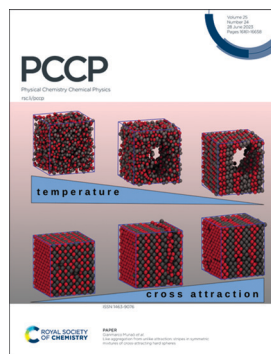


IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 25(24) 16161–16658 (2023)



Cover

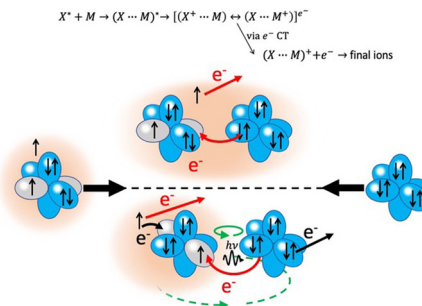
See Gianmarco Munaó *et al.*, pp. 16227–16237. Image reproduced by permission of Gianmarco Munaó from *Phys. Chem. Chem. Phys.*, 2023, 25, 16227.

REVIEW

16176

The role of precursor states in the stereo-dynamics of elementary processes

Stefano Falcinelli,* David Cappelletti, Franco Vecchiocattivi and Fernando Pirani

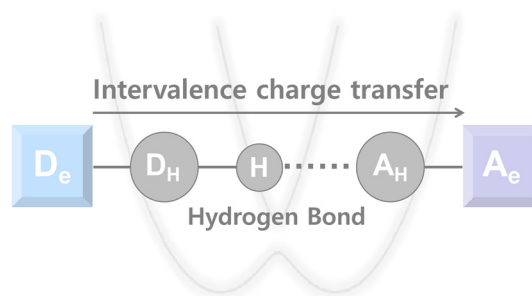


PERSPECTIVE

16201

Electronic coupling and electron transfer in hydrogen-bonded mixed-valence compounds

Juanjuan Li, Yuqing Shi and Tao Cheng*



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

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

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

All orders, with cheques made payable to the Royal Society of Chemistry, should be sent to the Royal Society of Chemistry Order Department, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK.

Tel +44 (0)1223 432398; E-mail: orders@rsc.org

2023 Annual (electronic) subscription price: £4448; US\$7835. Customers in Canada will be subject to a surcharge to cover GST. Customers in the EU subscribing to the electronic version only will be charged VAT.

If you take an institutional subscription to any Royal Society of Chemistry journal you are entitled to free, site-wide web access to that journal. You can arrange access via Internet Protocol (IP) address at www.rsc.org/ip

Customers should make payments by cheque in sterling payable on a UK clearing bank or in US dollars payable on a US clearing bank.

Whilst this material has been produced with all due care, the Royal Society of Chemistry cannot be held responsible or liable for its accuracy and completeness, nor for any consequences arising from any errors or the use of the information contained in this publication. The publication of advertisements does not constitute any endorsement by the Royal Society of Chemistry or Authors of any products advertised. The views and opinions advanced by contributors do not necessarily reflect those of the Royal Society of Chemistry which shall not be liable for any resulting loss or damage arising as a result of reliance upon this material. The Royal Society of Chemistry is a charity, registered in England and Wales, Number 207890, and a company incorporated in England by Royal Charter (Registered No. RC000524), registered office: Burlington House, Piccadilly, London W1J 0BA, UK. Telephone: +44 (0) 207 4378 6556.

Advertisement sales:

Tel +44 (0) 1223 432246;

Fax +44 (0) 1223 426017;

E-mail advertising@rsc.org

For marketing opportunities relating to this journal, contact marketing@rsc.org

PCCP

Physical Chemistry Chemical Physics – An international journal

rsc.li/pccp

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

Owner Societies

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

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

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

Honorary Board

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

K Kohse-Hoinghaus, Universitaet Bielefeld,
Germany
Y T Lee, Academia Sinica, Taiwan
W H Miller, Berkeley, USA
E Neher, Max Planck Institute for Biophysical
Chemistry, Germany
J Polanyi, Toronto, Canada

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

Editorial Board

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

H Kondoh, Keio University, Japan
A Krylov, University of Southern California,
USA
P Maiti, Indian Institute of Science, India
R Naaman, Weizmann Institute of Science,
Israel

A Rijs, Vrije Universiteit Amsterdam,
The Netherlands (Chair)
H Schaefer III, University of Georgia, USA
(Deputy Chair)
I Tamblin, University of Ottawa, Canada
Y Xu, University of Alberta, Canada
J Zhang, New York University Shanghai, China

Advisory Board

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

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

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

Information for Authors

Full details on how to submit material for publication in PCCP are given in the Instructions for Authors (available from <http://www.rsc.org/authors>). Submissions should be made via the journal's homepage: rsc.li/pccp

Authors may reproduce/republish portions of their published contribution without seeking permission from the Royal Society of Chemistry, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation)–Reproduced by permission of the Royal Society of Chemistry.

