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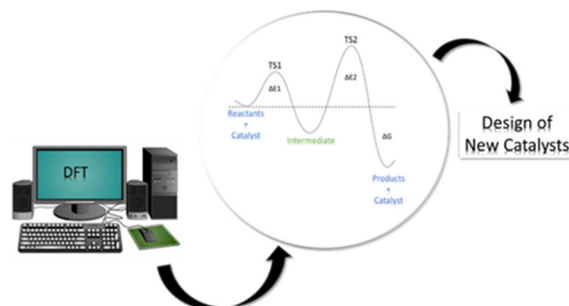
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TUTORIAL REVIEW

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

Valeria Butera

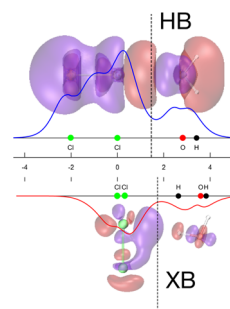


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The dawn of hydrogen and halogen bonds and their crucial role in collisional processes probing long-range intermolecular interactions

David Cappelletti,* Stefano Falcinelli and Fernando Pirani



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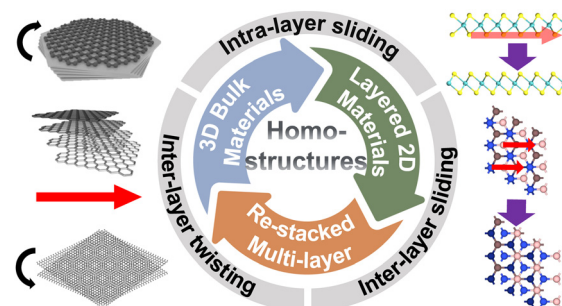


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Stacking engineering in layered homostructures: transitioning from 2D to 3D architectures

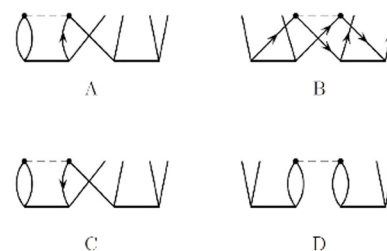
Jiamin Wang, Fang Cheng, Yan Sun,* Hai Xu* and Liang Cao*



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

Rodney J. Bartlett

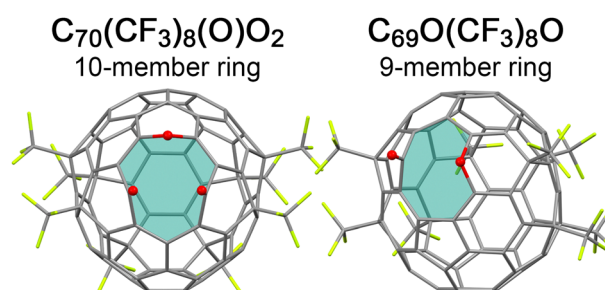
 T_2^2 Terms in CCD

COMMUNICATIONS

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Oxidative cage opening in the C₇₀ fullerene facilitated by preceding trifluoromethylation

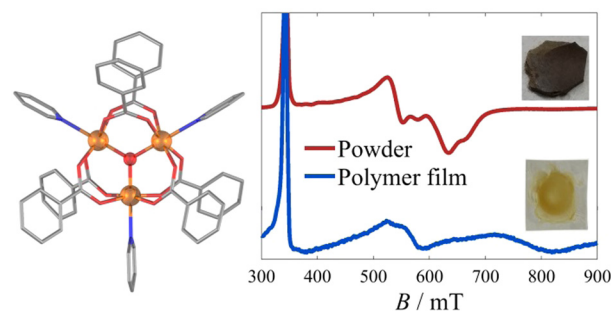
Sofia V. Gracheva, Nadezhda B. Tamm, Konstantin A. Lyssenko, Ilya N. Ioffe, Natalia S. Lukonina* and Alexey A. Goryunkov



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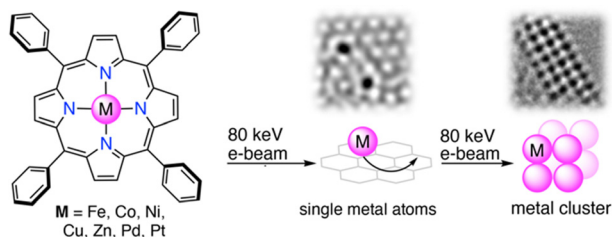
Matrix effects on the magnetic properties of a molecular spin triangle embedded in a polymeric film

