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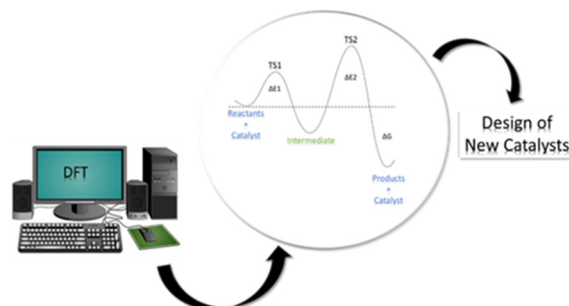
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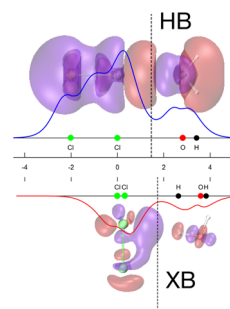


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David Cappelletti,* Stefano Falcinelli and Fernando Pirani



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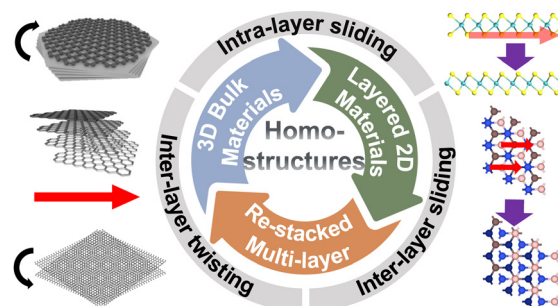


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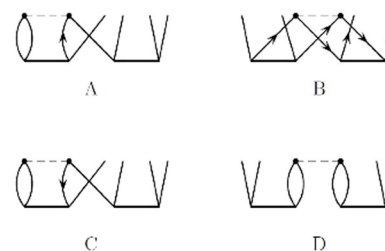
Jiamin Wang, Fang Cheng, Yan Sun,* Hai Xu* and Liang Cao*



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

Rodney J. Bartlett

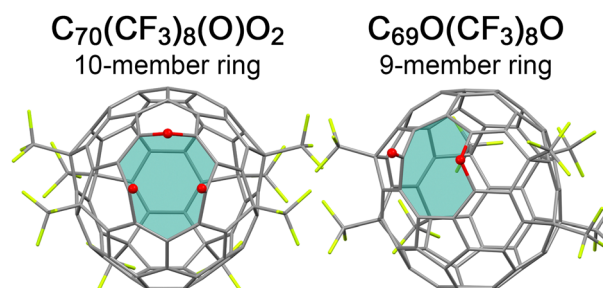
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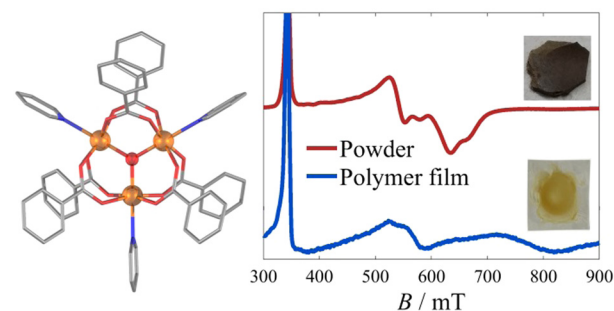
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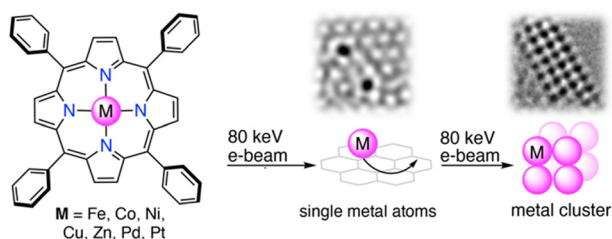
Matrix effects on the magnetic properties of a molecular spin triangle embedded in a polymeric film

