

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 26(10) 7933–8560 (2024)



Cover

See Dominik Lungerich *et al.*, pp. 8051–8061. Image reproduced by permission of Dominik Lungerich from *Phys. Chem. Chem. Phys.*, 2024, 26, 8051.



Inside cover

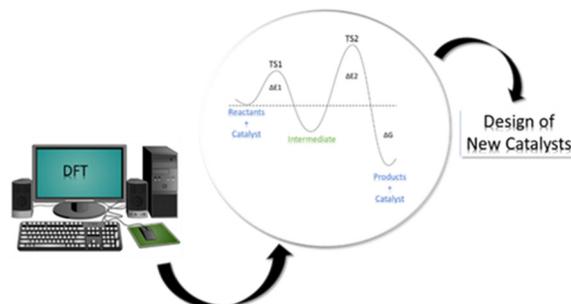
See Valentine I. Vullev *et al.*, pp. 8062–8076. Image reproduced by permission of Valentine I. Vullev from *Phys. Chem. Chem. Phys.*, 2024, 26, 8062.

TUTORIAL REVIEW

7950

Density functional theory methods applied to homogeneous and heterogeneous catalysis: a short review and a practical user guide

Valeria Butera

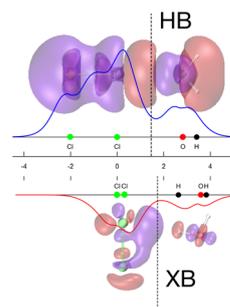


PERSPECTIVES

7971

The dawn of hydrogen and halogen bonds and their crucial role in collisional processes probing long-range intermolecular interactions

David Cappelletti,* Stefano Falcinelli and Fernando Pirani



Royal Society of Chemistry approved training courses

Explore your options.
Develop your skills.
Discover learning
that suits you.

**Courses in the classroom,
the lab, or online**

Find something for every
stage of your professional
development. Search our
database by:

- subject area
- location
- event type
- skill level

Members **get at least 10% off**

Visit rsc.li/cpd-training



**SAVE
10%**

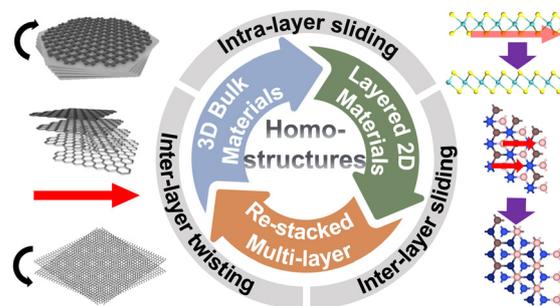


PERSPECTIVES

7988

Stacking engineering in layered homostructures: transitioning from 2D to 3D architectures

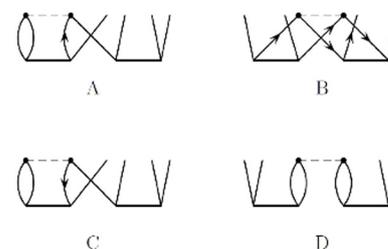
Jiamin Wang, Fang Cheng, Yan Sun,* Hai Xu* and Liang Cao*



8013

Perspective on Coupled-cluster Theory. The evolution toward simplicity in quantum chemistry

Rodney J. Bartlett

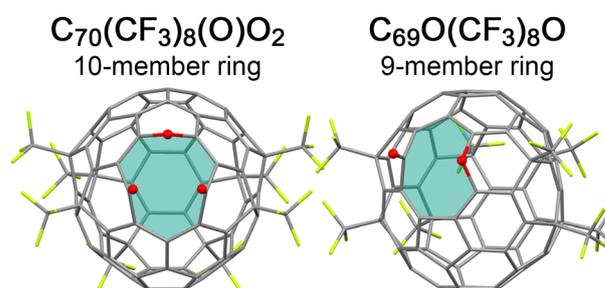
 T_2^2 Terms in CCD

COMMUNICATIONS

8038

Oxidative cage opening in the C₇₀ fullerene facilitated by preceding trifluoromethylation

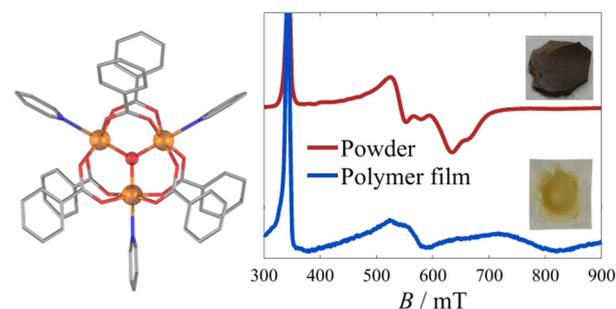
Sofia V. Gracheva, Nadezhda B. Tamm, Konstantin A. Lyssenko, Ilya N. Ioffe, Natalia S. Lukonina* and Alexey A. Goryunkov