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



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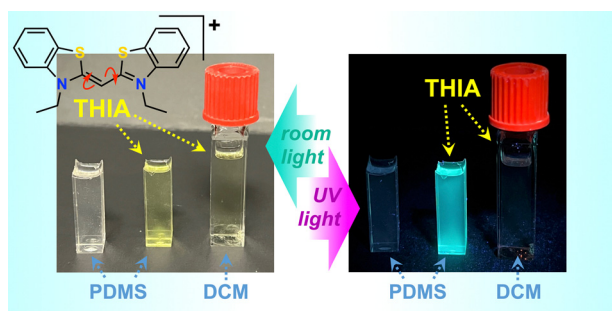
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Electron beam-induced demetallation of Fe, Co, Ni, Cu, Zn, Pd, and Pt metalloporphyrins: insights in e-beam chemistry and metal cluster formations

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

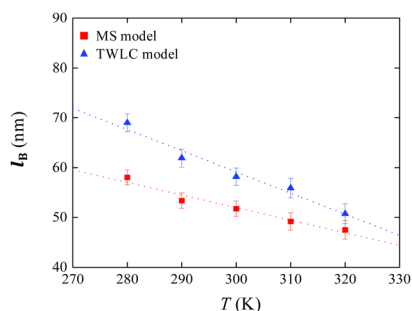
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Poly(dimethylsiloxane) as a room-temperature solid solvent for photophysics and photochemistry

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*

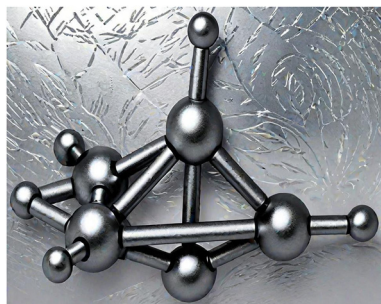
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Influence of temperature on bend, twist and twist-bend coupling of dsDNA

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

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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*

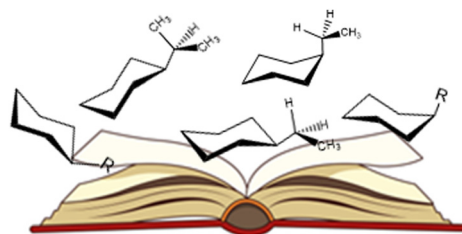


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Axial–equatorial equilibrium in substituted cyclohexanes: a DFT perspective on a small but complex problem

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

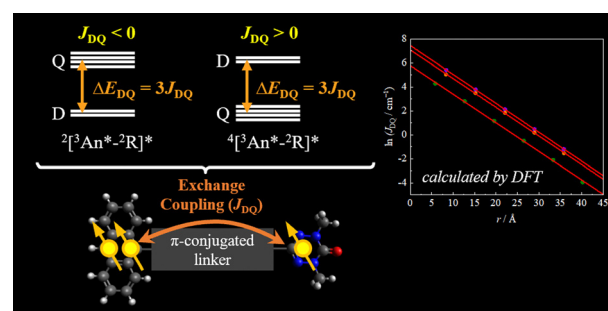


London forces vs. steric repulsion

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

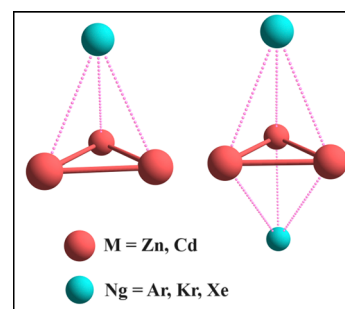
Ken Kato* and Yoshio Teki*



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Spodium bonding with noble gas atoms

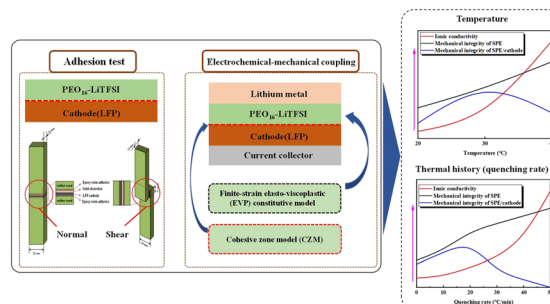
Farnaz Yashmin, Lakhya J. Mazumder, Pankaz K. Sharma* and Ankur K. Guha*