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



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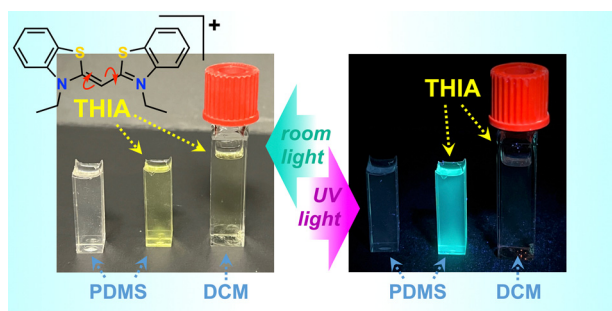
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Electron beam-induced demetallation of Fe, Co, Ni, Cu, Zn, Pd, and Pt metalloporphyrins: insights in e-beam chemistry and metal cluster formations

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

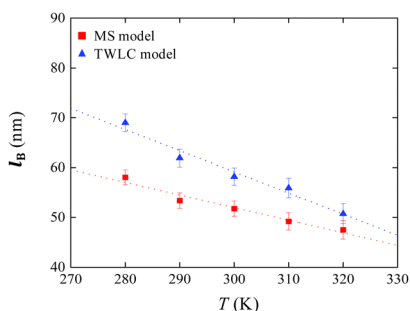
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John A. Clark, Samantha Robinson, Eli M. Espinoza, Duoduo Bao, James B. Derr, Luca Croft, Omar O'Mari, William H. Grover and Valentine I. Vullev*

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

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Breaking the plane: B₅H₅ is a three-dimensional structure

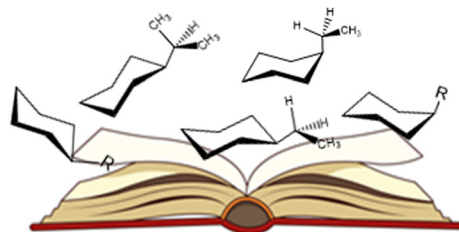
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Hanwei Li, Eric Brémond, Juan Carlos Sancho-García, Ángel José Pérez-Jiménez, Giovanni Scalmani, Michael J. Frisch and Carlo Adamo*

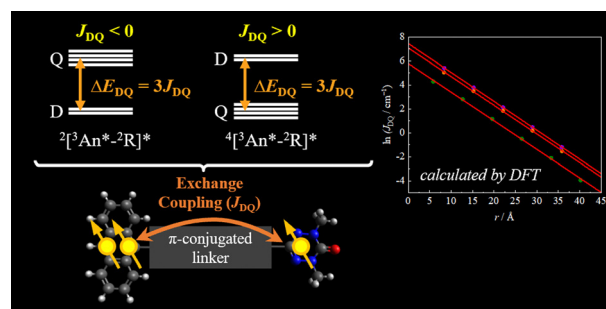


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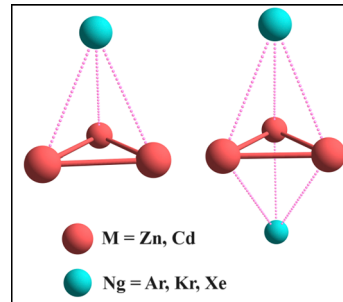
Ken Kato* and Yoshio Teki*



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Spodium bonding with noble gas atoms

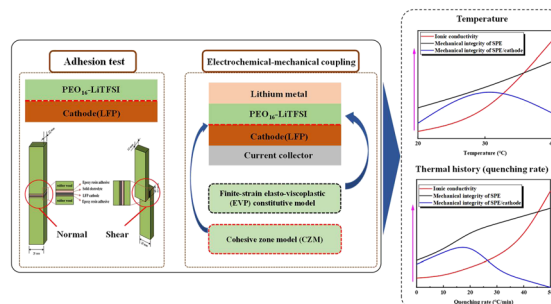
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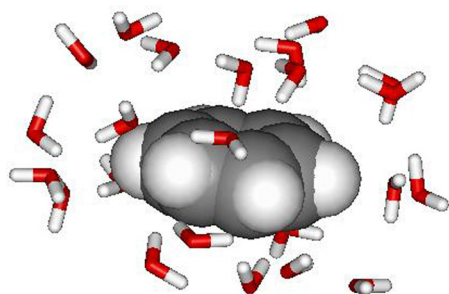
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Investigation on the mechanical integrity of a PEO-based polymer electrolyte in all-solid-state lithium batteries

