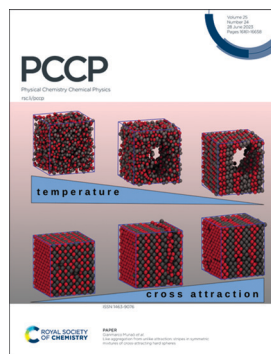


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Cover

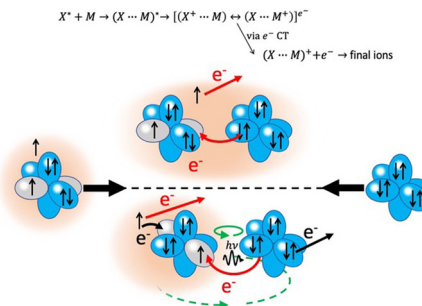
See Gianmarco Munaó *et al.*, pp. 16227–16237. Image reproduced by permission of Gianmarco Munaó from *Phys. Chem. Chem. Phys.*, 2023, 25, 16227.

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

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

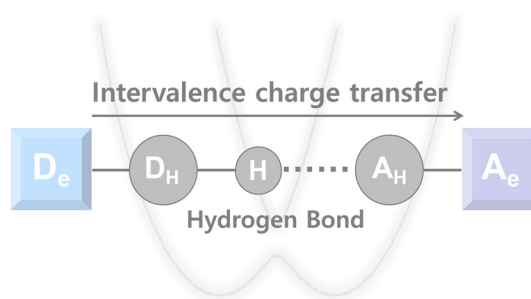


PERSPECTIVE

16201

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

Juanjuan Li, Yuqing Shi and Tao Cheng*



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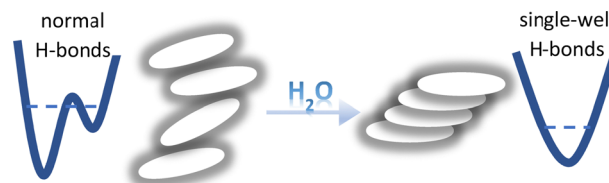


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Signatures of pancake bonding in hydrated eumelanin

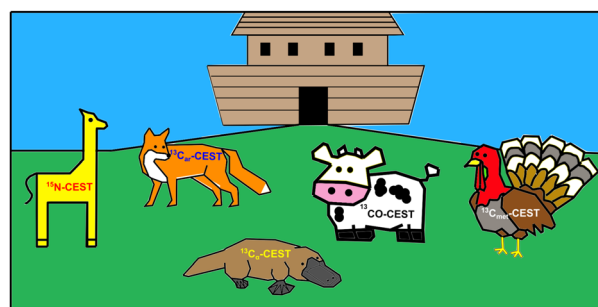
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ARCHE-NOAH: NMR supersequence with five different CEST experiments for studying protein conformational dynamics

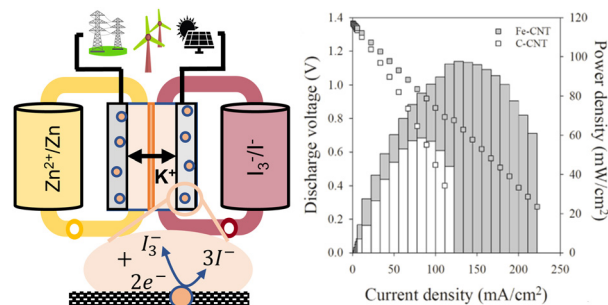
Rodrigo Cabrera Allpas, Alexandar L. Hansen and Rafael Brüschweiler*



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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*