8043

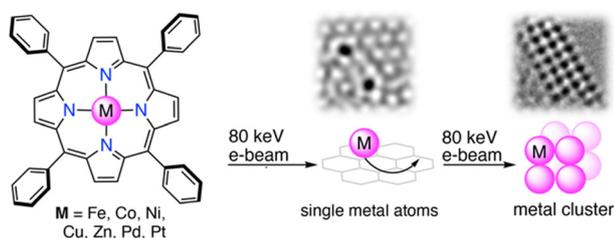
Matrix effects on the magnetic properties of a molecular spin triangle embedded in a polymeric film

Lorenzo Tesi,* Athanassios K. Boudalis,* Katja Drerup, Mario Ruben and Joris van Slageren



RESEARCH PAPERS

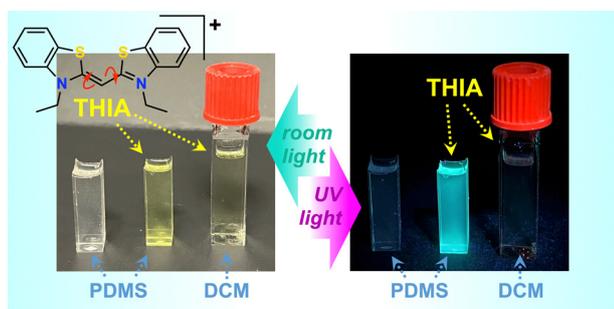
8051



Electron beam-induced demetallation of Fe, Co, Ni, Cu, Zn, Pd, and Pt metalloporphyrins: insights in e-beam chemistry and metal cluster formations

Jongseong Park, Sol Lee, Orein Francis Jafter, Jinwoo Cheon and Dominik Lungerich*

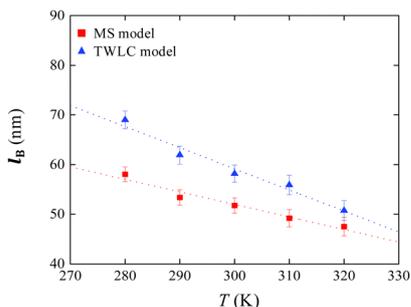
8062



Poly(dimethylsiloxane) as a room-temperature solid solvent for photophysics and photochemistry

John A. Clark, Samantha Robinson, Eli M. Espinoza, Duoduo Bao, James B. Derr, Luca Croft, Omar O'Mari, William H. Grover and Valentine I. Vullev*

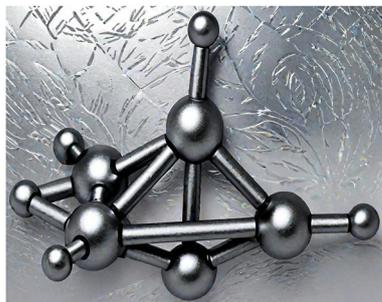
8077



Influence of temperature on bend, twist and twist–bend coupling of dsDNA

Zihao Zhang, Xuankang Mou, Yahong Zhang, Linli He and Shibei Li*

8089



Breaking the plane: B₅H₅ is a three-dimensional structure

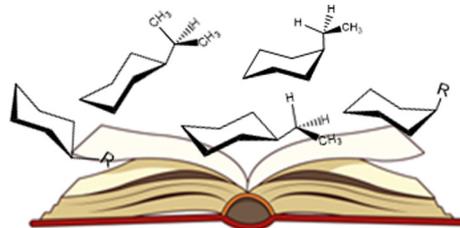
Gerardo Hernández-Juárez, Jorge Barroso, Alejandro Vásquez-Espinal, Filiberto Ortiz-Chi, William Tiznado, Fernando Murillo* and Gabriel Merino*



8094

Axial–equatorial equilibrium in substituted cyclohexanes: a DFT perspective on a small but complex problem

Hanwei Li, Eric Brémond, Juan Carlos Sancho-García, Ángel José Pérez-Jiménez, Giovanni Scalmani, Michael J. Frisch and Carlo Adamo*

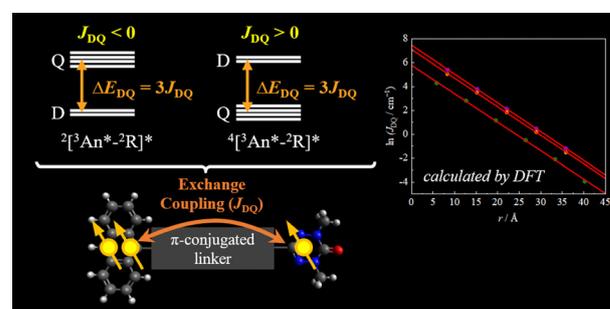


London forces vs. steric repulsion

8106

Theoretical investigation of multi-spin excited states of anthracene radical-linked π -conjugated spin systems by computational chemistry