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



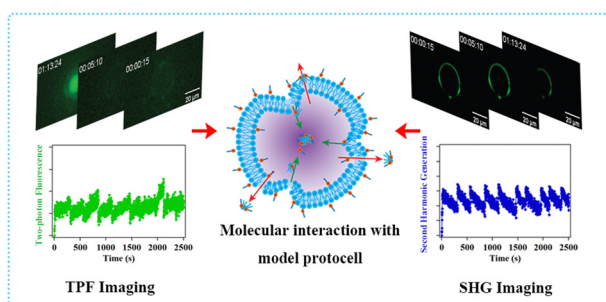
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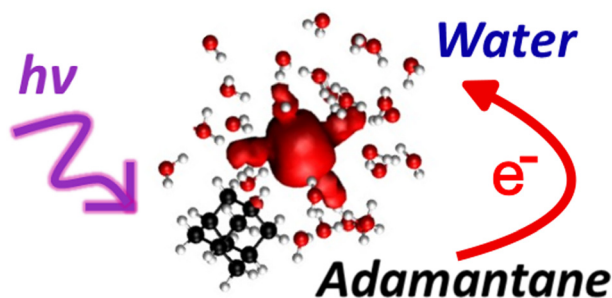
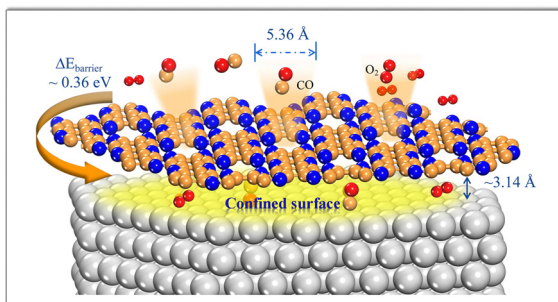


Photo-excited charge transfer from adamantane to electronic bound states in water

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

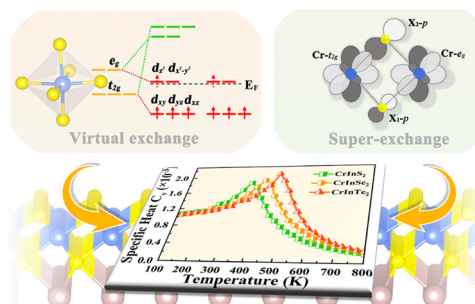
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Prediction of intrinsic room-temperature ferromagnetism in two-dimensional CrInX₂ (X = S, Se, Te) monolayers

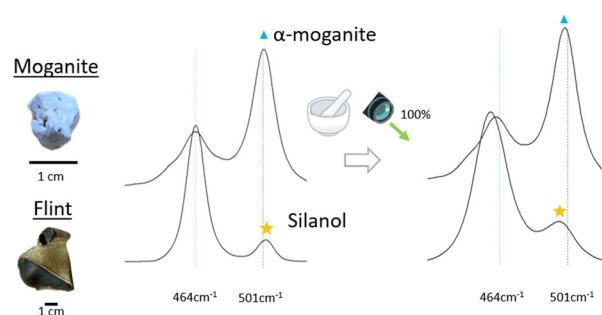
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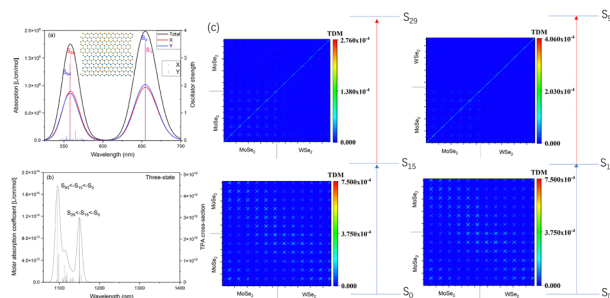
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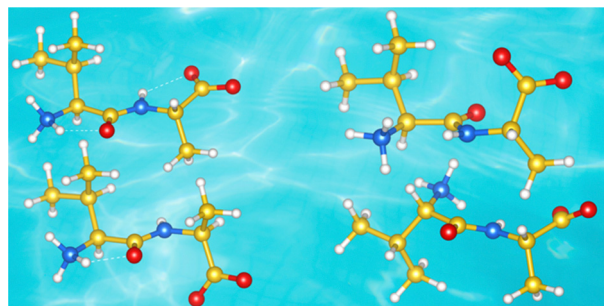
Ning Li, Na Zhang, Jingang Wang and Mengtao Sun*



