# **PCCP**

# Physical Chemistry Chemical Physics - An international journal

# rsc.li/pccp

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

# IN THIS ISSUE

ISSN 1463-9076 CODEN PPCPFQ 25(25) 16659-17060 (2023)



#### Cover

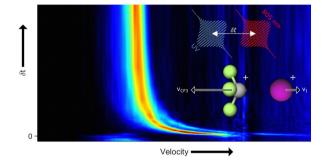
See Michael N. R. Ashfold et al., pp. 16672-16698. Image reproduced by permission of Stuart Crane from Phys. Chem. Chem. Phys., 2023, **25**, 16672.

#### **PERSPECTIVE**

#### 16672

# Molecular photodissociation dynamics revealed by Coulomb explosion imaging

Stuart W. Crane, Jason W. L. Lee, Michael N. R. Ashfold\* and Daniel Rolles

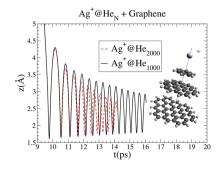


# **COMMUNICATIONS**

# 16699

Superfluid helium droplet-mediated surface-deposition of neutral and charged silver atomic species

Berta Fernández, Martí Pi and María Pilar de Lara-Castells\*



#### **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

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

H Schwarz, Technische Universität Berlin. Germany LP Simons, University of Oxford, UK G A Somorjai, University of California, Berkeley, USA I 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

H Kondoh, Keio University, Japan A Krylov, University of Southern California,

P Maiti, Indian Institute of Science, India R Naaman, Weizmann Institute of Science,

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

#### **Advisory Board**

C Adamo, ENSCP - Chimie ParisTech, France H Ågren, KTH Royal Institute of Technology,

K Ariga, National Institute for Materials Science, Japan

P Ayers, McMaster University, Canada A Ajayaghosh, CSIR-National Institute for Interdisciplinary Science and Technology

P Baglioni, University of Florence, Italy V Barone, Scuola Normale Superiore di Pisa.

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.

M DeVries, University of California Santa Barbara, USA

C Diaz, Universidad Complutense de Madrid,

I 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,

M Orozco, IRB Barcelona - Parc Científic de Barcelona, Spain K Pas, Monash University, Australia

G Patwari, Indian Institute of Technology Bombay, India M-P Pileni, Université Pierre et Marie Curie,

France M Pumera, Nanyang Technological University, Singapore

P Pyykkö, University of Helsinki, Finland M Rodgers, Wayne State University, USA S Sampath, Indian Institute of Science

Bangalore, India R Signorell, ETH Zurich, Switzerland T Schmidt, University of New South Wales, Australia

M Suhm, University of Göttingen, Germany A Suits, University of Missouri, USA D Sundholm, University of Helsinki, Finland T Suzuki, Kyoto University, Japan A Troisi, University of Warwick, UK S Vega, Weizmann Institute of Science, Israel D Waldeck, University of Pittsburgh, USA L-I Wan, Institute of Chemistry, Chinese

Academy of Sciences, China B Weckhuysen, Utrecht University, The Netherlands

X Yang, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China A Zehnacker-Rentien, Université Paris, France

#### Information for Authors

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

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

This journal is @ the Owner Societies.

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

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

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

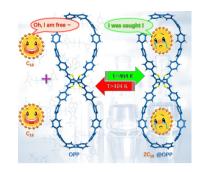
Registered charity number: 207890

#### COMMUNICATIONS

#### 16707

Molecular assembly with a figure-of-eight nanohoop as a strategy for the collection and stabilization of cyclo[18]carbon

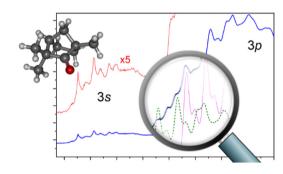
Zeyu Liu,\* Xia Wang, Tian Lu,\* Jiaojiao Wang, Xiufen Yan, Yang Wu and Jingbo Xu



# 16712

# The Rydberg 3p multiplet structure of the fenchone C band absorption

Ivan Powis\* and Dhirendra P. Singh

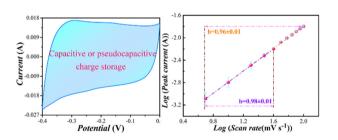


#### RESEARCH PAPERS

#### 16718

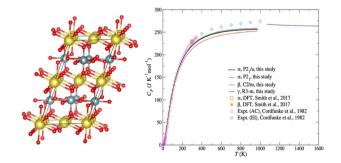
What about electrochemical behaviors for aurivillius-phase bismuth tungstate? Capacitive or pseudocapacitive