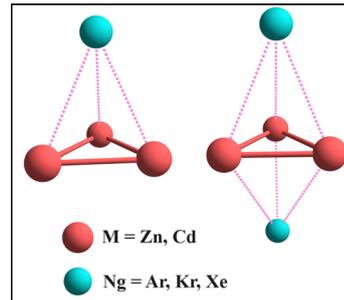
Ken Kato* and Yoshio Teki*



8115

Spodium bonding with noble gas atoms

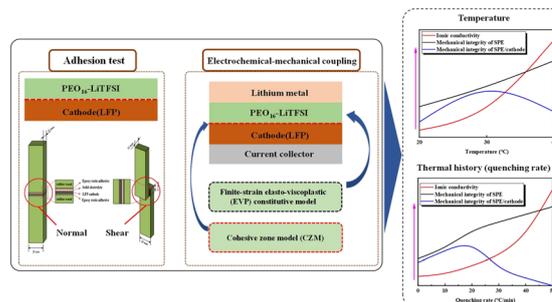
Farnaz Yashmin, Lakhya J. Mazumder, Pankaz K. Sharma* and Ankur K. Guha*



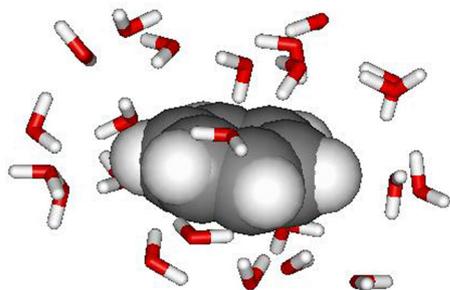
8125

Investigation on the mechanical integrity of a PEO-based polymer electrolyte in all-solid-state lithium batteries

Qinghua Yang, Detao Kong, Liang Fu, Yaolong He* and Hongjiu Hu



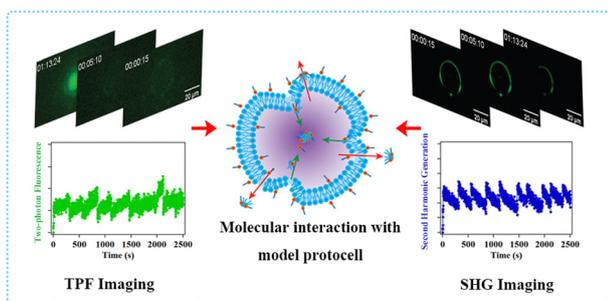
8141



Enthalpies and entropies of hydration from Monte Carlo simulations

William L. Jorgensen

8148



Monitoring the response of a model protocell to dye and surfactant molecules through second harmonic generation and fluorescence imaging

Bifei Li, Jianhui Li, Shujiao Chen, Qunhui Yuan,*
Chao Fang* and Wei Gan*

8158

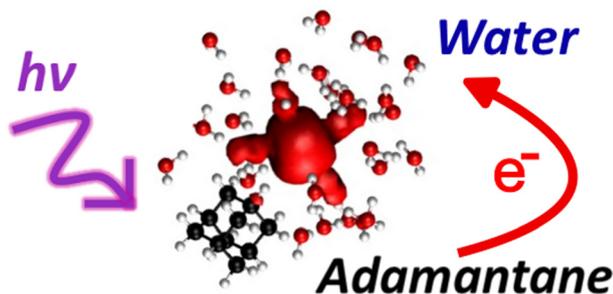
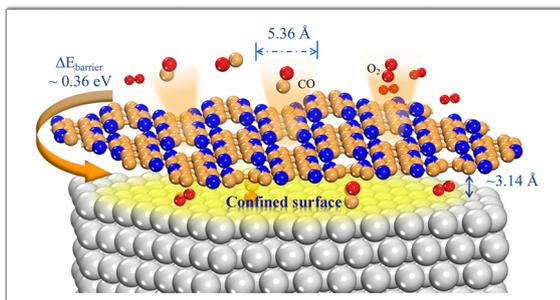


Photo-excited charge transfer from adamantane to electronic bound states in water

Xiangfei Wang, Pascal Krause, Thorren Kirschbaum,
Karol Palczynski, Joachim Dzubiella* and Annika Bande*

8177



The confined surface C₂N/Pt(111) as a highly efficient catalyst for CO oxidation

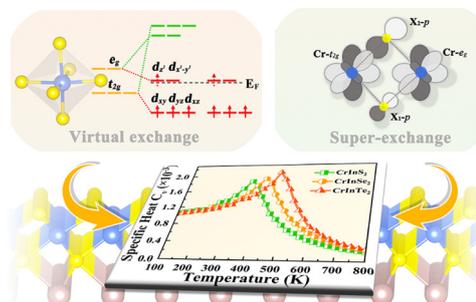
Yiqun Guo, Yongdao Chen and Xiangmei Duan*



8183

Prediction of intrinsic room-temperature ferromagnetism in two-dimensional CrInX_2 ($X = \text{S}, \text{Se}, \text{Te}$) monolayers

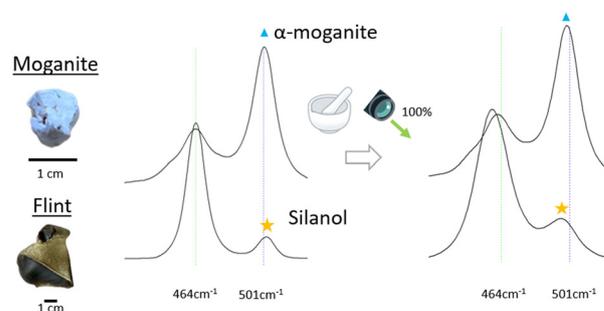
Yunfei Zhang, Shuo Zhang, Minghao Jia, Tian Wang, Lixiu Guan* and Junguang Tao*