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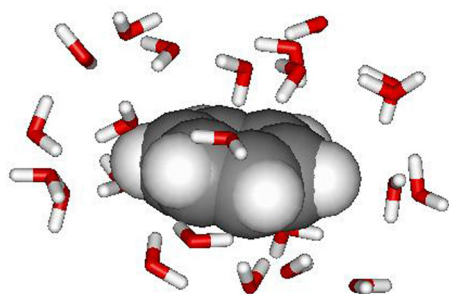
Investigation on the mechanical integrity of a PEO-based polymer electrolyte in all-solid-state lithium batteries

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



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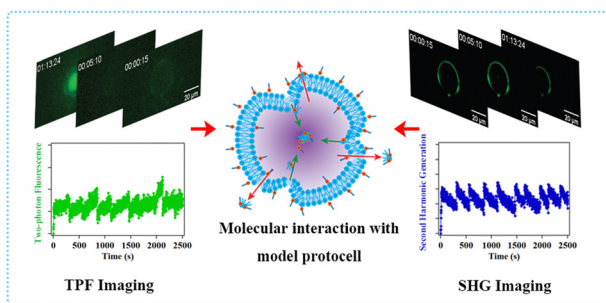
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Enthalpies and entropies of hydration from Monte Carlo simulations

William L. Jorgensen

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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*

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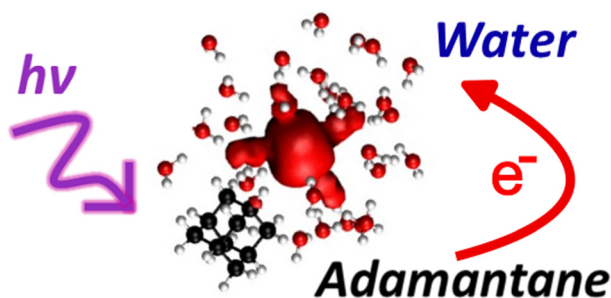
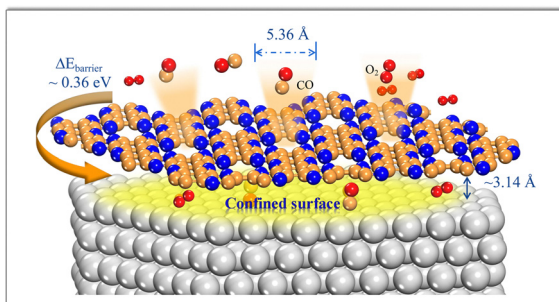


Photo-excited charge transfer from adamantane to electronic bound states in water

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

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

Yiqun Guo, Yongdao Chen and Xiangmei Duan*

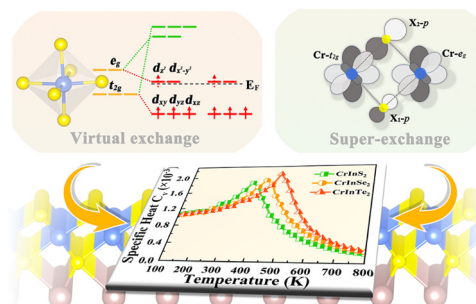


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Prediction of intrinsic room-temperature ferromagnetism in two-dimensional CrInX_2 ($X = \text{S, Se, Te}$) monolayers

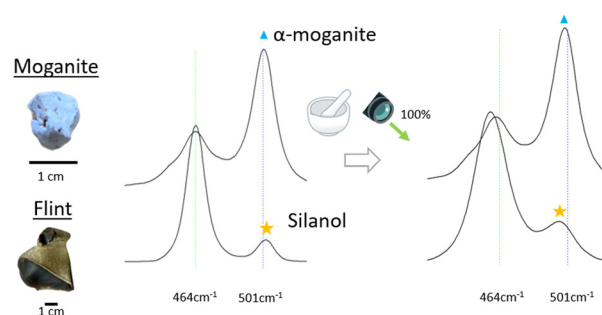
Yunfei Zhang, Shuo Zhang, Minghao Jia, Tian Wang, Lixiu Guan* and Junguang Tao*