Jian-Fei Gao, Jing-Feng Hou and Ling-Bin Kong\*

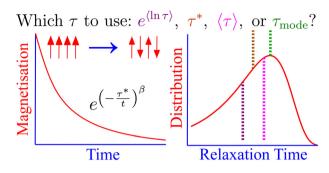


# Polymorphism and phase transitions in Na<sub>2</sub>U<sub>2</sub>O<sub>7</sub> from density functional perturbation theory

Philippe F. Weck,\* Carlos F. Jové-Colón and Eunja Kim



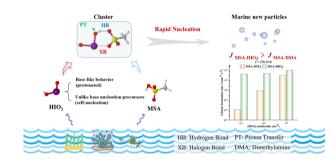
#### 16735



# Characterisation of magnetic relaxation on extremely long timescales

William J. A. Blackmore, Gemma K. Gransbury, Peter Evans, Jon G. C. Kragskow, David P. Mills\* and Nicholas F. Chilton\*

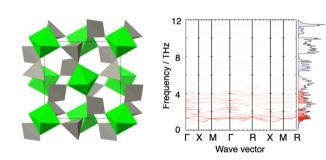
#### 16745



# Methanesulfonic acid and iodous acid nucleation: a novel mechanism for marine aerosols

Nan Wu, An Ning,\* Ling Liu, Haotian Zu, Danli Liang and Xiuhui Zhang\*

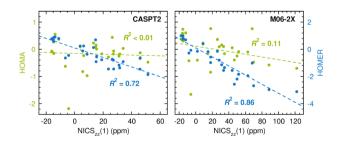
# 16753



# Phonon mechanism for the negative thermal expansion of zirconium tungstate, ZrW2O8

Leila H. N. Rimmer, Keith Refson and Martin T. Dove\*

#### 16763



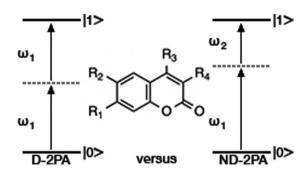
# HOMER: a reparameterization of the harmonic oscillator model of aromaticity (HOMA) for excited states

Enrique M. Arpa\* and Bo Durbeej\*

#### 16772

# Degenerate and non-degenerate two-photon absorption of coumarin dyes

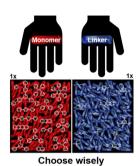
Ismael A. Elayan and Alex Brown\*



#### 16781

# Rationalizing the formation of porosity in mechanochemically-synthesized polymers

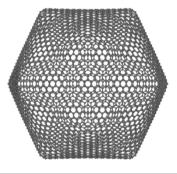
Annika Krusenbaum, Steffi Krause Hinojosa, Sven Fabig, Valentin Becker, Sven Grätz and Lars Borchardt\*



# 16790

# The largest fullerene

Michael Gatchell, Henning Zettergren and Klavs Hansen\*



#### 16796

# A tetrahydroacridine derivative and its conjugate with gold nanoparticles: promising agents for the treatment of Alzheimer's disease

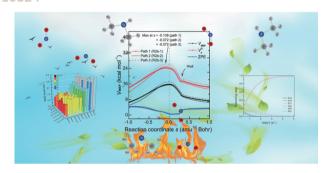
Ilona Mojzych, Anna Zawadzka, Katarzyna Kaczyńska, Piotr Wojciechowski, Dominika Zając, Maciej Chotkowski, Katarzyna Wiktorska, Jan K. Maurin and Maciej Mazur\*

# 16807 Unique interactions per cage-type i Hielscher et al Ballard and Sloar Number of Parameters describing Hydrate Phase

# A cage-specific hydrate equilibrium model for robust predictions of industrially-relevant mixtures

David J. Zhu, Bruce W. E. Norris, Zachary M. Aman\* and Eric F. May\*

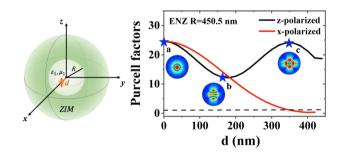
#### 16824



Advanced kinetic calculations with multi-path variational transition state theory for reactions between dimethylamine and nitrogen dioxide in atmospheric and combustion temperature ranges

Yanlei Shang

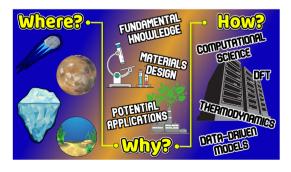
#### 16835



# Inhibition and enhancement of the spontaneous emission in spherical cavities surrounded by zero-index-materials

Yun Ma, Qi Liu, Lingxiao Shan, Xinchen Zhang, Yali Jia, Qihuang Gong and Ying Gu\*

#### 16844



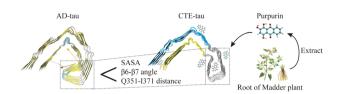
# Computational investigations of stable multiplecage-occupancy He clathrate-like hydrostructures