8195

Differentiating α -moganite, silanol and α -quartz by Raman spectroscopy

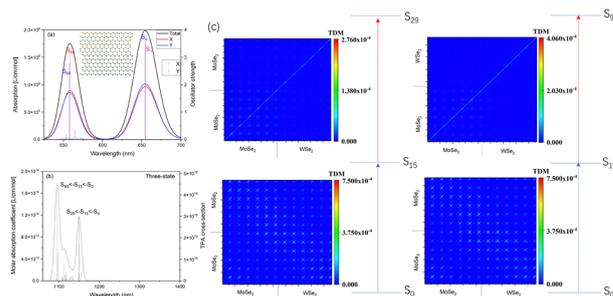
Yasumoto Tsukada,* Patrick Schmidt and Stephen A. Bowden



8200

Charge transfer excitons and directional fluorescence of in-plane lateral MoSe_2 - WSe_2 heterostructures

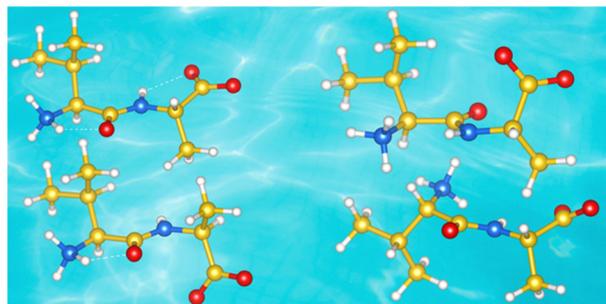
Ning Li, Na Zhang, Jingang Wang and Mengtao Sun*



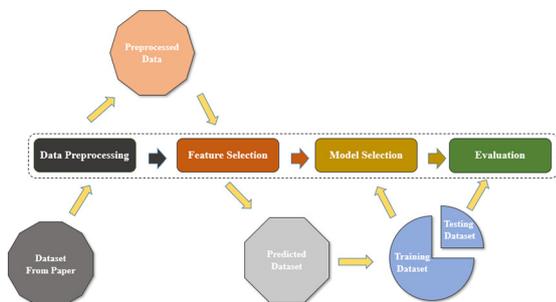
8210

Conformational preference of dipeptide zwitterions in aqueous solvents

Francisco Adasme-Carreño,* Alvaro Ochoa-Calle,* Marcelo Galván and Joel Ireta*



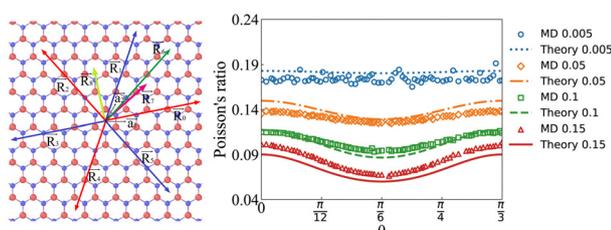
8219



Composition design and optimization of Fe–C–Mn–Al steel based on machine learning

Hong Cheng, Zhongping He,* Meiling Ge, Lun Che, Kaiyuan Zheng, Tianyu Si and Feng Zhao*

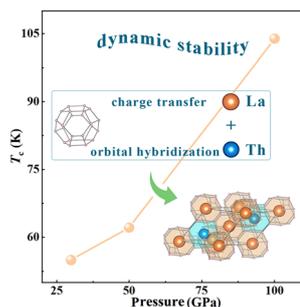
8228



Symmetry constraints on the orientation dependence of high-order elastic constants for the hexagonal boron nitride monolayer

Dong-Jian Yang, Peng Wei and Jin-Wu Jiang*

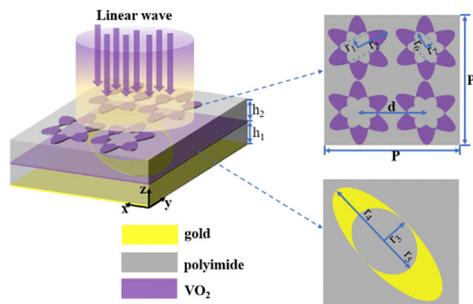
8237



High-temperature superconductivities and crucial factors influencing the stability of LaThH₁₂ under moderate pressures

Pengye Liu, Wendi Zhao, Zhao Liu,* Yilong Pan, Defang Duan and Tian Cui*

8247



Realization of multifunctional transformation based on the vanadium dioxide-assisted metamaterial structure

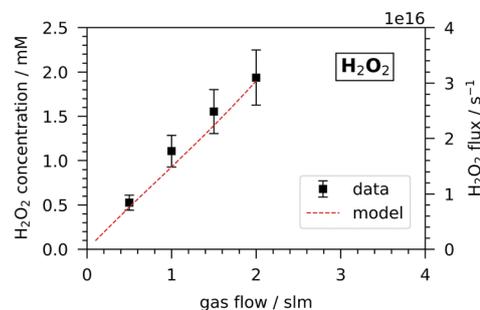
Xuehui Weng, Dexian Yan,* Yu Qiu, Xiangjun Li, Le Zhang and Jining Li



