Zhang\*

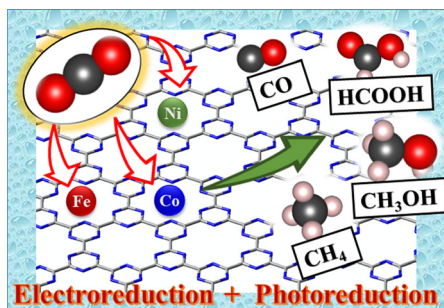
15777



### Reactions of oxygen atoms with fluorocarbon and its radiolysis products: matrix isolation and *ab initio* study

Ilya S. Sosulin, Ekaterina S. Shiryayeva, Daniil A. Tyurin and Vladimir I. Feldman\*

15788



### Boosting photo-assisted efficient electrochemical CO<sub>2</sub> reduction reaction on transition metal single-atom catalysts supported on the C<sub>6</sub>N<sub>6</sub> nanosheet

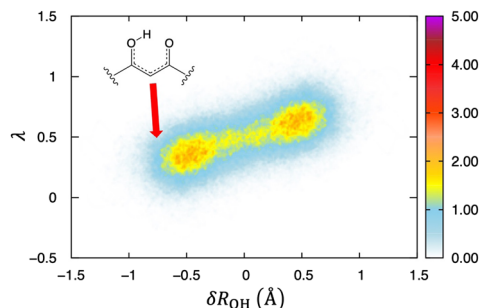
Supriti Dutta and Swapan K. Pati\*



15798

### Nuclear quantum and H/D isotope effects on intramolecular hydrogen bond in curcumin

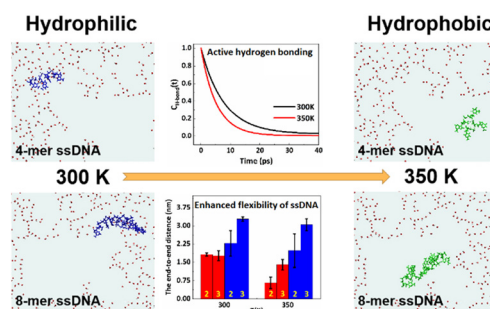
Taro Udagawa,\* Hinata Yabushita, Hikaru Tanaka, Kazuaki Kuwahata and Masanori Tachikawa



15807

### Dynamic behavior of the single-strand DNA molecules from the hydrophilic to hydrophobic regions on graphene oxide surface driven by heating

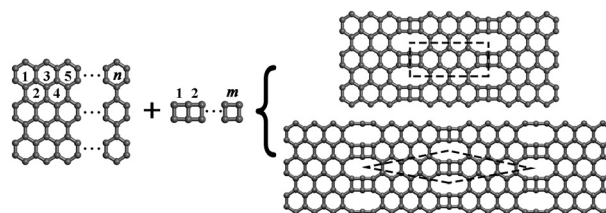
Mengjiao Wu, Yingying Huang, Li Yang, Yongshun Song\* and Xiaoling Lei\*