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

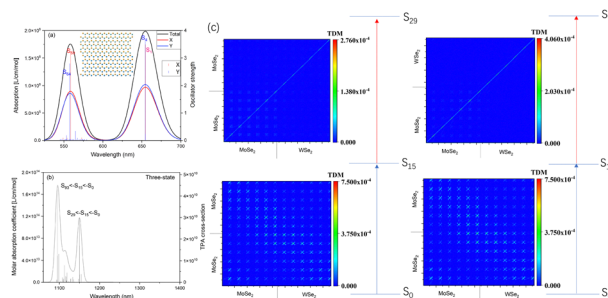
Yasumoto Tsukada,* Patrick Schmidt and Stephen A. Bowden



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

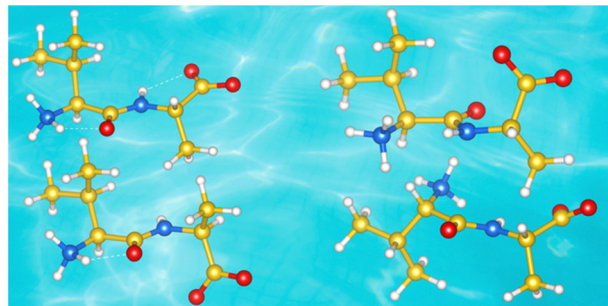
Ning Li, Na Zhang, Jingang Wang and Mengtao Sun*



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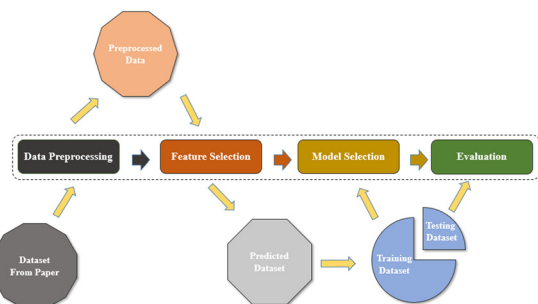
Conformational preference of dipeptide zwitterions in aqueous solvents

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



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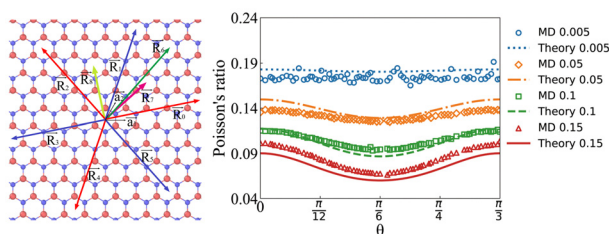
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Composition design and optimization of Fe–C–Mn–Al steel based on machine learning

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

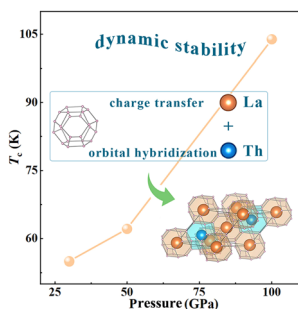
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Symmetry constraints on the orientation dependence of high-order elastic constants for the hexagonal boron nitride monolayer

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

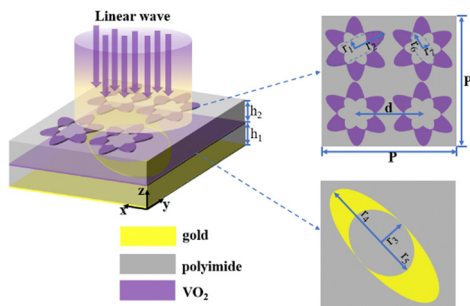
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High-temperature superconductivities and crucial factors influencing the stability of LaThH₁₂ under moderate pressures

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

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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

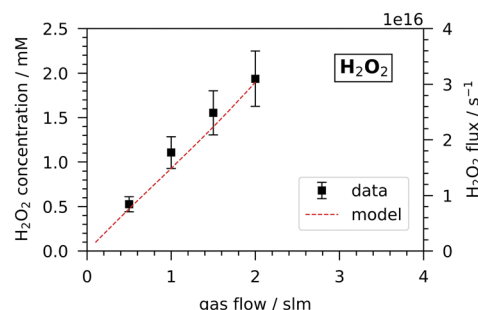


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Production and transport of plasma-generated hydrogen peroxide from gas to liquid