This journal is © the Owner Societies.

Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted

under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

© The paper used in this publication meets the requirements of ANSI/NISO Z39.48-1992 (Permanence of Paper).

Registered charity number: 207890

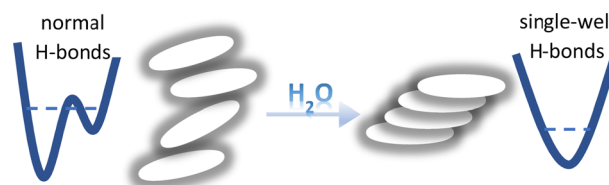


COMMUNICATIONS

16212

Signatures of pancake bonding in hydrated eumelanin

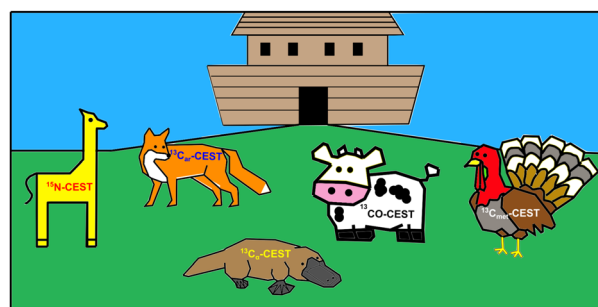
P. A. Abramov, O. I. Ivankov, A. B. Mostert and K. A. Motovilov*



16217

ARCHE-NOAH: NMR supersequence with five different CEST experiments for studying protein conformational dynamics

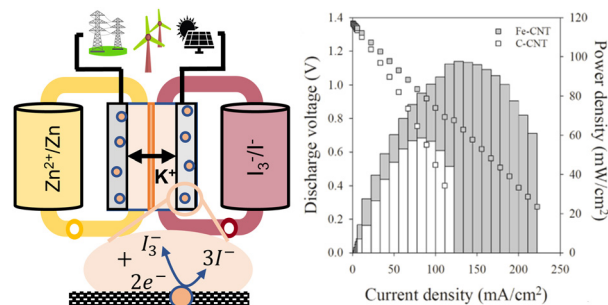
Rodrigo Cabrera Allpas, Alexandar L. Hansen and Rafael Brüschweiler*



16222

High power zinc iodine redox flow battery with iron-functionalized carbon electrodes

Abena A. Williams, Robert K. Emmett and Mark E. Roberts*

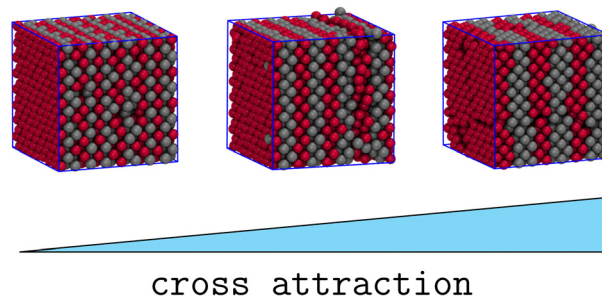


RESEARCH PAPERS

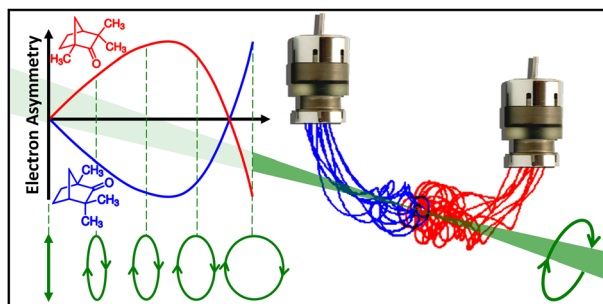
16227

Like aggregation from unlike attraction: stripes in symmetric mixtures of cross-attracting hard spheres

Gianmarco Munaò,* Dino Costa, Gianpietro Malescio, Jean-Marc Bomont and Santi Prestipino