15815

### A series of two-dimensional carbon allotropes with Dirac cone structure

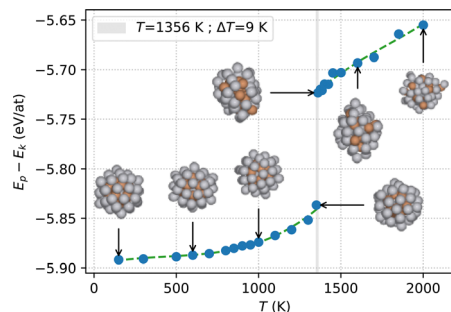
Guo Xiang Wang



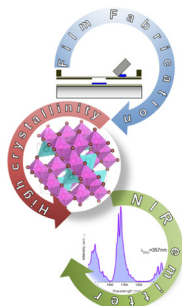
15822

### Melting of FePt nanoparticles studied using DFT

Paweł T. Jochym,\* Jan Łażewski and Przemysław Piekarczyk



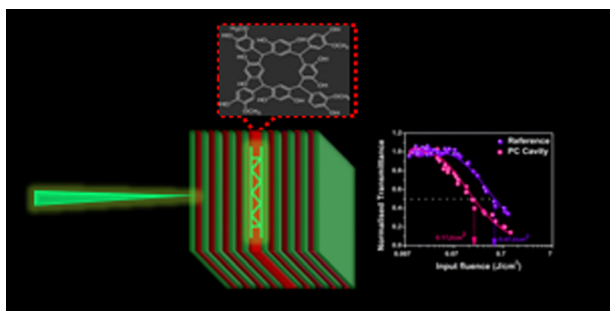
15829



### Cost-effective screen printing approach for Ce/Nd-doped ZnAl<sub>2</sub>O<sub>4</sub> films: tuning crystallinity induced by the substrate

Rocio E. Rojas-Hernandez,\* Fernando Rubio-Marcos, Jallouli Necib, Mati Danilson, José F. Fernandez and Irina Hussainova

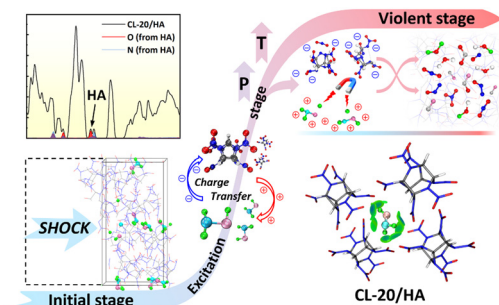
15839



### Photonic crystal cavity-mediated improved absorptive nonlinearity of C-4-hydroxy-3-methoxyphenilcalix[4]resorcinarene

Siji Alappattu John, Athulya Kadeprath Satheesan, Simi Pushpan K. and Chandrasekharan Keloth\*

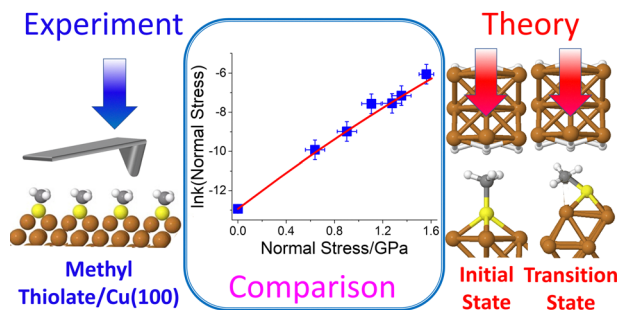
15846



### Reaction mechanism and electronic properties of host-guest energetic material CL-20/HA under high pressure by quantum-based molecular dynamics simulations

Yiwen Xiao, Lang Chen,\* Kun Yang, Jianying Lu and Junying Wu

15855



### Exploring mechanochemical reactions at the nanoscale: theory versus experiment

Nicholas Hopper, François Sidoroff, Resham Rana, Robert Bavisotto, Juliette Cayer-Barrioz, Denis Mazuyer and Wilfred T. Tysoe\*

