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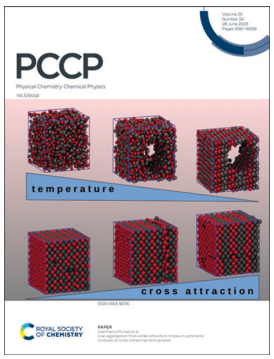

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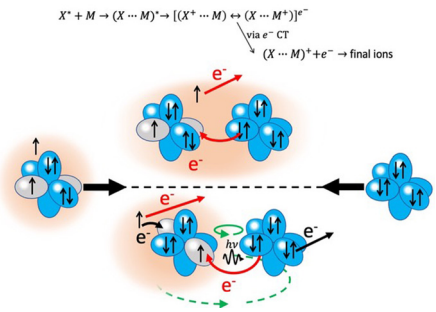
See Gianmarco Munaó *et al.*, pp. 16227–16237. Image reproduced by permission of Gianmarco Munaó from *Phys. Chem. Chem. Phys.*, 2023, **25**, 16227.

REVIEW

16176

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

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

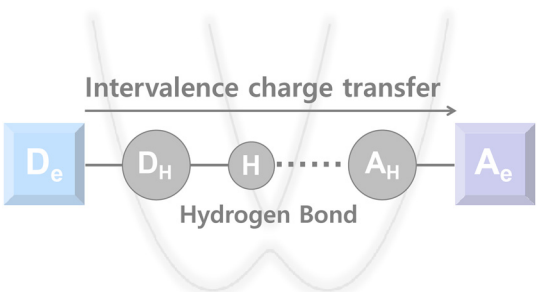


PERSPECTIVE

16201

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

Juanjuan Li, Yuqing Shi and Tao Cheng*



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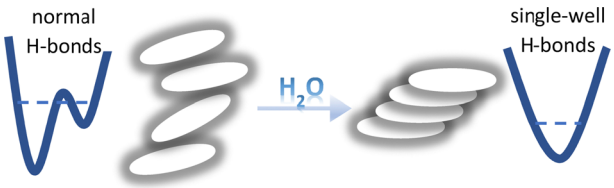
COMMUNICATIONS

16212

Signatures of pancake bonding in hydrated eumelanin

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



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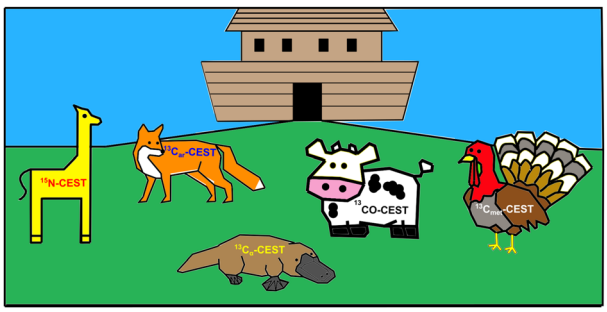
ARCHE-NOAH: NMR supersequence with five different CEST experiments for studying protein conformational dynamics

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



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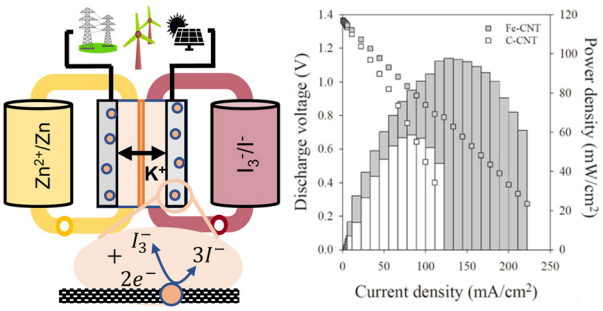
High power zinc iodine redox flow battery with iron-functionalized carbon electrodes