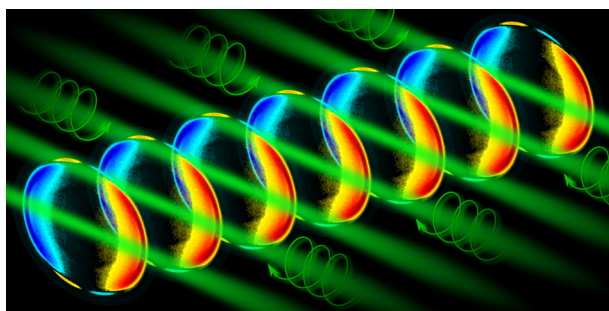
16238



Investigation of photoelectron elliptical dichroism for chiral analysis

Jason B. Greenwood* and Ian D. Williams

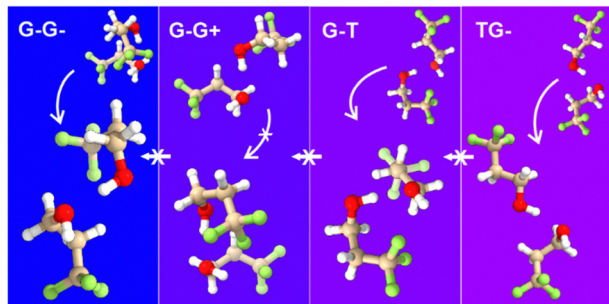
16246



Fast and precise chiroptical spectroscopy by photoelectron elliptical dichroism

Antoine Comby, Dominique Descamps, Stéphane Petit, Emmanuel Valzer, Morgan Wloch, Laurent Pouységu, Stéphane Quideau, Jana Bocková, Cornelia Meinert, Valérie Blanchet, Baptiste Fabre and Yann Mairesse*

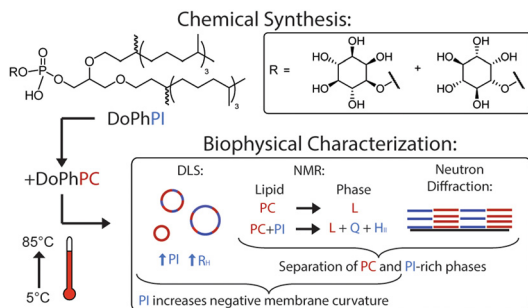
16264



Rotational spectroscopy of hydrogen-bonded binary trifluoro-propanol conformers: conformational diversity, preference and abundances in a jet expansion

Alex N. Mort, Fan Xie, Arsh S. Hazrah and Yunjie Xu*

16273



Membrane plasticity induced by *myo*-inositol derived archaeal lipids: chemical synthesis and biophysical characterization

Johal Ruiz, Josephine G. LoRicco, Laurent Soulère, Marta Salvador Castell, Axelle Grélard, Brice Kauffmann, Erick J. Dufourc, Bruno Demé, Florence Popowycz and Judith Peters*

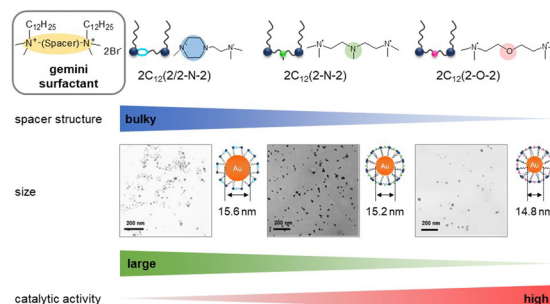


RESEARCH PAPERS

16288

Catalytic activity of gold nanoparticles protected by quaternary ammonium salt-based gemini surfactants with different spacer structures

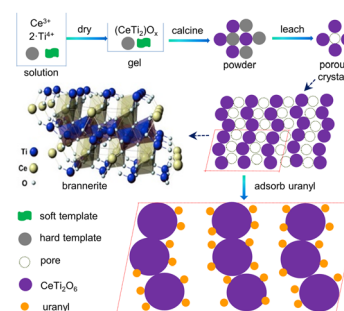
Tsukasa Morita, Shiho Yada and Tomokazu Yoshimura*



16294

Synthesis of hierarchical mesoporous cerium titanate brannerite and uranyl adsorption properties at pH 3.8