Raquel Yanes-Rodríguez and Rita Prosmiti\*

#### 16856

# Destabilization mechanism of R3-R4 tau protofilament by purpurin: a molecular dynamics study

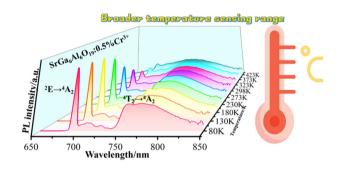
Jiagian Wan, Yu Zou, Ruiging Sun, Zhengdong Xu, Jiaxing Tang, Yehong Gong, Guanghong Wei\* and Qingwen Zhang\*



#### 16866

# Extending the optical temperature sensing range of Cr<sup>3+</sup> by synchronously tuning <sup>2</sup>E and <sup>4</sup>T<sub>2</sub> emission

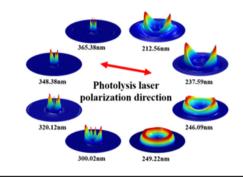
Jiaqi Ou, Shuangqiang Fang,\* Qiangqiang Zhu, Yue Zhai, Hong Zhang and Le Wang\*



#### 16872

# Slice imaging study of NO<sub>2</sub> photodissociation via the $1^2B_2$ and $2^2B_2$ states: the NO(X<sup>2</sup> $\Pi$ ) + O( $^3P_J$ ) product channel

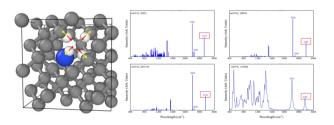
Zhaoxue Zhang, Shuaikang Yang, Zhenxing Li,\* Yao Chang, Zijie Luo, Yarui Zhao, Shengrui Yu,\* Kaijun Yuan\* and Xueming Yang



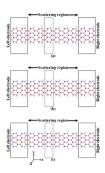
#### 16881

The search for a band of a defect predicted above 4000 cm<sup>-1</sup> in diamond through infrared vibrational spectra: a quantum mechanical investigation

Yanyan Zhang, Libin Zhang, Dongliang Zhang, Yichen Li, Sheng Liu, Bo Yang\* and Zhiyin Gan\*



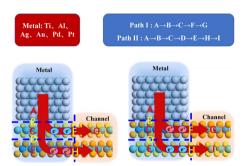
#### 16889



# Nitrogen-doped zinc oxide nanoribbons for potential resonant tunneling diode applications

M. Sankush Krishna,\* Sangeeta Singh and Brajesh Kumar Kaushik

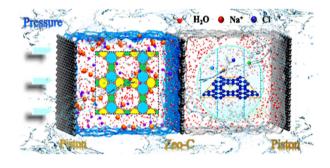
#### 16896



# Dual transmission channels at metal-MoS<sub>2</sub>/WSe<sub>2</sub> hetero-bilayer interfaces

Dongqing Zou, Wenkai Zhao,\* Yuqing Xu, Xiaoteng Li, Yuliang Liu and Chuanlu Yang\*

#### 16908

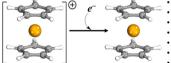


# Computational simulation-driven discovery of novel zeolite-like carbon materials as seawater desalination membranes

Kun Meng, Xiuhan Li, Yutao Niu, Changhong Zhang, Xiaohua Yu, Ju Rong, Hongying Hou\* and Hui Chen\*

#### 16921

# Absolute reduction potential ( $\mathring{E_{abs}}$ ) predictions for $Cp_2M^+/Cp_2M$ (M=Fe, Co and Ni)



- CCSD(T)-F12 (E<sub>CCSD(T)-F12</sub>) Core-valence correlation  $(E_{CV})$
- Relativistic effect (E<sub>SR</sub>) Spin-orbit coupling (E<sub>SO</sub>)
- Zero-point energy correction (E<sub>ZPVE</sub>)
- Gibbs free energy correction ( $\Delta G_{gas}$ )
- Solvation energy (ΔG<sub>solv</sub>)

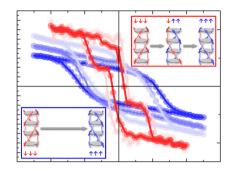
# Ferrocene/ferrocenium, cobaltocene/ cobaltocenium and nickelocene/nickelocenium: from gas phase ionization energy to one-electron reduction potential in solvated medium

Hongyan Zhao, Yi Pan and Kai-Chung Lau\*

#### 16921

Ferro- and ferrielectricity and negative piezoelectricity in thioamide-based supramolecular organic discotics

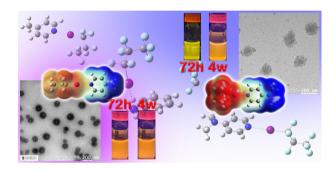
Indre Urbanaviciute, Miguel Garcia-Iglesias, Andrey Gorbunov, E. W. Meijer and Martijn Kemerink\*