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



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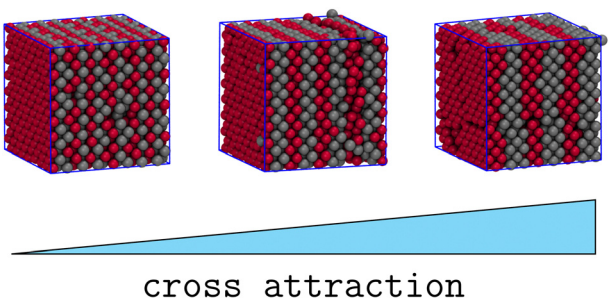
Like aggregation from unlike attraction: stripes in symmetric mixtures of cross-attracting hard spheres

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



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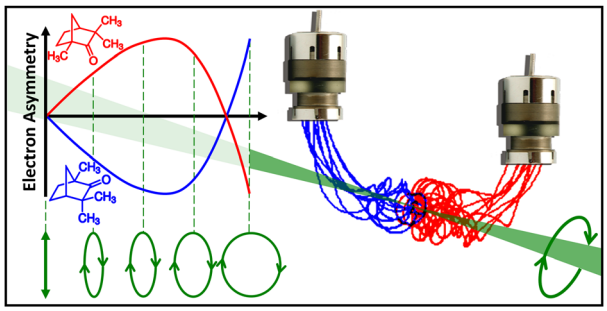
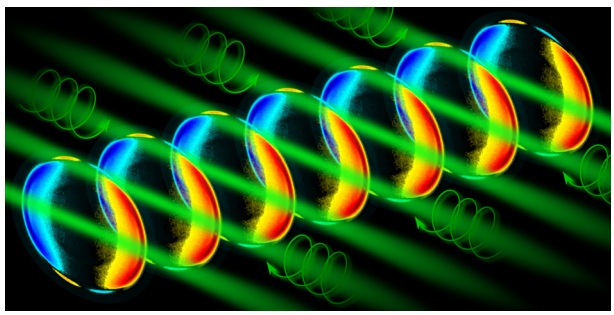


Investigation of photoelectron elliptical dichroism for chiral analysis

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*

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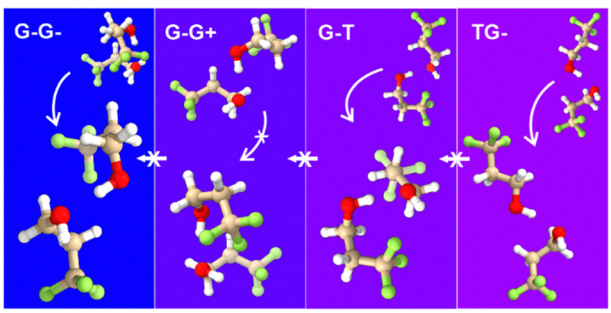

Rotational spectroscopy of hydrogen-bonded binary trifluoro-propanol conformers: conformational diversity, preference and abundances in a jet expansion

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

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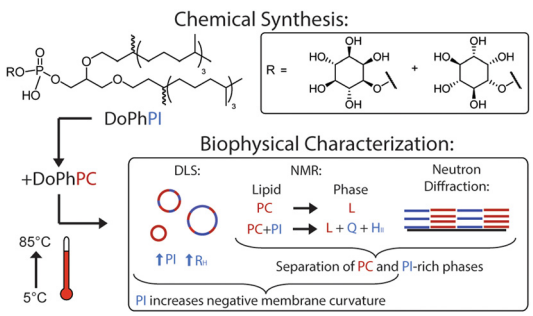

Membrane plasticity induced by *myo*-inositol derived archaeal lipids: chemical synthesis and biophysical characterization

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

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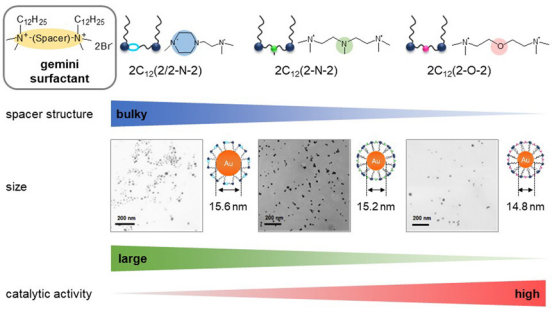
Catalytic activity of gold nanoparticles protected by quaternary ammonium salt-based gemini surfactants with different spacer structures