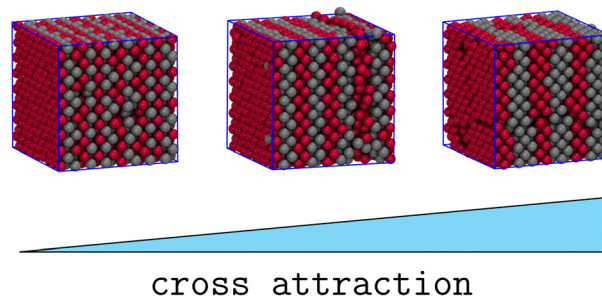


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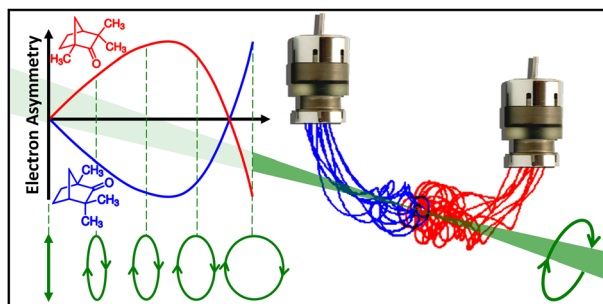
Like aggregation from unlike attraction: stripes in symmetric mixtures of cross-attracting hard spheres

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



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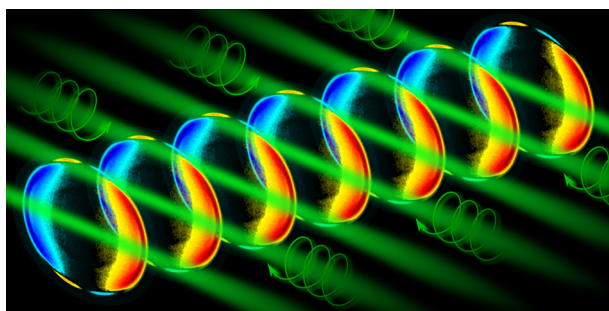
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Investigation of photoelectron elliptical dichroism for chiral analysis

Jason B. Greenwood* and Ian D. Williams

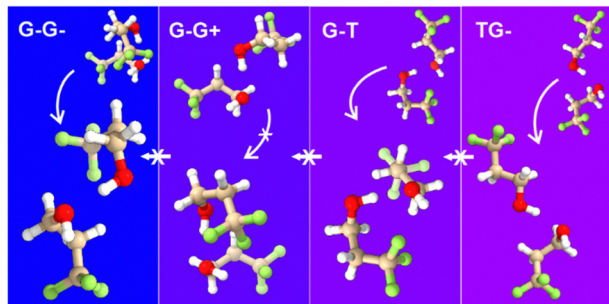
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Fast and precise chiroptical spectroscopy by photoelectron elliptical dichroism

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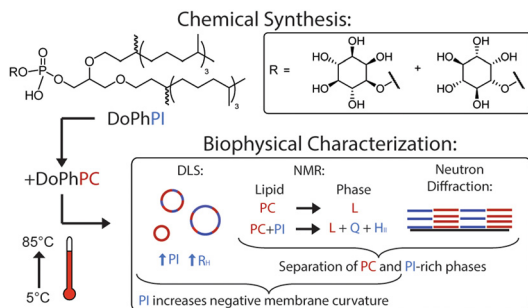
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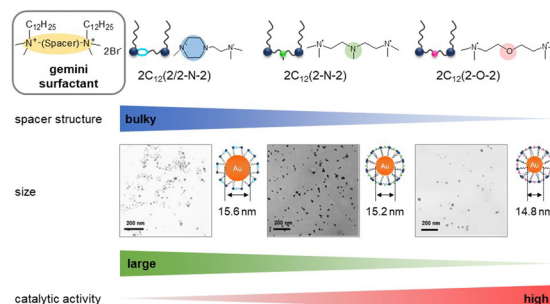


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Catalytic activity of gold nanoparticles protected by quaternary ammonium salt-based gemini surfactants with different spacer structures