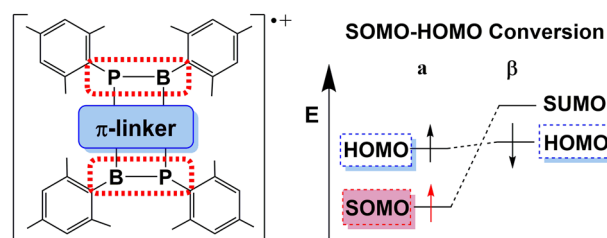
Steffen Schüttler, Anna Lena Schöne, Emanuel Jeß, Andrew R. Gibson and Judith Golda



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

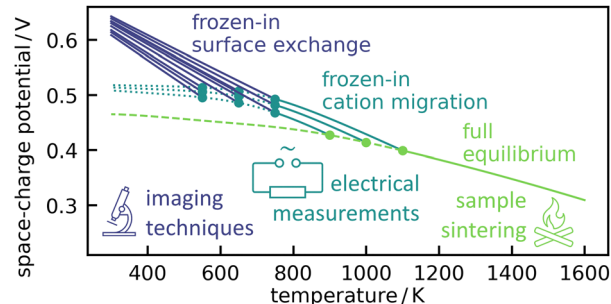
Li Zhang, Hongbo Li, Yanbin Zhu and Shoufeng Zhang*



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

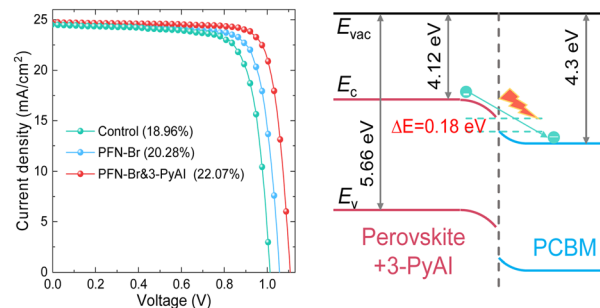
A. L. Usler,* F. Ketter and R. A. De Souza



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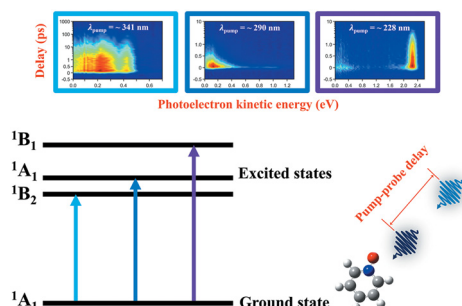
Multifunctional dual-interface layer enables efficient and stable inverted perovskite solar cells

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



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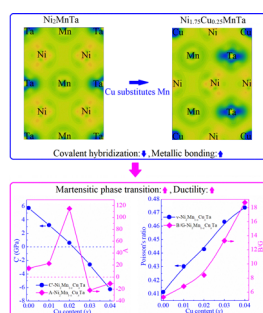
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Insights into ultrafast decay dynamics of electronically excited pyridine-*N*-oxide

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

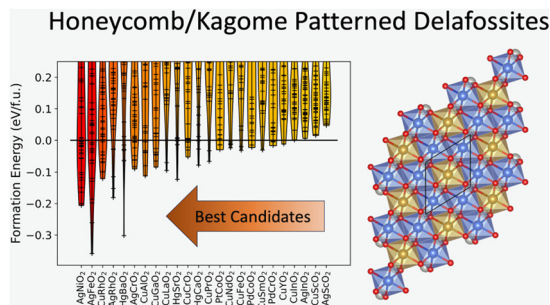
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Simultaneous improvement of martensitic phase transition and ductility in Cu-doped and/or alloyed all-d-metal Ni₂MnTa Heusler compounds

Guijiang Li,* Lei Xu and Zhenhua Cao

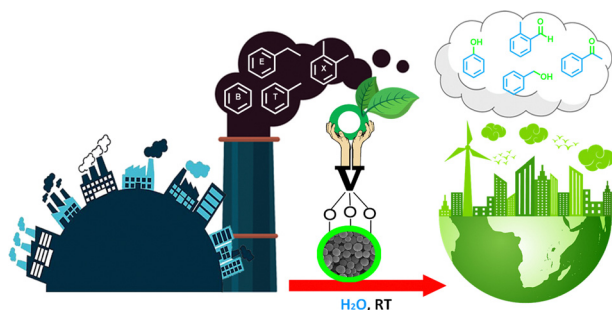
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Predictions of delafossite-hosted honeycomb and kagome phases