Tsukasa Morita, Shiho Yada and Tomokazu Yoshimura*



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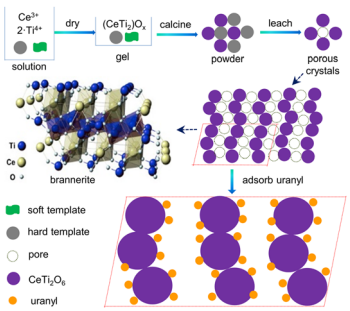
Synthesis of hierarchical mesoporous cerium titanate brannerite and uranyl adsorption properties at pH 3.8

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



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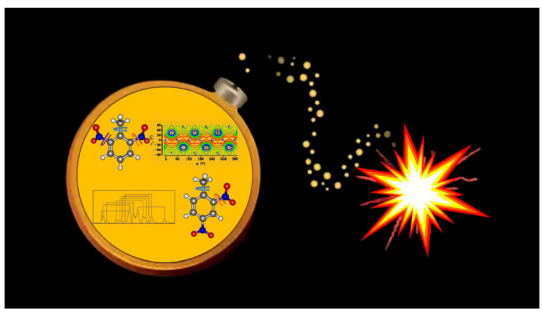
Microwave spectra of dinitrotoluene isomers: a new step towards the detection of explosive vapors

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



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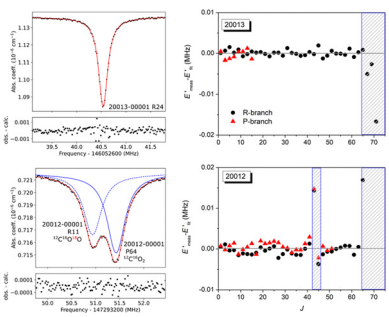
$^{12}CO_2$ transition frequencies with kHz-accuracy by saturation spectroscopy in the 1.99–2.09 μm region

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



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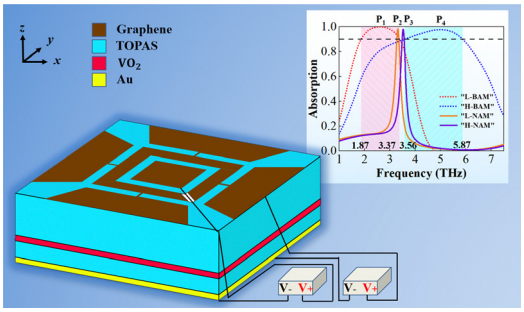

An electrical/thermal dual-controlled quad-functional terahertz metasurface absorber

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

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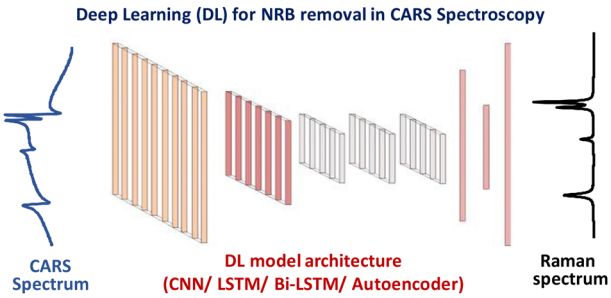

Evaluating different deep learning models for efficient extraction of Raman signals from CARS spectra

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

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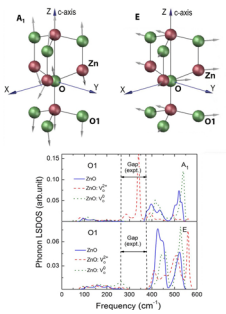

Structural and vibrational properties of wurtzite ZnO with oxygen-deficient defects: *ab initio* and potential-based calculations

Alexey N. Kislov* and Anatoly F. Zatsepin

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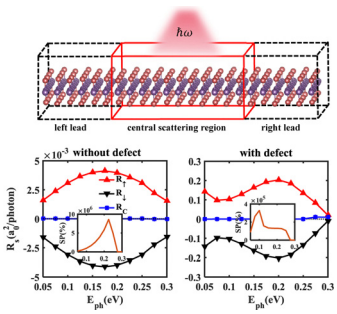