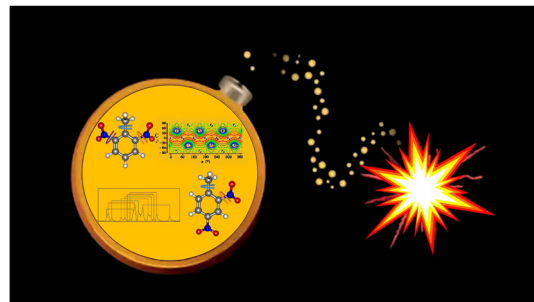
Linggen Kong,* Tao Wei, Inna Karatchevtseva and Nicholas Scales



16307

Microwave spectra of dinitrotoluene isomers: a new step towards the detection of explosive vapors

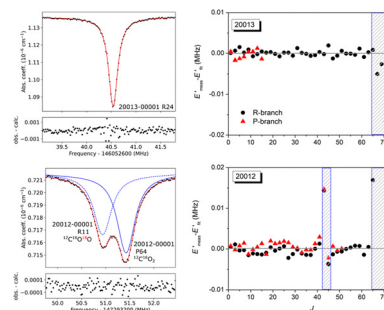
Mhamad Chrayteh,* Pascal Dréan, Manuel Goubet, Laurent H. Coudert, Anthony Roucou and Arnaud Cuisset*



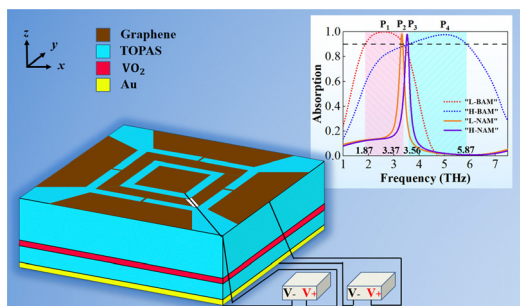
16319

¹²CO₂ transition frequencies with kHz-accuracy by saturation spectroscopy in the 1.99–2.09 μm region

H. Fleurbaey, P. Čermák, A. Campargue, S. Kassi, D. Romanini, O. Votava and D. Mondelain*



16331

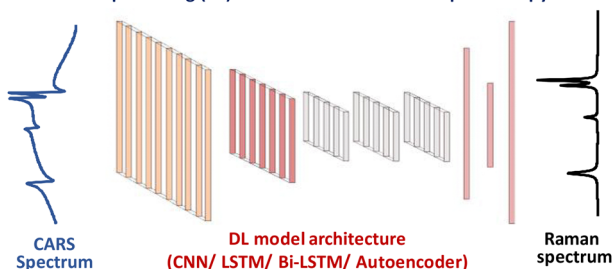


An electrical/thermal dual-controlled quad-functional terahertz metasurface absorber

Zhipeng Ding, Wei Su,* Lipengan Ye, Hong Wu and Hongbing Yao*

16340

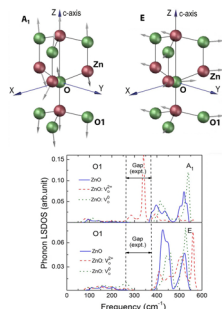
Deep Learning (DL) for NRB removal in CARS Spectroscopy



Evaluating different deep learning models for efficient extraction of Raman signals from CARS spectra

Rajendhar Junjuri,* Ali Saghi, Lasse Lensu and Erik M. Vartiainen

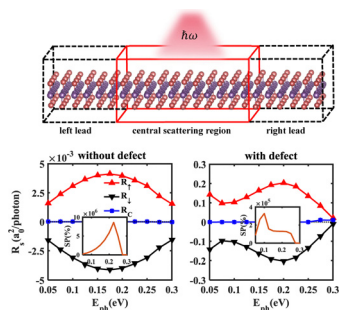
16354



Structural and vibrational properties of wurtzite ZnO with oxygen-deficient defects: *ab initio* and potential-based calculations

Alexey N. Kislov* and Anatoly F. Zatsopin

16363



The photogalvanic effect induced by quantum spin Hall edge states from first-principles calculations

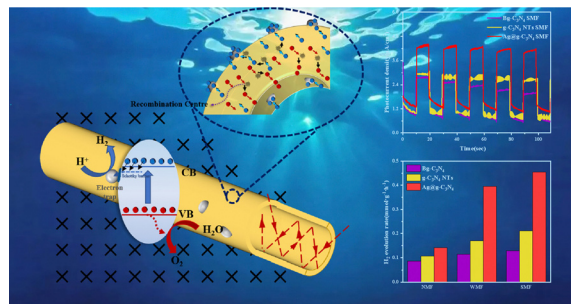
Yaqing Yang, Liwen Zhang, Xiaohong Zheng,* Jun Chen, Liantuan Xiao, Suotang Jia and Lei Zhang*