#### 16938

Fluorescent nano-sized aggregates of halogen bonded complexes formed using perfluoropropyl iodides: a systematic comparison between two isomeric halogen bond acceptors, aniline and 4-methyl pyridine

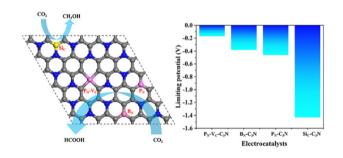
Haiyan Fan, Lazzat Nurtay, Nurgul Daniyeva and Enrico Benassi\*



# 16952

Unravelling the adsorption and electroreduction performance of CO<sub>2</sub> and N<sub>2</sub> over defective and B, P, Si-doped C<sub>3</sub>Ns: a DFT study

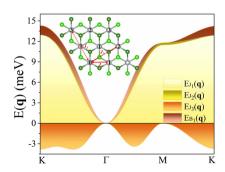
Dandan Wang, Xueting Liu, Huiru Yang, Ziang Zhao, Yucheng Liu, Xin Qu, Lihua Yang, Ming Feng\* and Zaicheng Sun\*



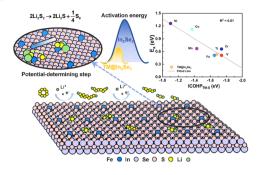
#### 16962

Same effect of biquadratic exchange interaction and Heisenberg linear interaction in a spin spiral

Lingzi Jiang, Can Huang, Bingjie Liu, Yanfei Pan, Jiyu Fan, Daning Shi,\* Chunlan Ma\* and Yan Zhu\*



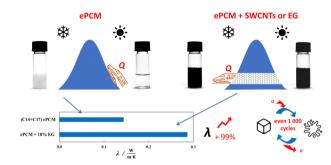
#### 16968



# Identification of linear scaling relationships in polysulfide conversion on α-In<sub>2</sub>Se<sub>3</sub>-supported single-atom catalysts

Hui Wang, Lin Zou, Min Li and Long Zhang\*

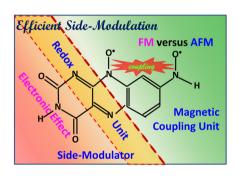
# 16979



# Alkane-based eutectic phase change materials doped with carbon nanomaterials

Mikołaj Więckowski,\* Marek Królikowski, Łukasz Scheller and Marzena Dzida

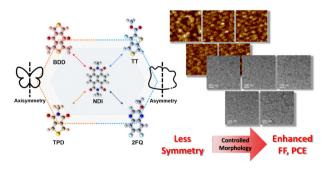
# 16991



# Magnetic coupling modulation in meta-nitroxidefunctionalized isoalloxazine magnets with redox-active units as efficient side-modulators

Rabia Malik and Yuxiang Bu\*

#### 17001



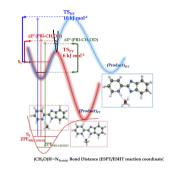
# Naphthalene diimide-based random terpolymers with axisymmetric and asymmetric electron acceptors for controllable morphology and enhanced fill factors in all-polymer solar cells

Geunhyung Park, Yongjoon Cho, Seunglok Lee, Seungju Kim, Kyu Cheol Lee\* and Changduk Yang\*

#### 17010

A combined spectroscopic and computational investigation on the solvent-to-chromophore excited-state proton transfer in the 2,2'-pyridylbenzimidazole-methanol complex

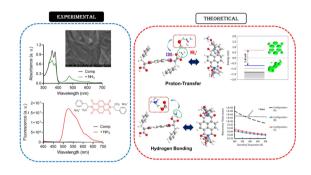
Ramesh Jarupula, Saurabh Khodia, Muhammed Shabeeb and Surajit Maity\*



#### 17021

Site-specific ammonia adsorption and transduction on a naphthalimide derivative molecule - a complementary analysis involving ab initio calculation and experimental verification

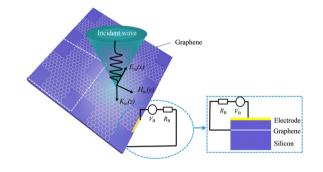
Aditya Tiwari, Rikitha S. Fernandes, Nilanjan Dey\* and Sayan Kanungo\*



# 17034

Polarization-independent plasmon-induced transparency and slow light effects in a fully continuous symmetric cross-shaped monolayer graphene structure

Can Wan, Cuixiu Xiong,\* Meng Tan, Chengya Wei, Jie Wang and Saiwen Zhang



# 17043

GO nanosheets decorated with SnS nanoparticles: excellent photocatalytic performance under visible-light irradiation

Elham Kharatzadeh\* and Marzieh Khademalrasool\*