The photogalvanic effect induced by quantum spin Hall edge states from first-principles calculations

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

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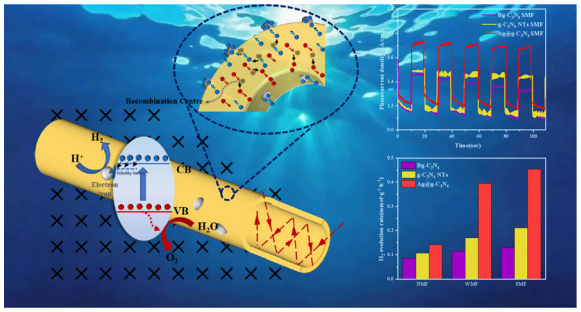
Enhanced photocatalytic activity of Ag@g-C_3N_4 nanotubes by regulating photogenerated carriers to bypass the recombination center under the Lorentz force

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



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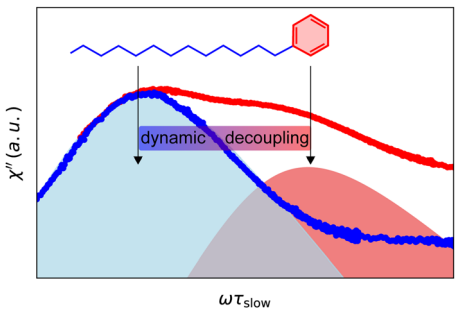
Influence of intramolecular dynamics on the relaxation spectra of simple liquids

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



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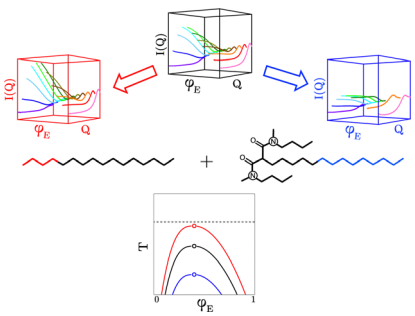
Critical fluctuations in liquid–liquid extraction organic phases controlled by extractant and diluent molecular structure

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



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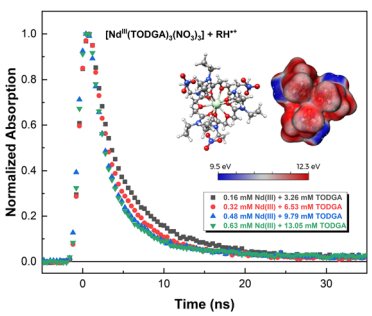
Impact of lanthanide ion complexation and temperature on the chemical reactivity of *N,N,N′,N′*-tetraoctyl diglycolamide (TODGA) with the dodecane radical cation

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*



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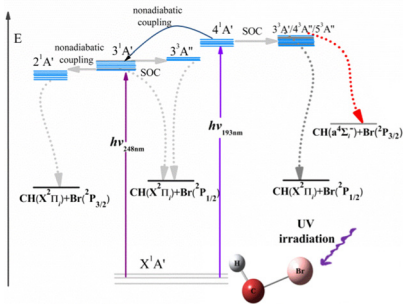

An *ab initio* study on the electronic excited states and photodissociation mechanism of bromocarbene molecule

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

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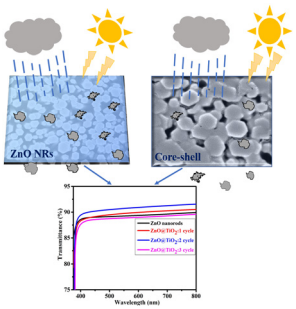
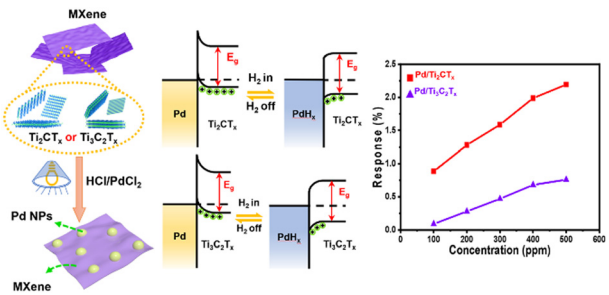