8255

Production and transport of plasma-generated hydrogen peroxide from gas to liquid

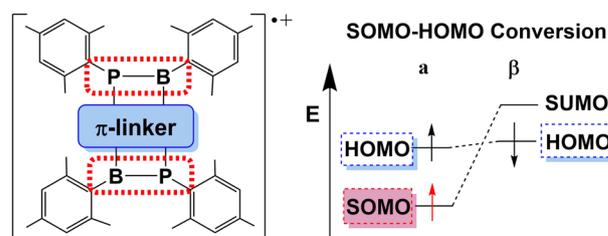
Steffen Schüttler, Anna Lena Schöne, Emanuel Jeß, Andrew R. Gibson and Judith Golda



8273

A quantum-chemical insight into SOMO–HOMO conversion in phosphorus–boron cation radicals

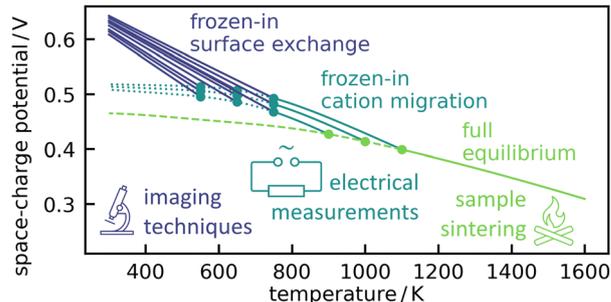
Li Zhang, Hongbo Li, Yanbin Zhu and Shoufeng Zhang*



8287

How space-charge behaviour at grain boundaries in electroceramic oxides is modified by two restricted equilibria

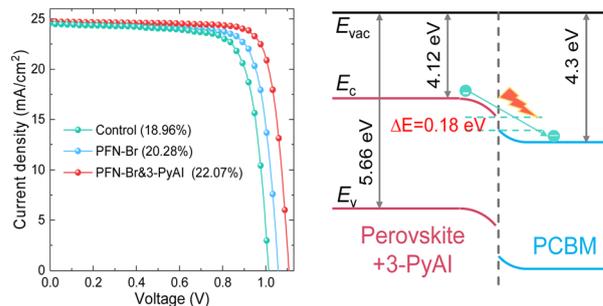
A. L. Usler,* F. Ketter and R. A. De Souza



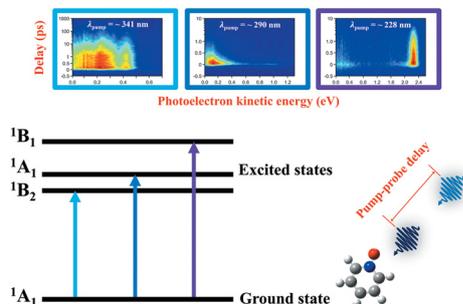
8299

Multifunctional dual-interface layer enables efficient and stable inverted perovskite solar cells

Chaofeng Wang, Yi Guo, Shuang Liu, Jiajia Huang, Xiaohui Liu, Jing Zhang, Ziyang Hu, Yuejin Zhu and Like Huang*



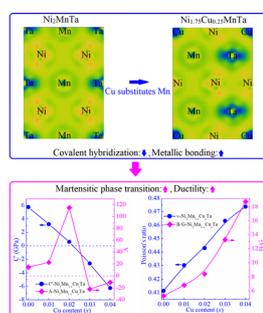
8308



Insights into ultrafast decay dynamics of electronically excited pyridine-*N*-oxide

Baihui Feng, Wenping Wu, Shuaikang Yang, Zhigang He, Benjie Fang, Dongyuan Yang,* Guorong Wu* and Xueming Yang

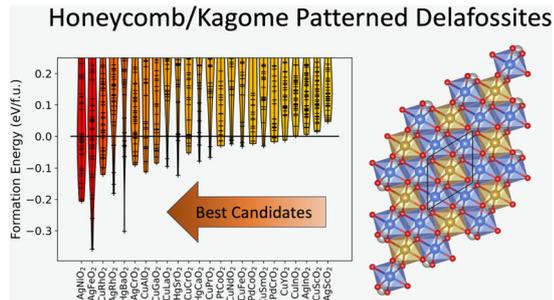
8318



Simultaneous improvement of martensitic phase transition and ductility in Cu-doped and/or alloyed all-d-metal Ni₂MnTa Heusler compounds