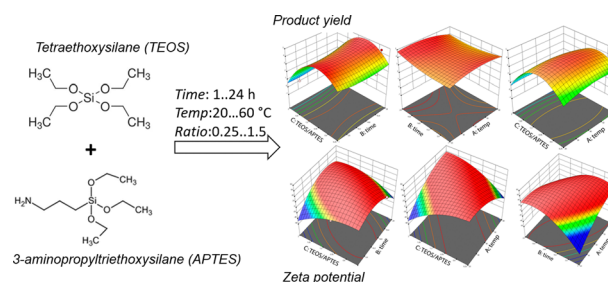


## RESEARCH PAPERS

15862

### A statistical design approach to the sol–gel synthesis of (amino)organosilane hybrid nanoparticles

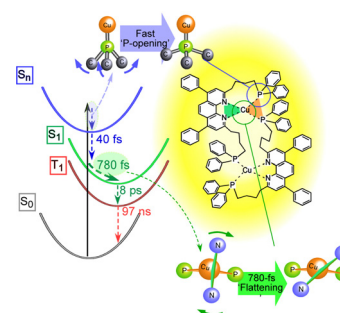
Lyubov Bondarenko,\* Yaroslav Saveliev, Dmitry Chernyaev, Rose Baimuratova, Gulzhian Dzhardimalieva, Artur Dzeranov, Elena Kelbysheva and Kamila Kydralieva



15873

### Structural change dynamics of heteroleptic Cu(I) complexes observed by ultrafast emission spectroscopy

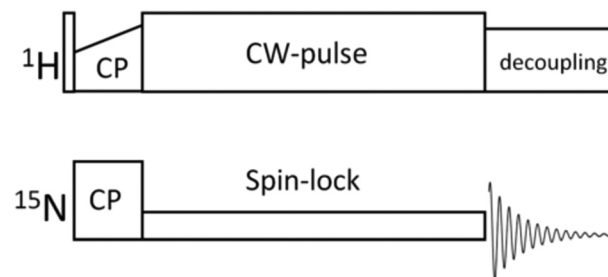
Masashi Sanga, Kosuke Nakamura, Munetaka Iwamura,\* Koichi Nozaki, Hiroyuki Takeda,\* Yu Monma and Osamu Ishitani



15885

### Rocking motion in solid proteins studied by the $^{15}\text{N}$ proton-decoupled $R_{1\rho}$ relaxometry

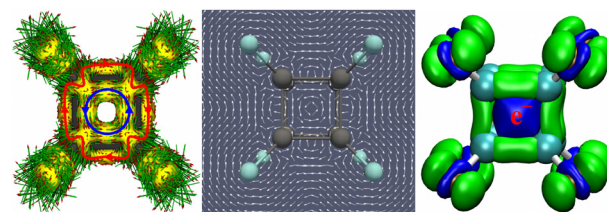
Alexey Krushelnitsky,\* Günter Hempel, Hannes Jurack and Tiago Mendes Ferreira



15897

### Bonding character, electronic properties, and electronic transitions of perfluorocubane as a small electron acceptor

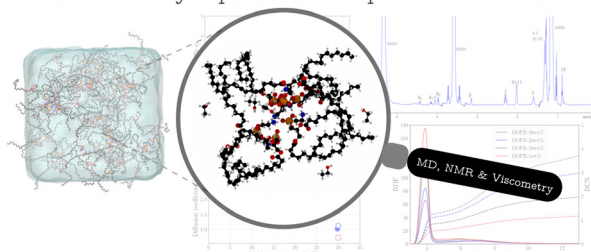
Xiaojun Li,\* Shuna Li, Jun Lu, Hongjiang Ren, Mengqi Zhang and Wangdi Zhang



## RESEARCH PAPERS

15905

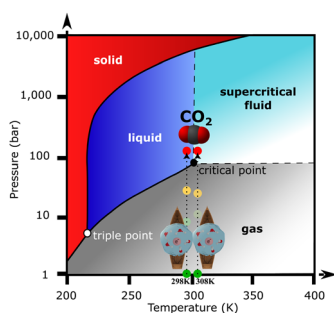
Simulation insight and interpretation of results from NMR and viscometry experiments in lipid-ethanol mixtures



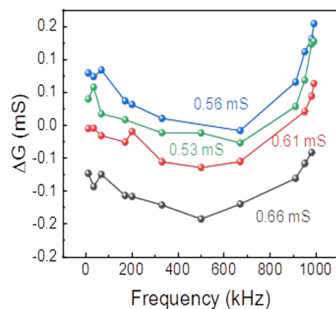
## Phase equilibrium, dynamics and rheology of phospholipid-ethanol mixtures: a combined molecular dynamics, NMR and viscometry study