Fabrication of porous and visible light active ZnO nanorods and ZnO@TiO_2 core–shell photocatalysts for self-cleaning applications

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

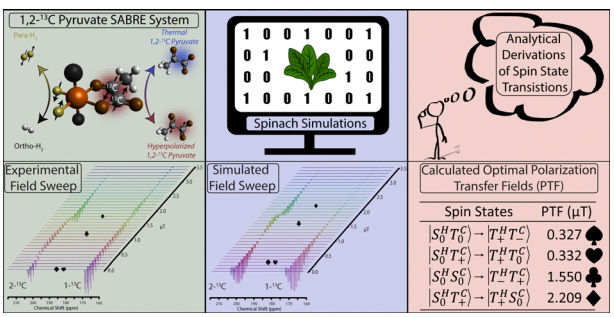
16438



A comparative study of H_2 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-$^{13}C_2$]pyruvate hyperpolarization by parahydrogen in reversible exchange at micro Tesla fields

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

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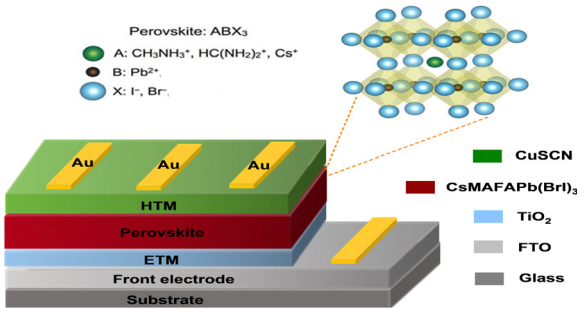
16459

Understanding Auger recombination in perovskite solar cells

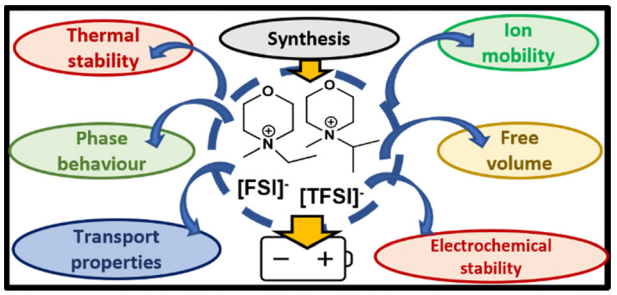
Ali K. Al-Mousoi, Mustafa K. A. Mohammed,* Anjan Kumar, Rahul Pandey,* Jaya Madan, Davoud Dastan, M. Khalid Hossain, P. Sakthivel, G. Anandha babu and Zaher Mundher Yaseen



16469

New organic ionic plastic crystals utilizing the morpholinium cation

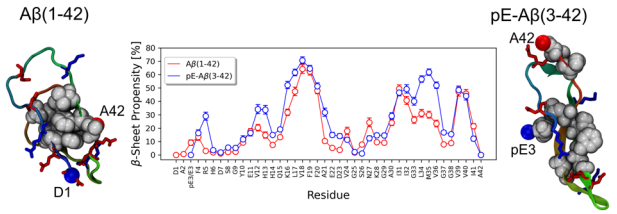
Azra Sourjah, Colin S. M. Kang, Cara M. Doherty, Durga Acharya, Luke A. O'Dell and Jennifer M. Pringle*



16483

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

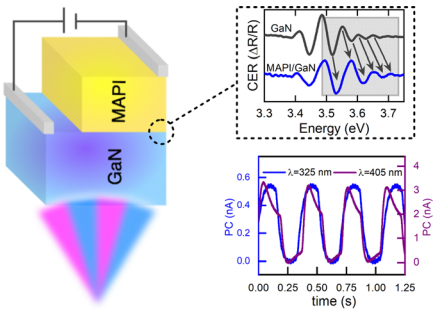
Soumav Nath, Alexander K. Buell and Bogdan Barz*