Guijiang Li,* Lei Xu and Zhenhua Cao

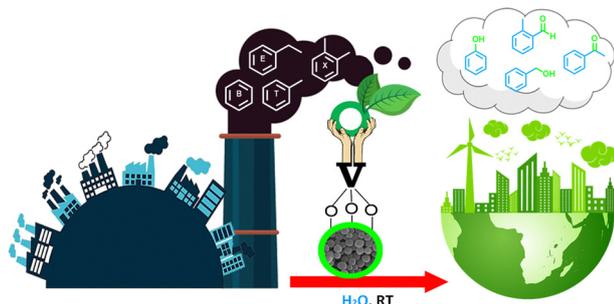
8327



Predictions of delafossite-hosted honeycomb and kagome phases

Jaron T. Krogel, Tomohiro Ichibha, Kayahan Saritas, Mina Yoon and Fernando A. Reboredo*

8334



Silica nanoparticles and kaolin clay decorated with VO²⁺ in aerobic oxidative destruction of BTEX contaminants

Pegah Mohammadpour, Elham Safaei* and Constantinos D. Zeinalipour-Yazdi

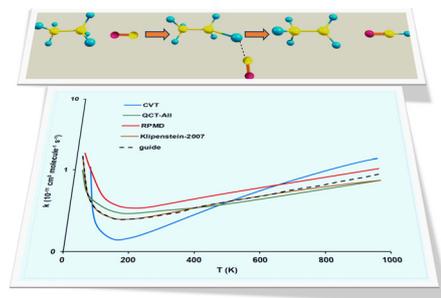


RESEARCH PAPERS

8344

Kinetic study of the CN + C₂H₆ hydrogen abstraction reaction based on an analytical potential energy surface

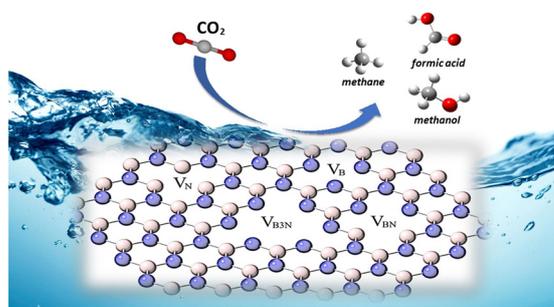
Joaquin Espinosa-Garcia* and Somnath Bhowmick*



8356

A DFT study of CO₂ electroreduction catalyzed by hexagonal boron-nitride nanosheets with vacancy defects

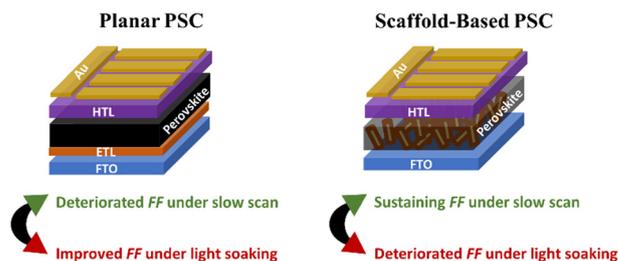
Dušan N. Sredojević,* Ivana Vukoje, Đorđe Trpkov and Edward N. Brothers



8366

Synergetic interfacial conductivity modulation dictating hysteresis evolution in perovskite solar cells under operation

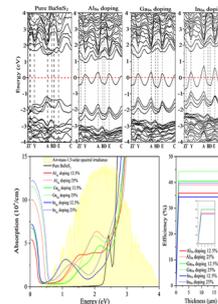
Rana Yekani, Han Wang, Stephanie Bessette, Raynald Gauvin and George Demopoulos*



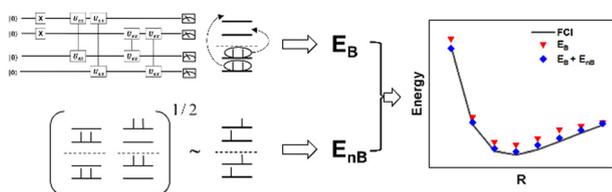
8380

Group-IIIA element doped BaSnS₂ as a high efficiency absorber for intermediate band solar cell from a first-principles insight

Yang Xue, Changqing Lin, Jiancheng Zhong, Dan Huang* and Clas Persson*



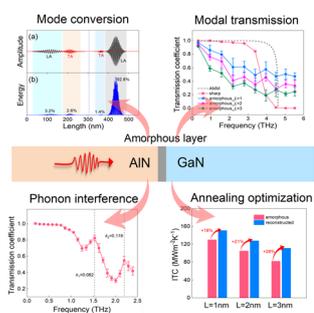
8390



Variational quantum eigensolver for closed-shell molecules with non-bosonic corrections

Kyungmin Kim, Sumin Lim, Kyujin Shin,* Gwonhak Lee, Yousung Jung, Woomin Kyoung, June-Koo Kevin Rhee* and Young Min Rhee*

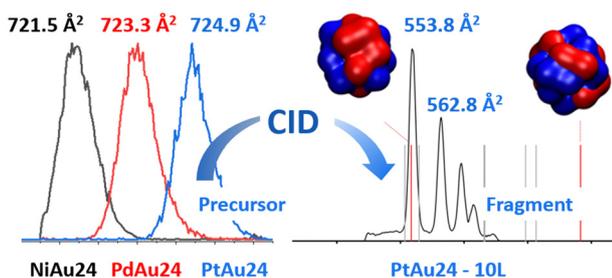
8397



Phonon dynamic behaviors induced by amorphous layers at heterointerfaces

Quanjie Wang, Jie Zhang, Yucheng Xiong, Shouhang Li, Vladimir Chernysh and Xiangjun Liu*