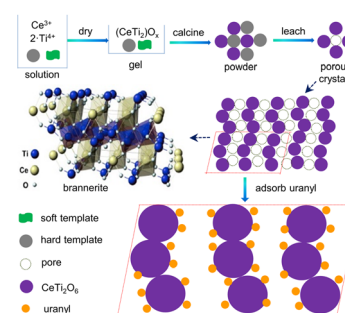
Tsukasa Morita, Shiho Yada and Tomokazu Yoshimura*



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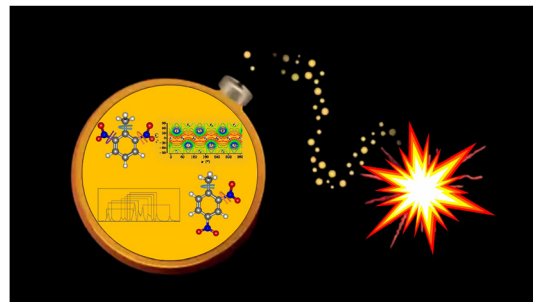
Linggen Kong,* Tao Wei, Inna Karatchevtseva and Nicholas Scales



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

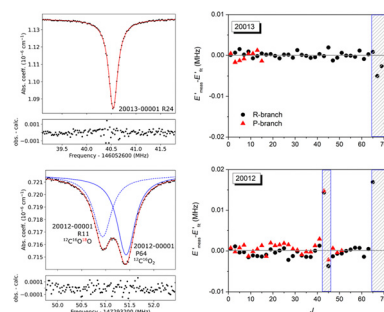
Mhamad Chrayteh,* Pascal Dréan, Manuel Goubet, Laurent H. Coudert, Anthony Roucou and Arnaud Cuisset*



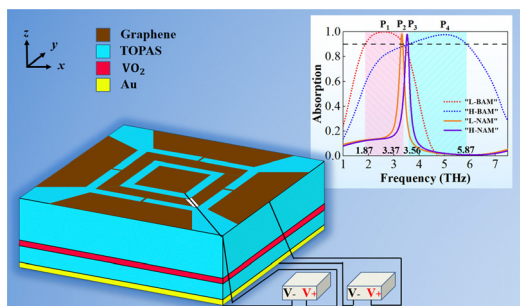
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¹²CO₂ transition frequencies with kHz-accuracy by saturation spectroscopy in the 1.99–2.09 μm region

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



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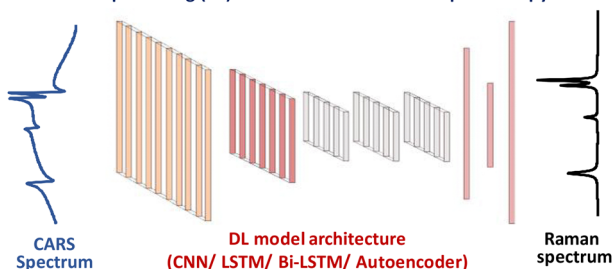


An electrical/thermal dual-controlled quad-functional terahertz metasurface absorber

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

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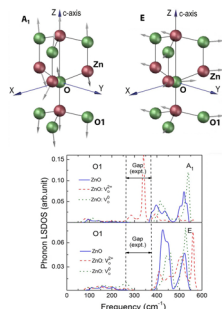
Deep Learning (DL) for NRB removal in CARS Spectroscopy



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

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

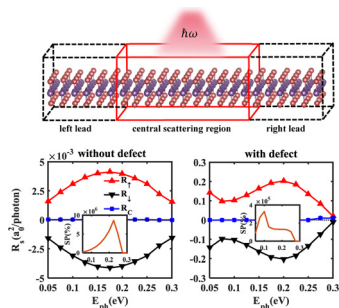
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Structural and vibrational properties of wurtzite ZnO with oxygen-deficient defects: *ab initio* and potential-based calculations