16371

Enhanced photocatalytic activity of Ag@*C*₃*N*₄ nanotubes by regulating photogenerated carriers to bypass the recombination center under the Lorentz force

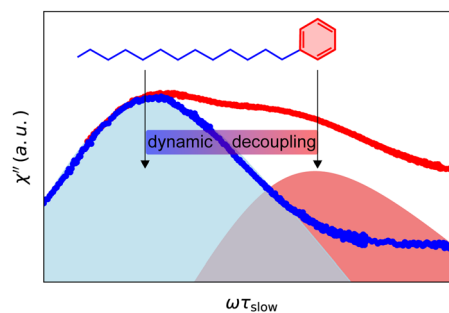
Libin Yang,* Chang Bo, Runjin Wu, Shijia Xu, Qian Li, Yan Ding and Chenyu Gao



16380

Influence of intramolecular dynamics on the relaxation spectra of simple liquids

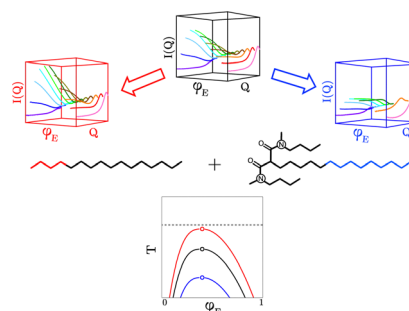
Rolf Zeißler,* Florian Pabst, Till Böhmer and Thomas Blochowicz



16389

Critical fluctuations in liquid–liquid extraction organic phases controlled by extractant and diluent molecular structure

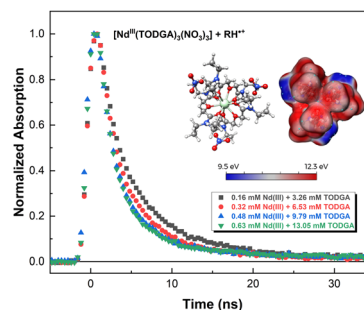
Brittany L. Bonnett, Dina Sheyfer, Pubudu N. Wimalasiri, Srikanth Nayak, Jyotsana Lal, Qingteng Zhang, Soenke Seifert, G. Brian Stephenson* and Michael J. Servis*



16404

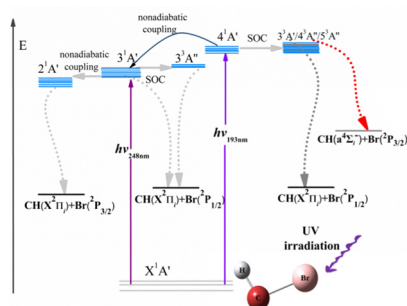
Impact of lanthanide ion complexation and temperature on the chemical reactivity of *N,N,N',N'*-tetraoctyl diglycolamide (TODGA) with the dodecane radical cation

Gregory P. Horne,* Cristian Celis-Barros, Jacy K. Conrad, Travis S. Grimes, Jeffrey R. McLachlan, Brian M. Rotermund, Andrew R. Cook and Stephen P. Mezyk*



RESEARCH PAPERS

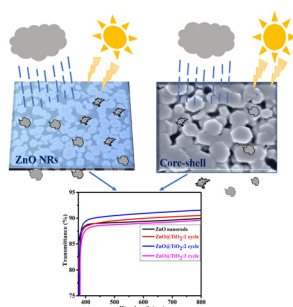
16414



An *ab initio* study on the electronic excited states and photodissociation mechanism of bromocarbene molecule

Shimin Shan, ErPing Sun, Yongquan Gao, Zirun Li, Haifeng Xu* and Bing Yan*

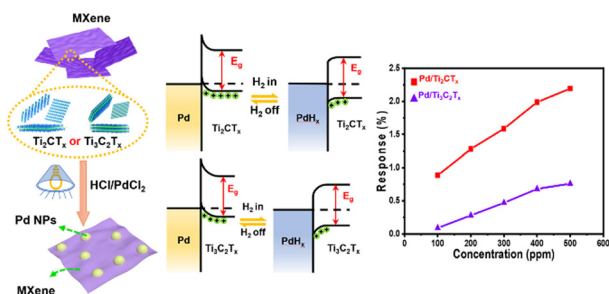
16423



Fabrication of porous and visible light active ZnO nanorods and ZnO@TiO₂ core-shell photocatalysts for self-cleaning applications