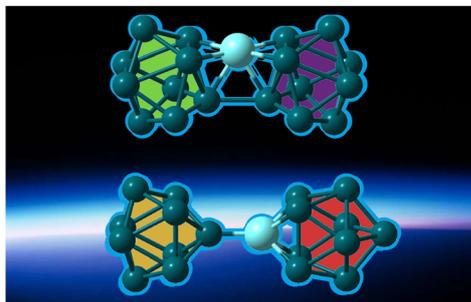
8408



Cyclic ion mobility of doped $[MAu_{24}L_{18}]^{2-}$ superatoms and their fragments ($M = Ni, Pd$ and Pt ; $L =$ alkynyl)

Frank Henrich, Shun Ito, Patrick Weis, Marco Neumaier, Shinjiro Takano, Tatsuya Tsukuda and Manfred M. Kappes*

8419



$[Ag(Sn_9-Sn_9)]^{5-}$ and $[(\eta^4-Sn_9)Ag(\eta^1-Sn_9)]^{7-}$, as aggregates of spherical aromatic building blocks. Persistence of aromaticity upon cluster gathering

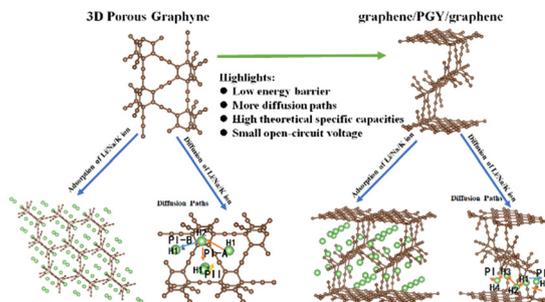
Peter L. Rodriguez-Kessler and Alvaro Muñoz-Castro*



8426

Graphyne-based 3D porous structure and its sandwich-type graphene structure for alkali metal ion battery anode materials

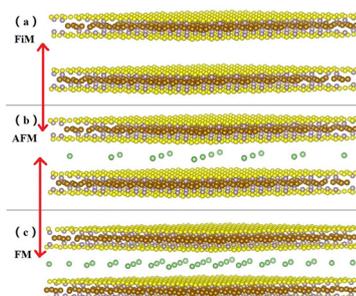
Haidong Liu, Xiaowei Li,* Haotian Chen, Jin Chen and Zixun Shi



8436

Li-ion intercalation-driven control of two-dimensional magnetism in van der Waals FePS₃ bilayers

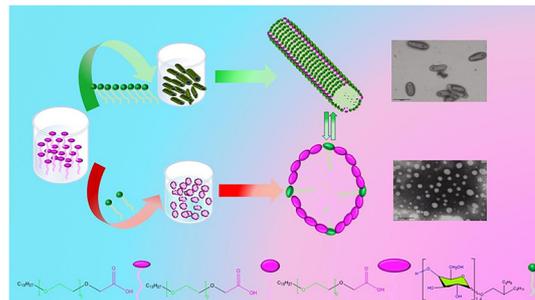
Dong Chen,* Chunlei Wang and Chengxiao Peng



8448

Self-assembly mechanism, physicochemical analyses and application performance investigations of branched alkyl glycosides with alcohol ether carboxylic acids of varied epoxide numbers

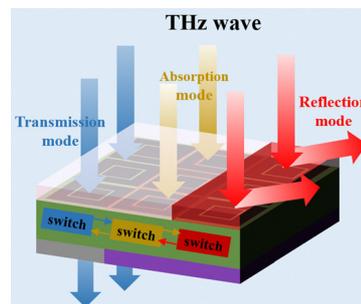
Yukai Wang, Zihui Zhang, Liang Bai,* Xiuquan Yang,* Yunqin Qi, Jiahao Li, Yuan Zhou, Zhiyu Wu and Ziyu Qin



8460

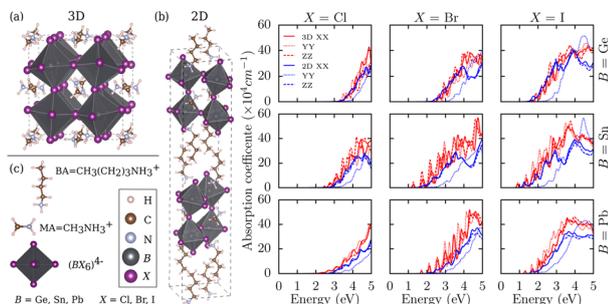
Thermal controlled multi-functional metasurface for freely switching of absorption, reflection, and transmission

Zhipeng Ding, Wei Su,* Lipengan Ye, Yuanhang Zhou, Wenlong Li, Jianfei Zou, Bin Tang and Hongbing Yao*