16492

The influence of Fermi level position at the GaN surface on carrier transfer across the $MAPbI_3$/GaN interface

Ewelina Zdanowicz,* Artur P. Herman, Łukasz Przypis, Katarzyna Opołczyńska, Jarosław Serafińczuk, Mikołaj Chlipała, Czesław Skierbiszewski and Robert Kudrawiec



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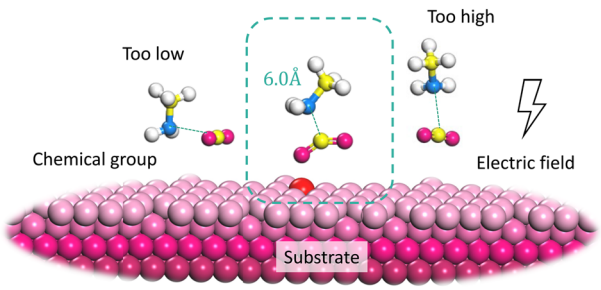
16499



Frustrated amino functional group coupling with electric field makes CO_2 activation easier

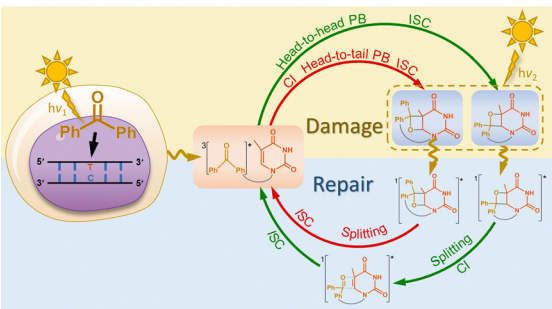
Nian Wu

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*

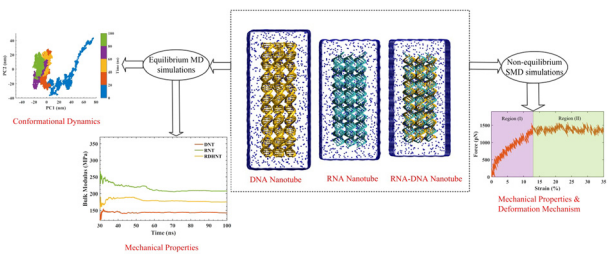
16520



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*

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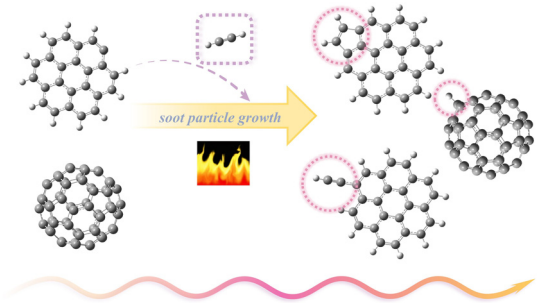
16550

A theoretical study on the effect of C_{60} particles on the growth of coronene radical based on HACA pathway

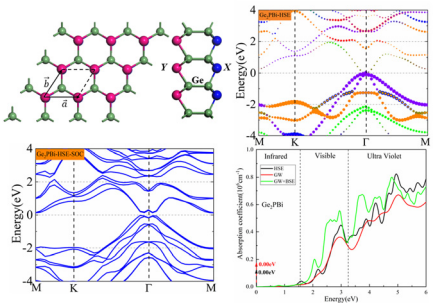
Shanshan Ruan, Ying Shi, Chunlan Qin, Kangwei Xu, Chenliang He and Lidong Zhang*



16559

Spin–orbit splitting and piezoelectric properties of Janus Ge_2XY (X ≠ Y = P, As, Sb and Bi)