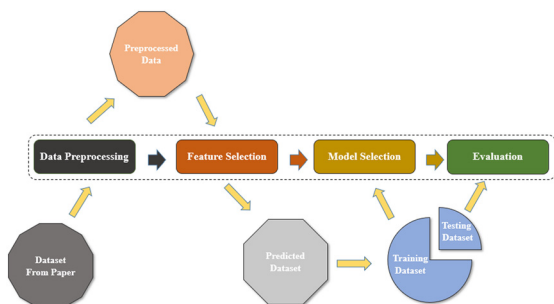
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Conformational preference of dipeptide zwitterions in aqueous solvents

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



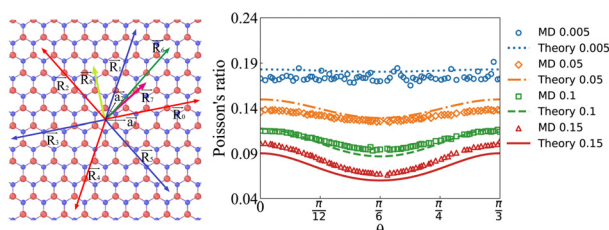
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Composition design and optimization of Fe–C–Mn–Al steel based on machine learning

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

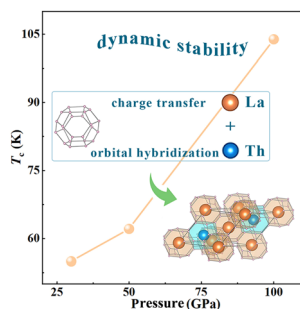
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Symmetry constraints on the orientation dependence of high-order elastic constants for the hexagonal boron nitride monolayer

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

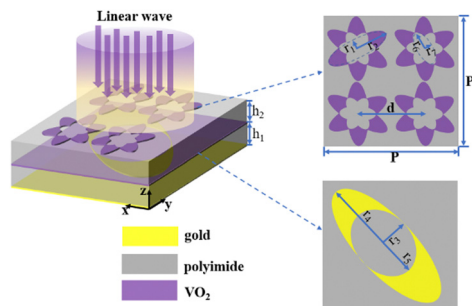
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High-temperature superconductivities and crucial factors influencing the stability of LaThH₁₂ under moderate pressures

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

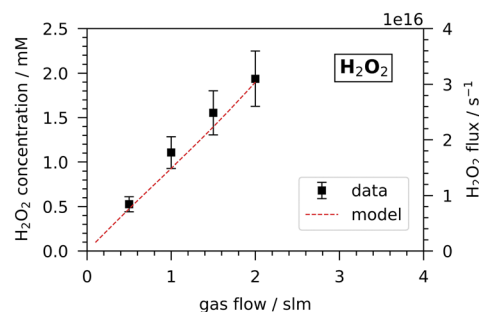
Xuehui Weng, Dexian Yan,* Yu Qiu, Xiangjun Li, Le Zhang and Jining Li



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

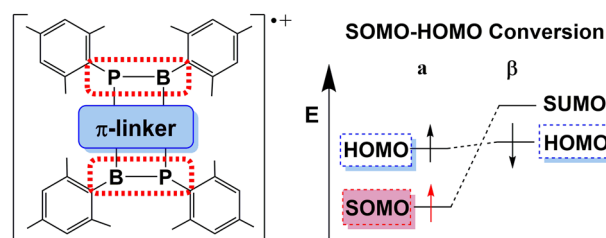
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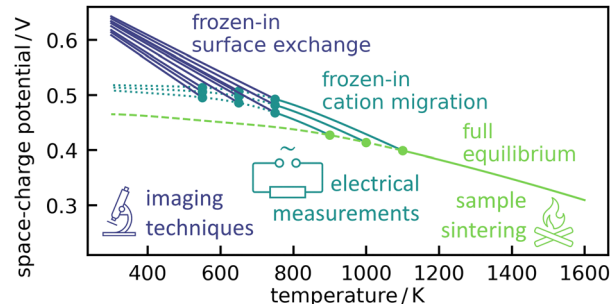
Li Zhang, Hongbo Li, Yanbin Zhu and Shoufeng Zhang*