Fredrik Grote, Alexander Lyubartsev,\*  
Sergey V. Dvinskikh, Vibhu Rinwa and Jan Holmbäck

15916

Reactivity of presolvated and solvated electrons with CO<sub>2</sub> in water up to 118 bar at 298 and 308 KDenis S. Dobrovolskii, Mehran Mostafavi and  
Sergey A. Denisov\*

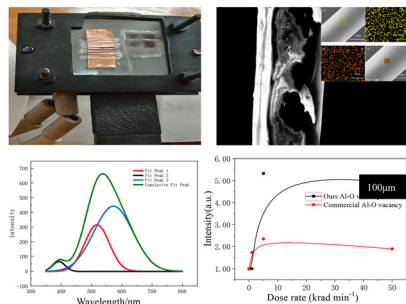
15920



## Tuning Bienenstock-Cooper-Munro learning rules in a two-terminal memristor for neuromorphic computing

Zeyang Li, Peilin Liu, Guanghong Yang, Caihong Jia\* and  
Weifeng Zhang\*

15929



## Promotional effects of cerium in ytterbium doped fibers on proton irradiation damage

Yang Shao, Yuting Wang\* and Xin Ju\*

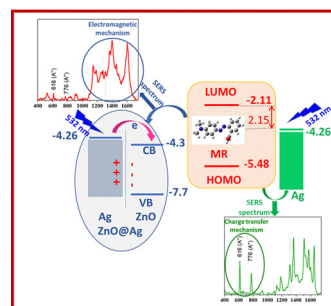


## RESEARCH PAPERS

15941

### Enhanced Raman scattering based on a ZnO/Ag nanostructured substrate: an in-depth study of the SERS mechanism

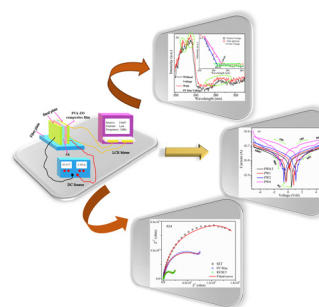
Thu Trang Tran, Xuan Hoa Vu, Thi Lan Ngo, Thi Thu Ha Pham,\* Dac Dien Nguyen and Van Dang Nguyen



15953

### Tunable, reversible resistive switching behavior of PVA-zirconia nanocomposite films and validation of the trap-assisted switching mechanism by the selective application of external bias voltages

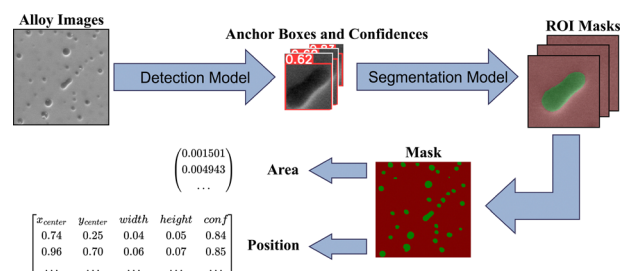
Riju Karmakar, Amit Kumar Das, Bilwadal Dutta, Subhojyoti Sinha,\* Saikat Santra, Subhamay Pramanik, Probooth Kumar Kuri and Ajit Kumar Meikap\*



15970

### Accurate identification and measurement of the precipitate area by two-stage deep neural networks in novel chromium-based alloys

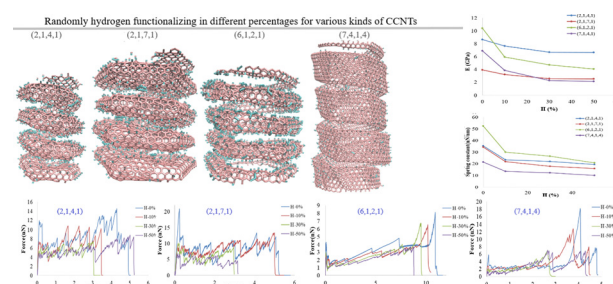
Zeyu Xia, Kan Ma, Sibao Cheng,\* Thomas Blackburn, Ziling Peng, Kewei Zhu, Weihang Zhang, Dunhui Xiao, Alexander J Knowles and Rossella Arcucci