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

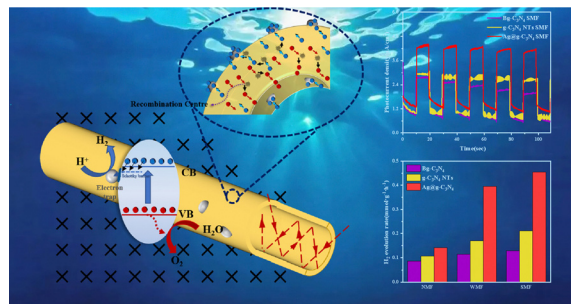
Yaqing Yang, Liwen Zhang, Xiaohong Zheng,* Jun Chen, Liantuan Xiao, Suotang Jia and Lei Zhang*



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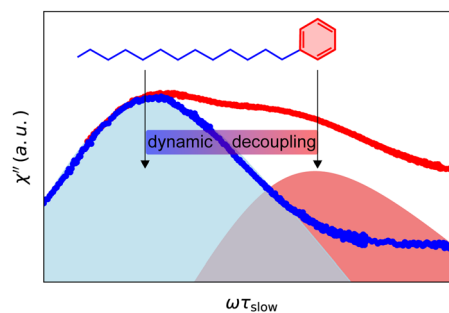
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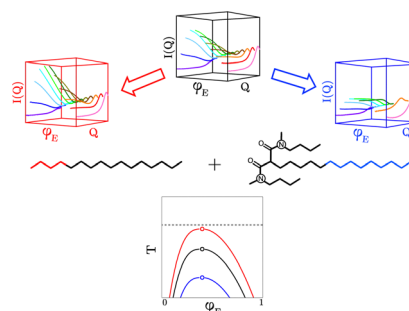
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Critical fluctuations in liquid–liquid extraction organic phases controlled by extractant and diluent molecular structure

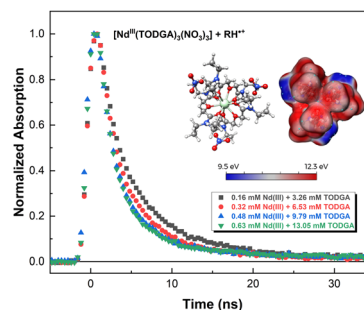
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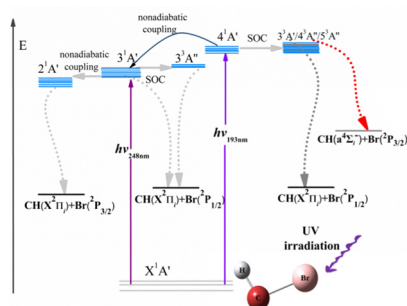
Impact of lanthanide ion complexation and temperature on the chemical reactivity of *N,N,N',N'*-tetraoctyl diglycolamide (TODGA) with the dodecane radical cation

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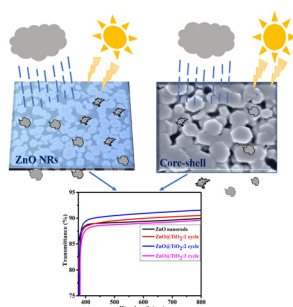
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An *ab initio* study on the electronic excited states and photodissociation mechanism of bromocarbene molecule

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

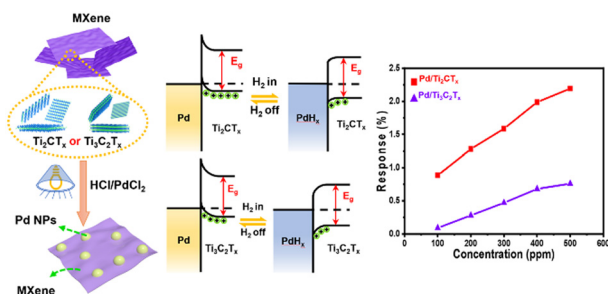
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Fabrication of porous and visible light active ZnO nanorods and ZnO@TiO₂ core-shell photocatalysts for self-cleaning applications