RESEARCH PAPERS

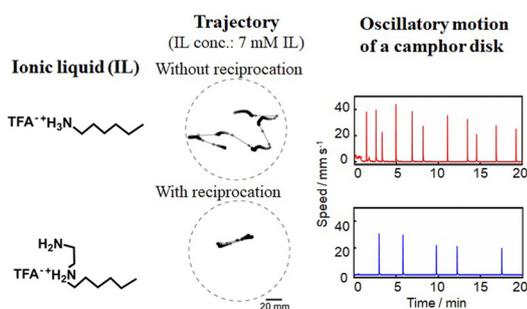
8469



Contrasting the stability, octahedral distortions, and optoelectronic properties of 3D MABX₃ and 2D (BA)₂(MA)B₂X₇ (B = Ge, Sn, Pb; X = Cl, Br, I) perovskites

João G. Danelon, Ramiro M. Santos, Alexandre C. Dias, Juarez L. F. Da Silva and Matheus P. Lima*

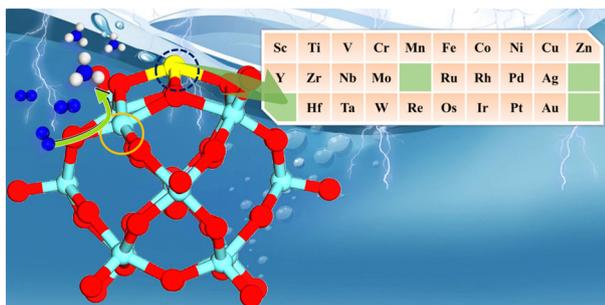
8488



Self-propelled motion controlled by ionic liquids

Er Hua,* Jun Gao, Yu Xu, Muneyuki Matsuo and Satoshi Nakata*

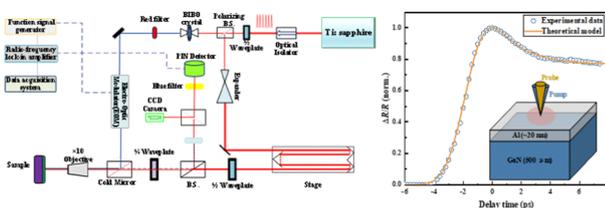
8494



Design of high performance nitrogen reduction electrocatalysts by doping defective polyoxometalate with a single atom promoter

Linghui Lin, Ruijie Ma, Rong Jiang* and Sen Lin*

8504



Nonequilibrium electron-phonon coupling across the interfaces between Al nanofilm and GaN

Jiao Chen, Wenlong Bao, Zhaoliang Wang,* Ke Xu and Dawei Tang

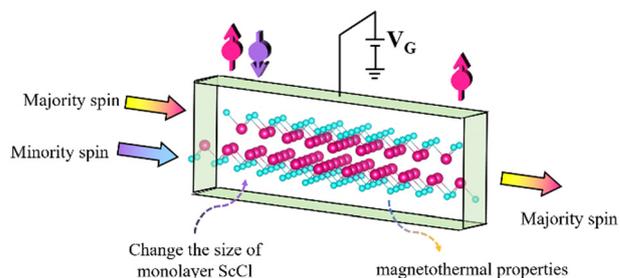


RESEARCH PAPERS

8515

Electronic structure and magnetothermal properties of two-dimensional ScCl

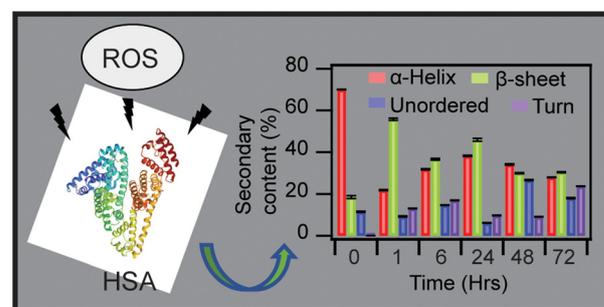
Hao-Jia Wu, Dan Wang, Hua-Yun Geng and Xiang-Rong Chen*



8528

Oxidative stress induced conformational changes of human serum albumin

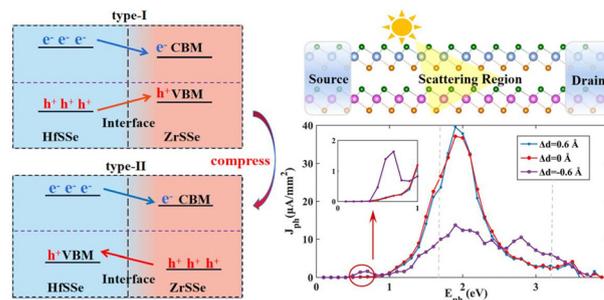
Debdip Brahma, Akshay Narayan Sarangi, Rupal Kaushik and Amar Nath Gupta*



8539

A strategy for boosting photovoltaic performance based on a two-dimensional ZrSSe/HfSSe van der Waals heterostructure

Keying Han, Defeng Guo,* Yuxin Han, Pei Zhao, Yan Liang* and Qiang Wang*



8547

Temperature-dependent decomposition of the CL-20/MTNP cocrystal after phase separation

Fang Yang, Zongwei Yang, Qian Yu, Zhongping Liu, Gang Li, Chuande Zhao* and Yong Tian*