Ajay Kumar, Dipali Nayak, Pooja Sahoo, Barun Kumar Nandi, V. K. Saxena and R. Thangavel*

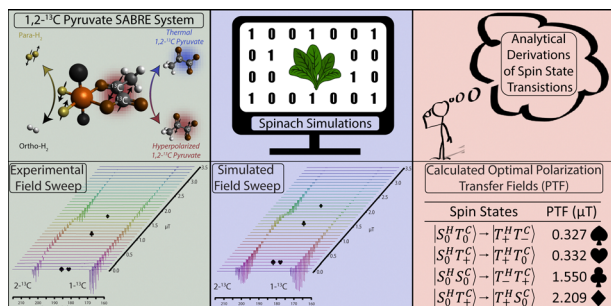
16438



A comparative study of H₂ sensing performance of stoichiometric polymorphs of titanium carbide MXenes loaded with Pd nanodots

Zhiwei Yang, Lijuan Dong, Qian Chen, Zeyi Wang, Jiacheng Cao, Mengwei Dong, Jian Wang, Jian Zhang* and Xiao Huang*

16446



Spin dynamics of [1,2-¹³C₂]pyruvate hyperpolarization by parahydrogen in reversible exchange at micro Tesla fields

Austin Browning, Keilian Macculloch, Patrick TomHon, Iuliia Mandzheva, Eduard Y. Chekmenev, Boyd M. Goodson, Sören Lehmkuhl* and Thomas Theis*

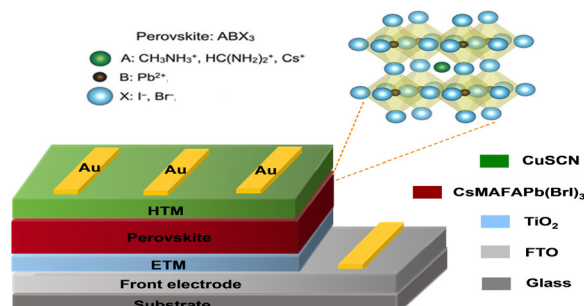


RESEARCH PAPERS

16459

Understanding Auger recombination in perovskite solar cells

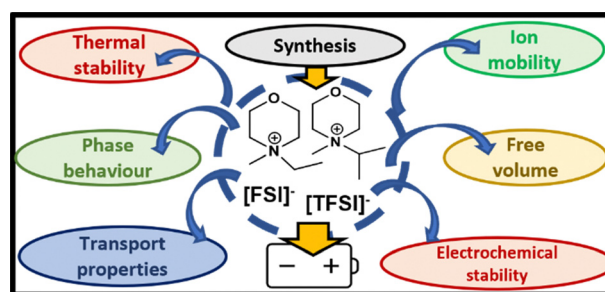
Ali K. Al-Mousoi, Mustafa K. A. Mohammed,*
Anjan Kumar, Rahul Pandey,* Jaya Madan,
Davoud Dastan, M. Khalid Hossain, P. Sakthivel,
G. Anandha babu and Zaher Mundher Yaseen



16469

New organic ionic plastic crystals utilizing the morpholinium cation

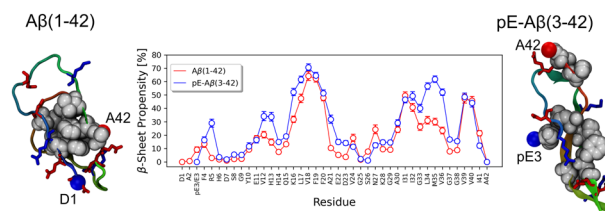
Azra Sourjah, Colin S. M. Kang, Cara M. Doherty,
Durga Acharya, Luke A. O'Dell and Jennifer M. Pringle*



16483

Pyroglutamate-modified amyloid $\beta(3-42)$ monomer has more β -sheet content than the amyloid $\beta(1-42)$ monomer

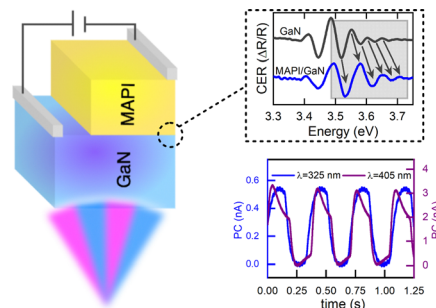
Soumav Nath, Alexander K. Buell and Bogdan Barz*