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

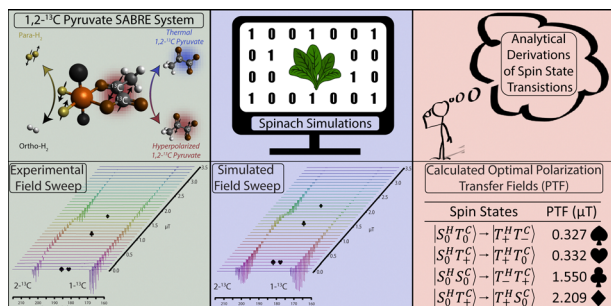
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A comparative study of H₂ sensing performance of stoichiometric polymorphs of titanium carbide MXenes loaded with Pd nanodots

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

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

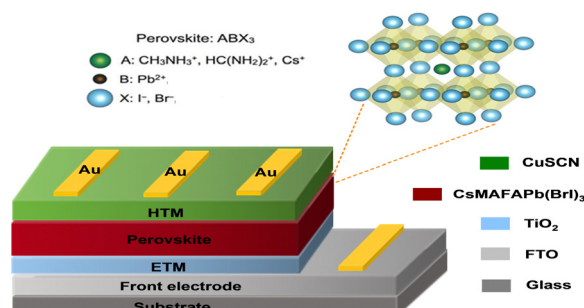


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Understanding Auger recombination in perovskite solar cells

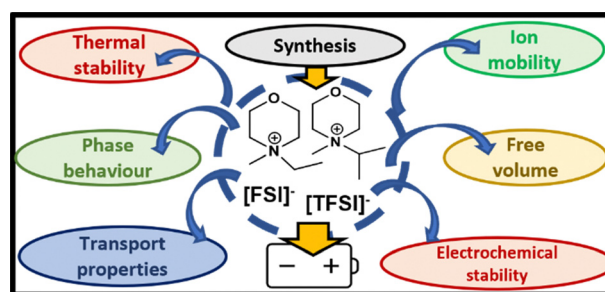
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Anjan Kumar, Rahul Pandey,* Jaya Madan,
Davoud Dastan, M. Khalid Hossain, P. Sakthivel,
G. Anandha babu and Zaher Mundher Yaseen



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New organic ionic plastic crystals utilizing the morpholinium cation

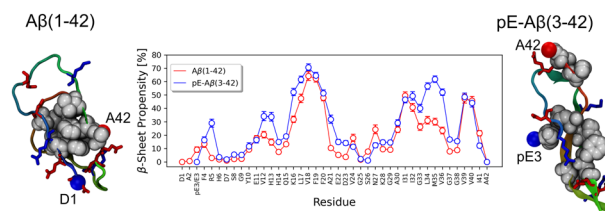
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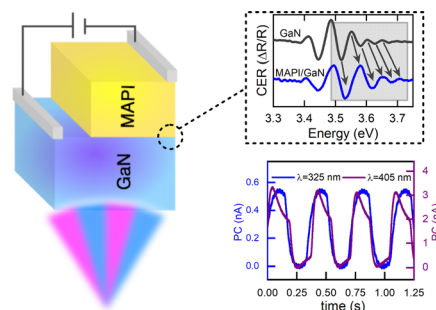
Soumav Nath, Alexander K. Buell and Bogdan Barz*



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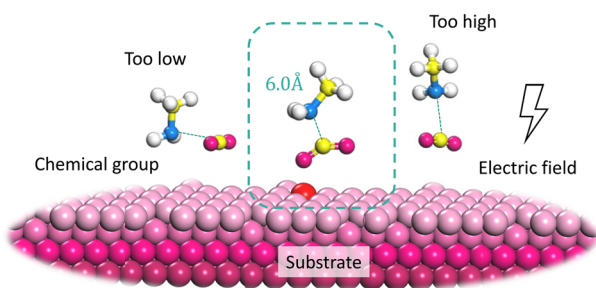
The influence of Fermi level position at the GaN surface on carrier transfer across the MAPbI₃/GaN interface