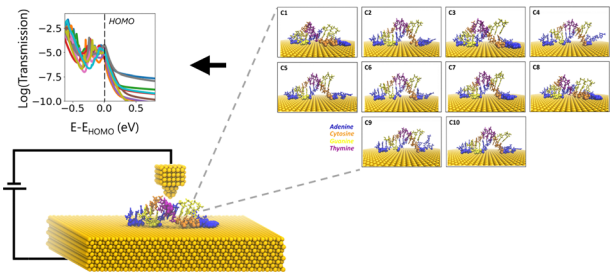
Hui-Ying Liu, Yue-Yi Wang, Ze-Yan Chen, Ting-Ping Hou, Kai-Ming Wu and Heng-Fu Lin*



16570

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

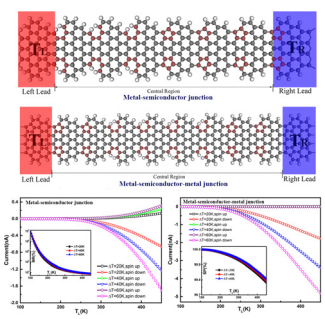
Busra Demir, Hashem Mohammad, M. P. Anantram and Ersin Emre Oren*



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



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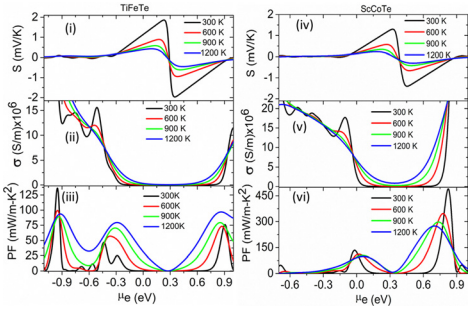
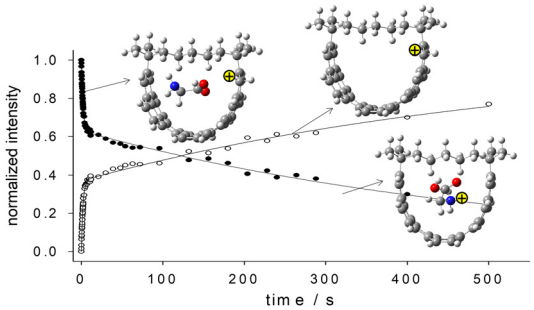
16587



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*

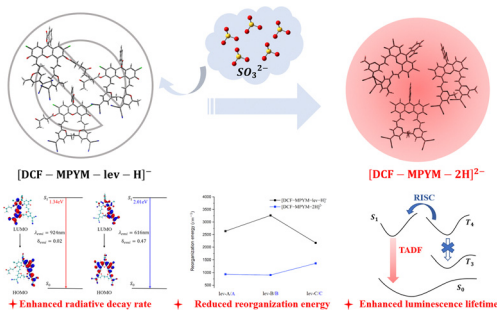
16597



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*

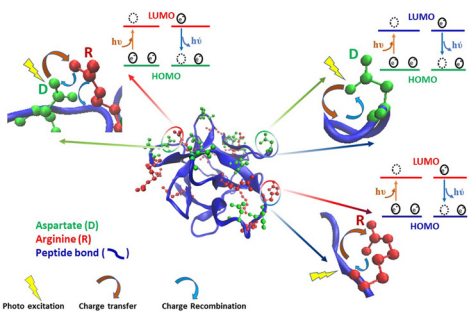
16613



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*

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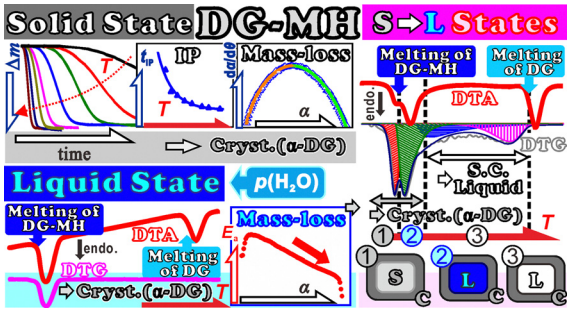
16643

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

Kazuki Kato, Masami Hara and Nobuyoshi Koga*



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