15988

### Unraveling the effect of hydrogenation on the mechanical properties of coiled carbon nanotubes: a molecular dynamics study

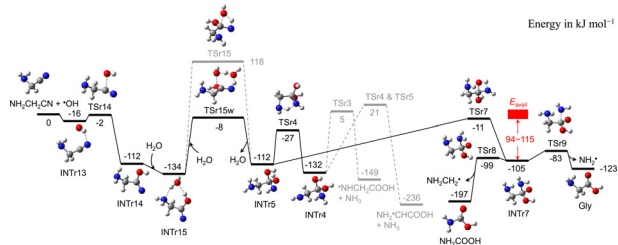
Mahdi Azhari Saray, Mostafa Baghani, Ali Rajabpour, Ali Sharifian\* and Majid Baniassadi\*



16001

## Mechanisms of glycine formation from aminoacetonitrile in space

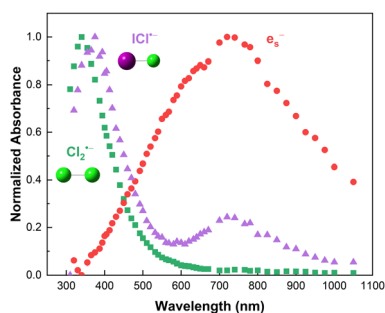
Joong Chul Choe



16009

## Impact of iodide ions on the speciation of radiolytic transients in molten LiCl–KCl eutectic salt mixtures

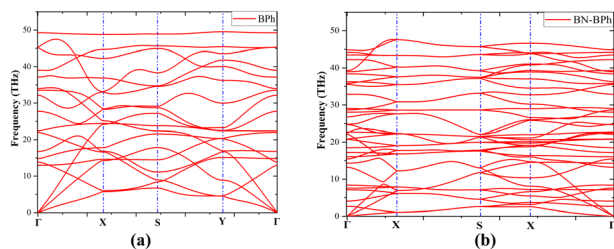
Jacy K. Conrad,\* Kazuhiro Iwamatsu, Michael E. Woods, Ruchi Gakhar, Bobby Layne, Andrew R. Cook and Gregory P. Horne\*



16018

## 2D BN-biphenylene: structure stability and properties tenability from a DFT perspective

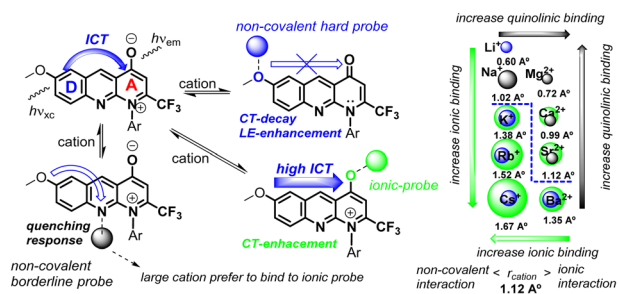
Mukesh Singh and Brahmananda Chakraborty\*



16030

## Exploring binding chemistry of alkali/alkaline earth cations in solution through modulation of intramolecular charge-transfer in an excited ambidentate organic fluorophore

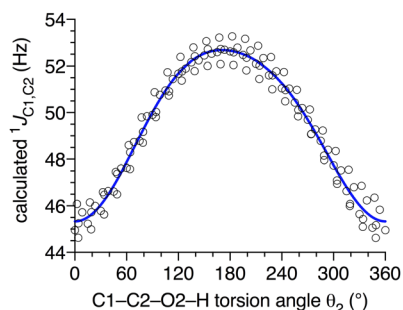
Angel H. Romero,\* Lourdes Gotopo, Gustavo Cabrera and Hugo Cerecetto