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

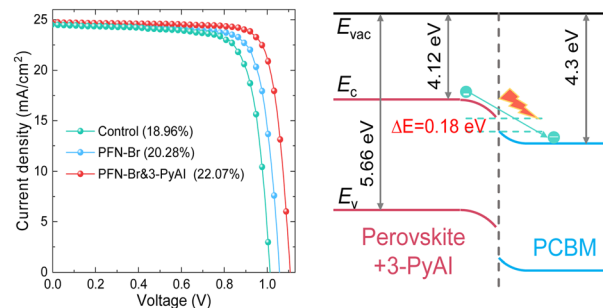
A. L. Usler,* F. Ketter and R. A. De Souza



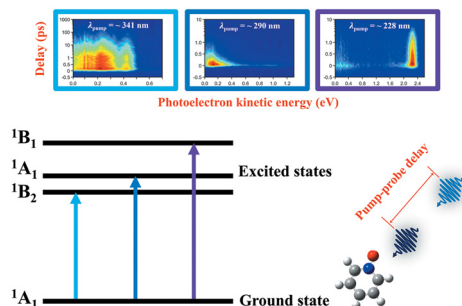
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Multifunctional dual-interface layer enables efficient and stable inverted perovskite solar cells

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



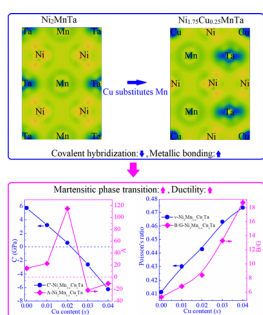
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Insights into ultrafast decay dynamics of electronically excited pyridine-*N*-oxide

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

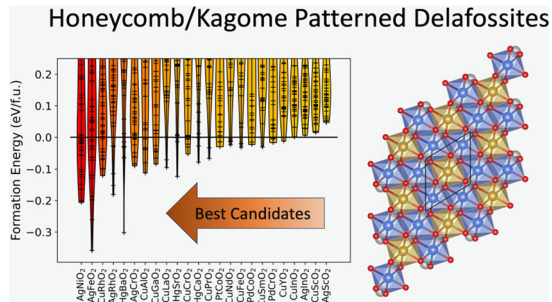
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Simultaneous improvement of martensitic phase transition and ductility in Cu-doped and/or alloyed all-d-metal Ni₂MnTa Heusler compounds

Guijiang Li,* Lei Xu and Zhenhua Cao

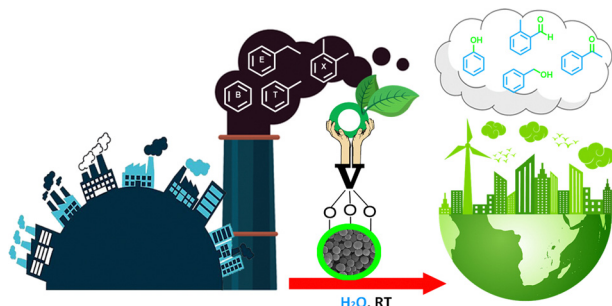
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Predictions of delafossite-hosted honeycomb and kagome phases

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

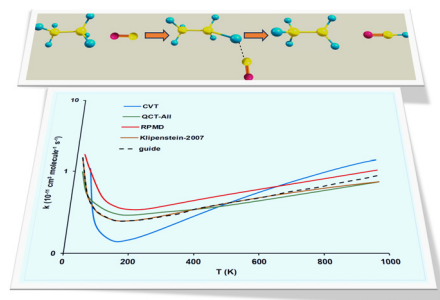


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Kinetic study of the CN + C₂H₆ hydrogen abstraction reaction based on an analytical potential energy surface