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

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

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

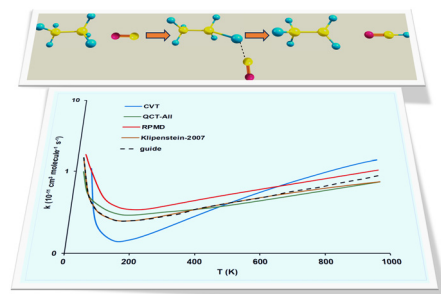


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Kinetic study of the $\text{CN} + \text{C}_2\text{H}_6$ hydrogen abstraction reaction based on an analytical potential energy surface

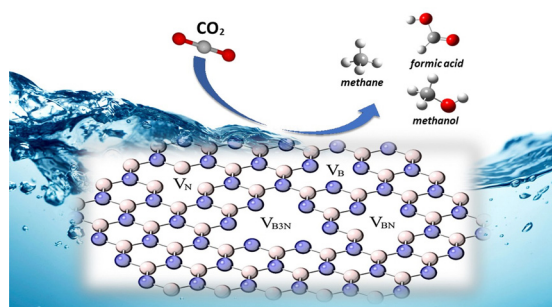
Joaquin Espinosa-Garcia* and Somnath Bhowmick*



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A DFT study of CO_2 electroreduction catalyzed by hexagonal boron-nitride nanosheets with vacancy defects

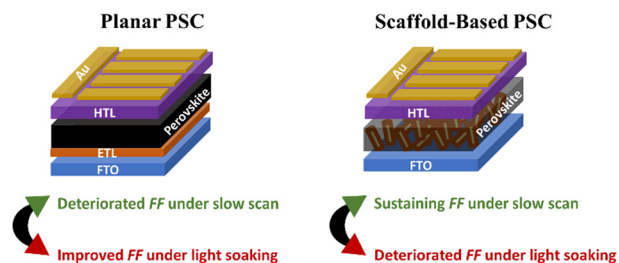
Dušan N. Sredojević,* Ivana Vukoje, Đorđe Trpkov and Edward N. Brothers



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

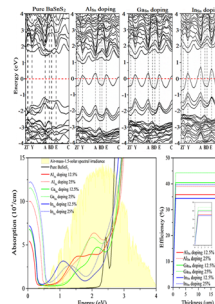
Rana Yekani, Han Wang, Stephanie Bessette, Raynald Gauvin and George Demopoulos*



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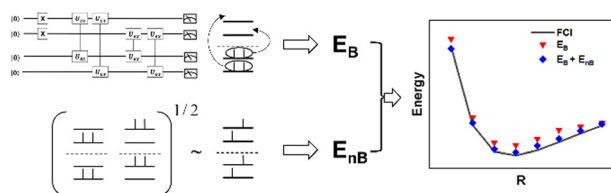
Group-IIIA element doped BaSnS_2 as a high efficiency absorber for intermediate band solar cell from a first-principles insight

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



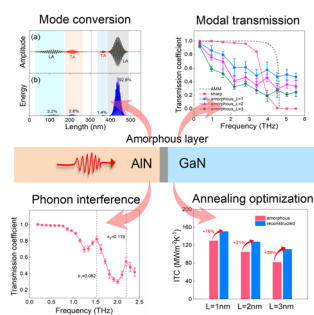
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**Variational quantum eigensolver for closed-shell molecules with non-bosonic corrections**

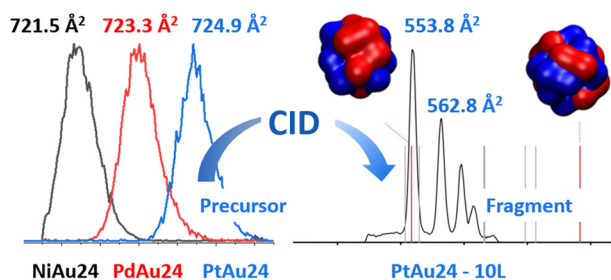
Kyungmin Kim, Sumin Lim, Kyujin Shin,* Gwonhak Lee, Yousung Jung, Woomin Kyoung, June-Koo Kevin Rhee* and Young Min Rhee*