16048

### One-bond $^{13}\text{C}$ – $^{13}\text{C}$ spin-coupling constants in saccharides: a comparison of experimental and calculated values by density functional theory using solid-state $^{13}\text{C}$ NMR and X-ray crystallography

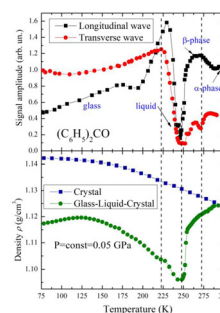
Timothy Tetrault, Reagan J. Meredith, Mi-Kyung Yoon, Christopher Canizares, Allen G. Oliver, Ian Carmichael and Anthony S. Serianni\*



16060

### Benzophenone glass, supercooled liquid, and crystals: elastic properties and phase transitions

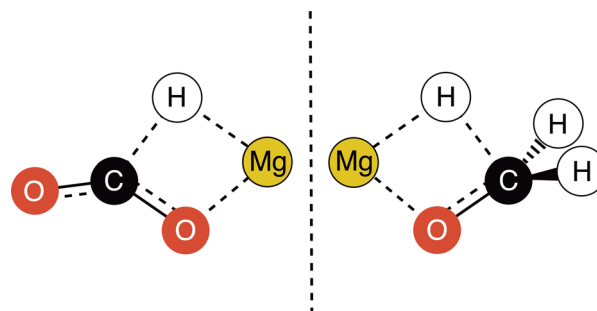
Elena L. Gromnitskaya,\* Igor V. Danilov, Fedor I. Zubkov and Vadim V. Brazhkin



16065

### Gas phase models of hydride transfer from divalent alkaline earth metals to $\text{CO}_2$ and $\text{CH}_2\text{O}$

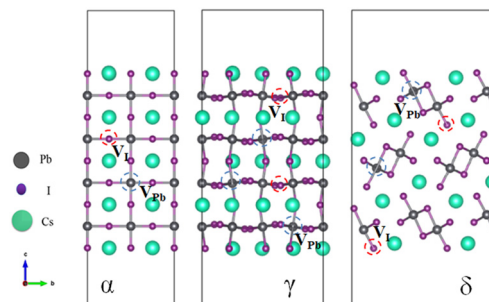
Christian Sant Gjermestad, Mauritz Johan Ryding and Einar Uggerud\*



16077

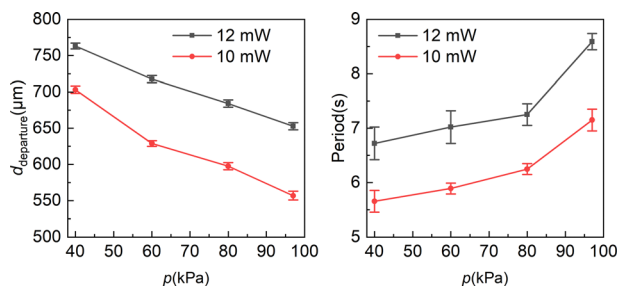
### Intrinsic defects on $\alpha$ , $\gamma$ and $\delta$ - $\text{CsPbI}_3$ (001) surfaces and implications for the $\alpha/\gamma$ to $\delta$ phase transition