16492

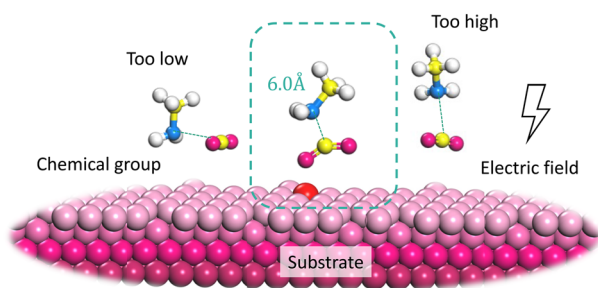
The influence of Fermi level position at the GaN surface on carrier transfer across the MAPbI₃/GaN interface

Ewelina Zdanowicz,* Artur P. Herman, Łukasz Przepis,
Katarzyna Opotczyńska, Jarostaw Serafińczuk,
Mikotaj Chlipata, Czesław Skierbiszewski and
Robert Kudrawiec



RESEARCH PAPERS

16499



Frustrated amino functional group coupling with electric field makes CO₂ activation easier

Nian Wu

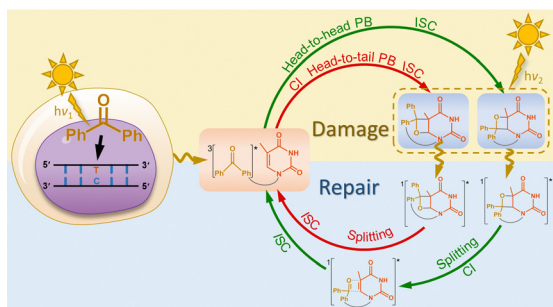
16507



The protein environment restricts the intramolecular charge transfer character of the luciferine/luciferase complex

Henar Mateo-delaFuente, Davide Avagliano, Marco Garavelli* and Juan J. Nogueira*

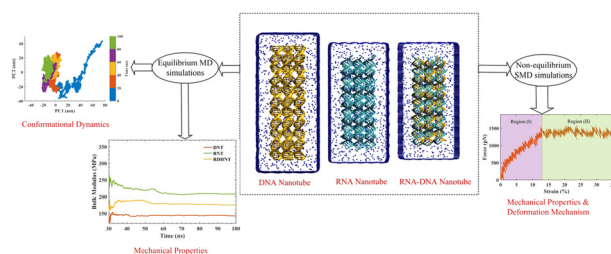
16520



Mechanisms and energetics of benzophenone photosensitized thymine damage and repair from Paternò–Büchi cycloaddition

Yingli Su, Yan Shen, Xiangyuan Li and Haisheng Ren*

16527



Conformational dynamics and mechanical properties of biomimetic RNA, DNA, and RNA–DNA hybrid nanotubes: an atomistic molecular dynamics study

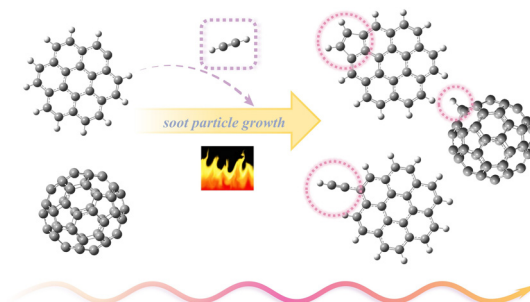
Ehsan Torkan and Mehdi Salmani-Tehrani*



16550

A theoretical study on the effect of C₆₀ particles on the growth of coronene radical based on HACA pathway

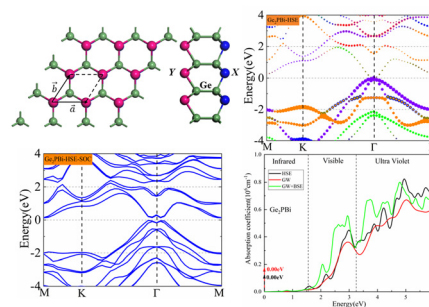
Shanshan Ruan, Ying Shi, Chunlan Qin, Kangwei Xu, Chenliang He and Lidong Zhang*



16559

Spin-orbit splitting and piezoelectric properties of Janus Ge₂XY (X ≠ Y = P, As, Sb and Bi)