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**Phonon dynamic behaviors induced by amorphous layers at heterointerfaces**

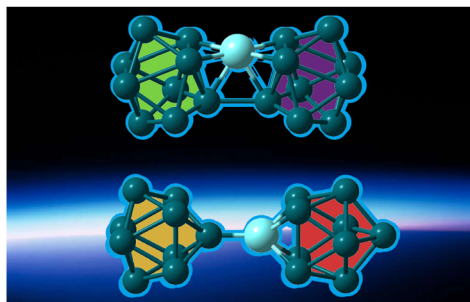
Quanjie Wang, Jie Zhang, Yucheng Xiong, Shouhang Li, Vladimir Chernysh and Xiangjun Liu*

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

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

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 **$[\text{Ag}(\text{Sn}_9\text{-Sn}_9)]^{5-}$ and $[(\eta^4\text{-Sn}_9)\text{Ag}(\eta^1\text{-Sn}_9)]^{7-}$, as aggregates of spherical aromatic building blocks. Persistence of aromaticity upon cluster gathering**

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

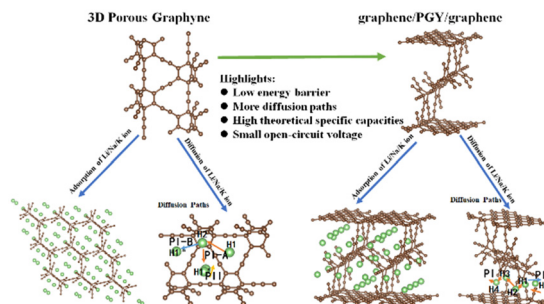


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Graphyne-based 3D porous structure and its sandwich-type graphene structure for alkali metal ion battery anode materials

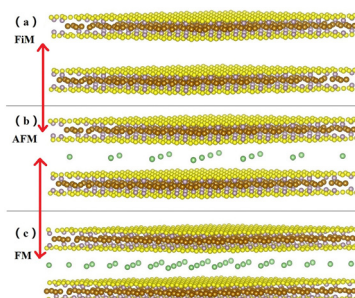
Haidong Liu, Xiaowei Li,* Haotian Chen, Jin Chen and Zixun Shi



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

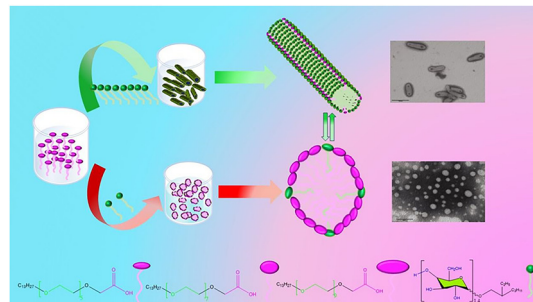
Dong Chen,* Chunlei Wang and Chengxiao Peng



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

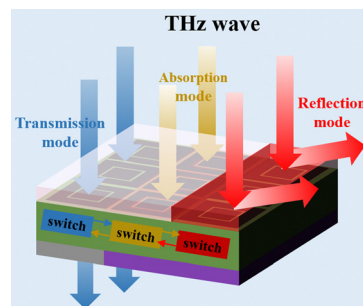
Yukai Wang, Zhihui Zhang, Liang Bai,* Xiuquan Yang,* Yunqin Qi, Jiahao Li, Yuan Zhou, Zhiyu Wu and Ziyu Qin



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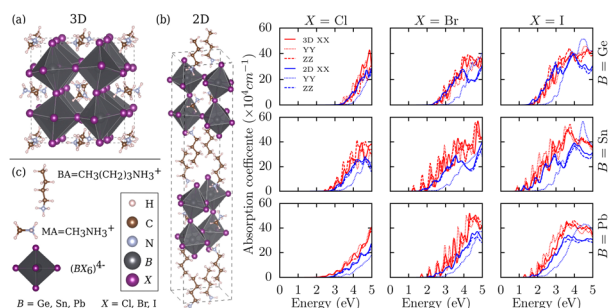
Thermal controlled multi-functional metasurface for freely switching of absorption, reflection, and transmission