Na Wang\* and Yaqiong Wu



## RESEARCH PAPERS

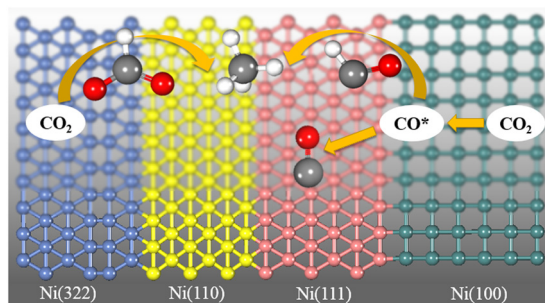
16086



### Influence of subatmospheric pressure on bubble evolution on the $\text{TiO}_2$ photoelectrode surface

Xinyi Luo, Qiang Xu,\* Tengfei Nie, Yonglu She, Xingmiao Ye and Liejin Guo

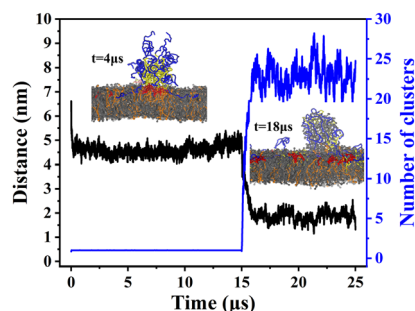
16105



### Meso-scale study of crystal-plane effects of Ni catalysts on $\text{CO}_2$ hydrogenation

Xiaolei Wang, Ning Liu, Ruinian Xu, Biaohua Chen,\* Chengna Dai and Gangqiang Yu

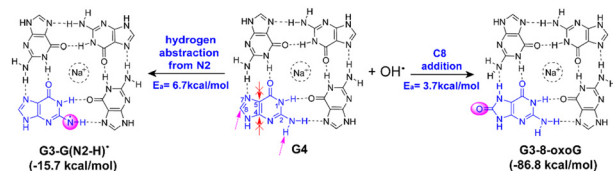
16114



### Delivery mechanism of doxorubicin by PEG-DPPE micelles on membrane invasion by dynamic simulations

Lina Zhao, Meina Ren, Yanjiao Wang, Hailong An\* and Fude Sun\*

16126



### Theoretical insights into the reaction mechanism of hydroxyl radicals and guanine in G-quadruplex DNA

Yinghui Wang\* and Simin Wei\*

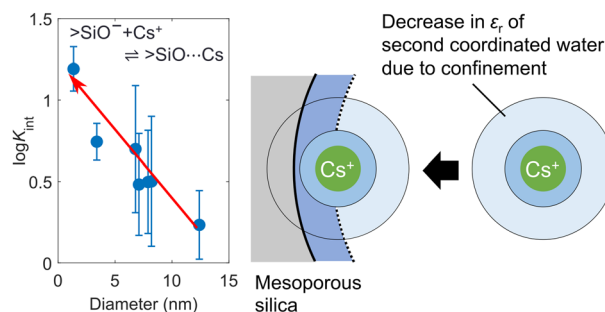


## RESEARCH PAPERS

16135

**Adsorption of cesium and strontium on mesoporous silicas**

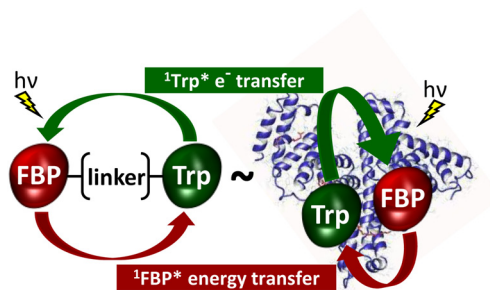
Kento Murota,\* Yoshio Takahashi and Takumi Saito



16148

**Topological effects in ultrafast photoinduced processes between flurbiprofen and tryptophan in linked dyads and within human serum albumin**

Lorena Tamarit, Laura García-Gabarda, M. Consuelo Jiménez, Miguel A. Miranda\* and Ignacio Vayá\*



## CORRECTION

16157

**Correction: Helium nanodroplets as an efficient tool to investigate hydrogen attachment to alkali cations**

Siegfried Kollotzek,\* José Campos-Martínez,\* Massimiliano Bartolomei, Fernando Pirani, Lukas Tiefenthaler, Marta I. Hernández, Teresa Lázaro, Eva Zunzunegui-Bru, Tomás González-Lezana, José Bretón, Javier Hernández-Rojas, Olof Echt and Paul Scheier