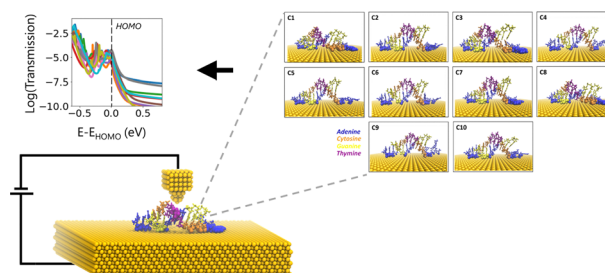
Hui-Ying Liu, Yue-Yi Wang, Ze-Yan Chen, Ting-Ping Hou, Kai-Ming Wu and Heng-Fu Lin*



16570

DNA–Au (111) interactions and transverse charge transport properties for DNA-based electronic devices

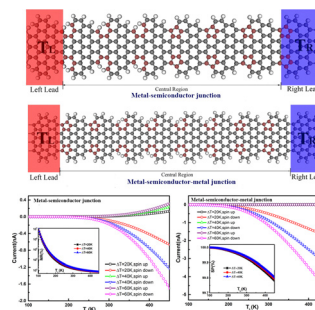
Busra Demir, Hashem Mohammad, M. P. Anantram and Ersin Emre Oren*



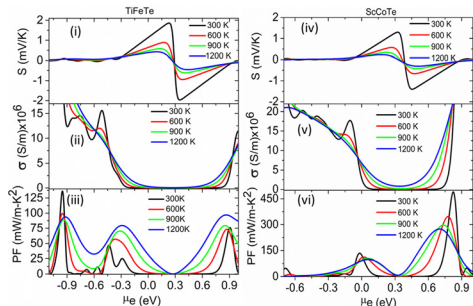
16578

The spin caloritronic transport properties of newly designed devices consisting of a sawtooth graphene nanoribbon and its derived five-member ring structure

Yun Ni,* Kun Chen, Ni Hu, Gang Deng, Jian Liu and Mingyan Chen



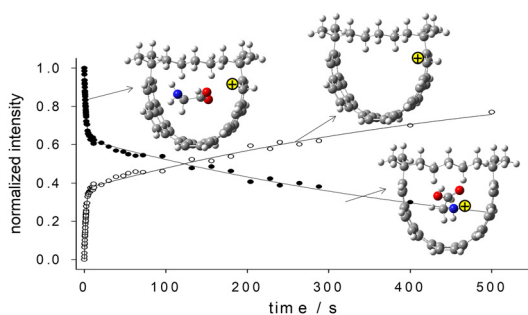
16587



Investigation of the electronic structure, mechanical, and thermoelectric properties of novel semiconductor compounds: XYTe (X = Ti/Sc; Y = Fe/Co)

Aquil Ahmad and Chia-Jyi Liu*

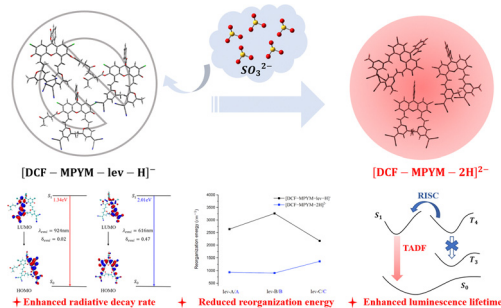
16597



Glycine in a basket: protonated complexes of 1,1,*n,n*-tetramethyl[*n*](2,11)teropyrenophane (*n* = 7, 8, 9) with glycine in the gas-phase

Yanyang Chen, Parisa Ghods Ghasemabadi, Graham J. Bodwell, Maria Demireva and Travis D. Fridgen*

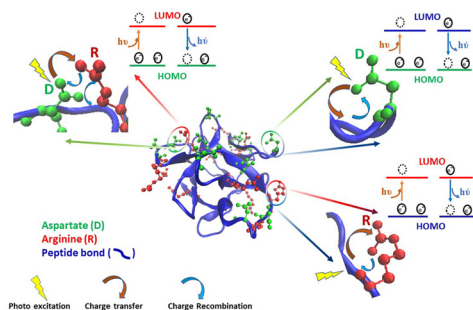
16613



Exploring the luminescence properties and sensing mechanism of a turn-on TADF probe for sulfite

Xiaofei Wang, Qun Zhang, Zhimin Wu, Xiaofang Li, Kai Zhang, Yuzhi Song, Jianzhong Fan, Lili Lin,* Chuan-Kui Wang* and Zhongjie Wang*

16626



Protein charge transfer spectra in a monomeric protein with no lysine

Shah Ekramul Alom and Rajaram Swaminathan*



16643

Thermal dehydration of D-glucose monohydrate in solid and liquid states

Kazuki Kato, Masami Hara and Nobuyoshi Koga*