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



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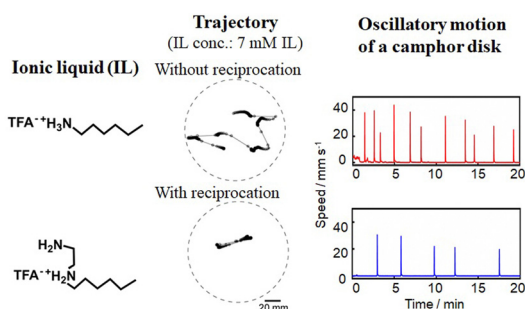
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Contrasting the stability, octahedral distortions, and optoelectronic properties of 3D MABX₃ and 2D (BA)₂(MA)B₂X₇ (B = Ge, Sn, Pb; X = Cl, Br, I) perovskites

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

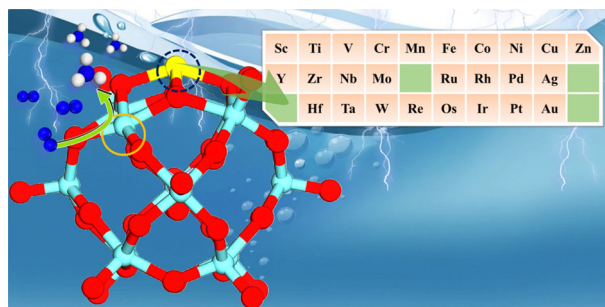
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Self-propelled motion controlled by ionic liquids

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

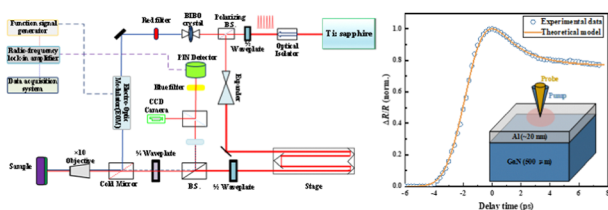
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Design of high performance nitrogen reduction electrocatalysts by doping defective polyoxometalate with a single atom promoter

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

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

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

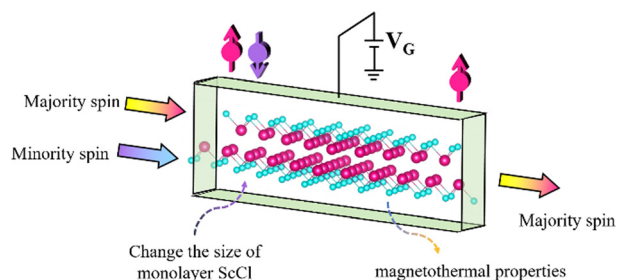


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Electronic structure and magnetothermal properties of two-dimensional ScCl

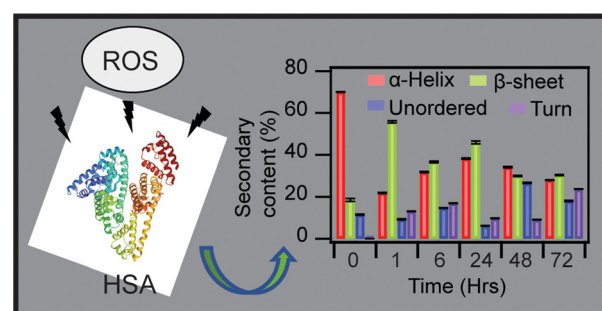
Hao-Jia Wu, Dan Wang, Hua-Yun Geng and Xiang-Rong Chen*



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Oxidative stress induced conformational changes of human serum albumin

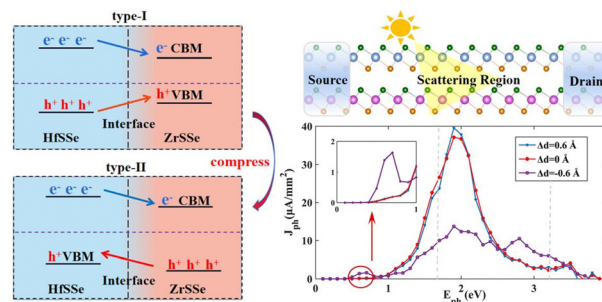
Debdip Brahma, Akshay Narayan Sarangi, Rupal Kaushik and Amar Nath Gupta*



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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*



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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*