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



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

Nian Wu

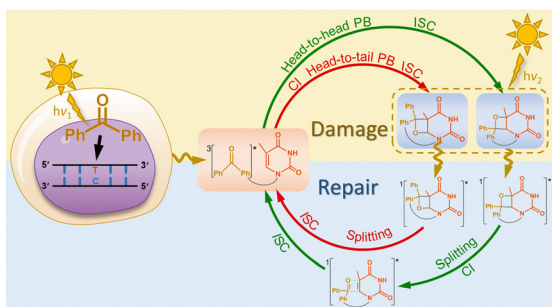
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The protein environment restricts the intramolecular charge transfer character of the luciferine/luciferase complex

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

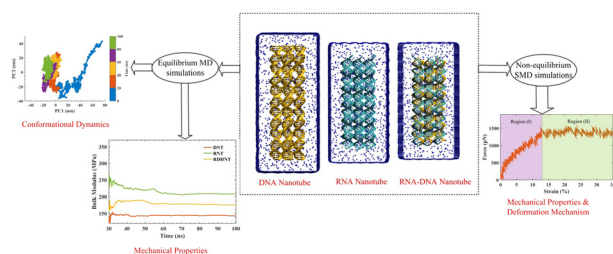
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Mechanisms and energetics of benzophenone photosensitized thymine damage and repair from Paternò–Büchi cycloaddition

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

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

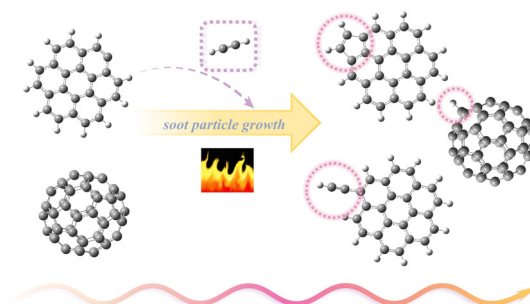
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A theoretical study on the effect of C₆₀ particles on the growth of coronene radical based on HACA pathway

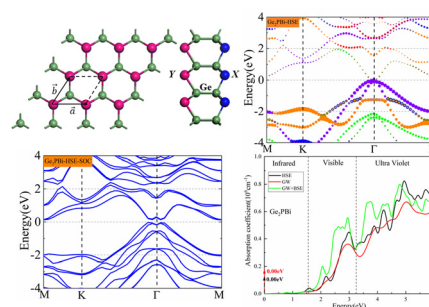
Shanshan Ruan, Ying Shi, Chunlan Qin, Kangwei Xu, Chenliang He and Lidong Zhang*



16559

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

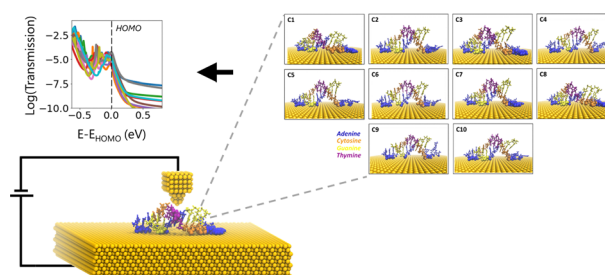
Hui-Ying Liu, Yue-Yi Wang, Ze-Yan Chen, Ting-Ping Hou, Kai-Ming Wu and Heng-Fu Lin*



16570

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

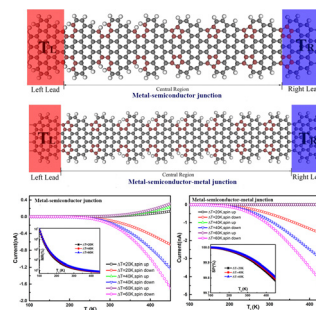
Busra Demir, Hashem Mohammad, M. P. Anantram and Ersin Emre Oren*



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



16643

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

Kazuki Kato, Masami Hara and Nobuyoshi Koga*