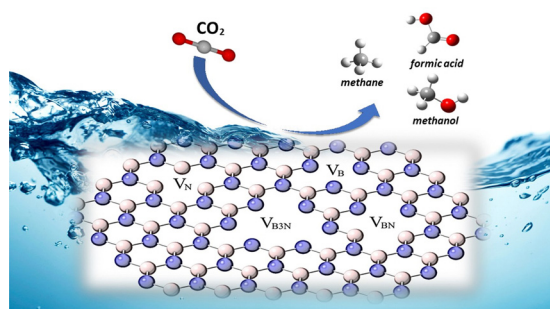
Joaquin Espinosa-Garcia* and Somnath Bhowmick*



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

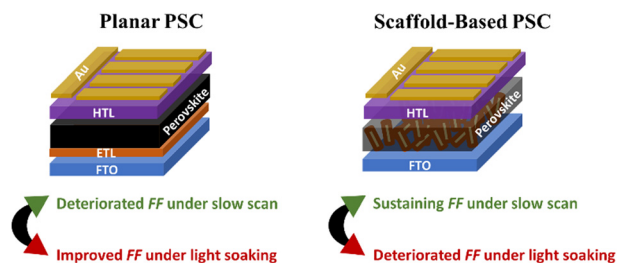
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Synergetic interfacial conductivity modulation dictating hysteresis evolution in perovskite solar cells under operation

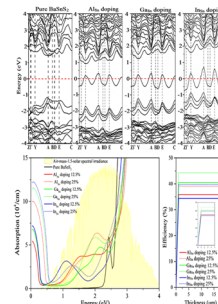
Rana Yekani, Han Wang, Stephanie Bessette, Raynald Gauvin and George Demopoulos*



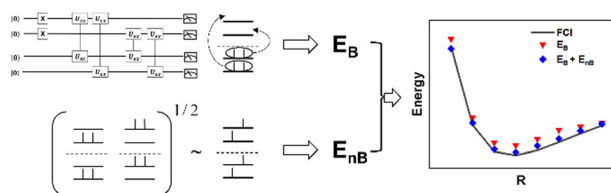
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Group-IIIA element doped BaSnS₂ as a high efficiency absorber for intermediate band solar cell from a first-principles insight

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



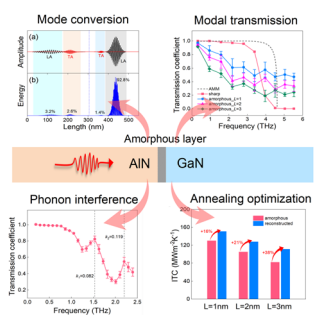
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Variational quantum eigensolver for closed-shell molecules with non-bosonic corrections

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

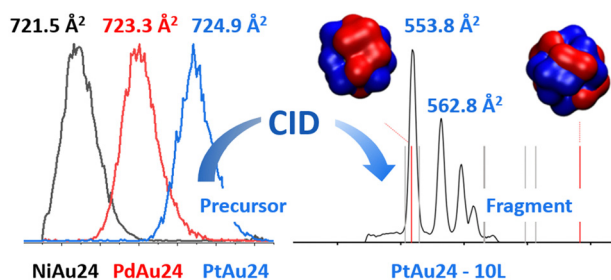
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Phonon dynamic behaviors induced by amorphous layers at heterointerfaces

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

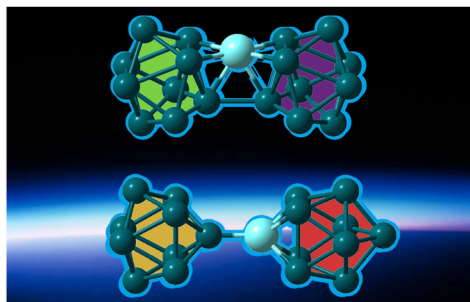
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Cyclic ion mobility of doped $[MAu_{24}L_{18}]^{2-}$ superatoms and their fragments ($M = Ni, Pd$ and Pt ; $L =$ alkynyl)

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

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

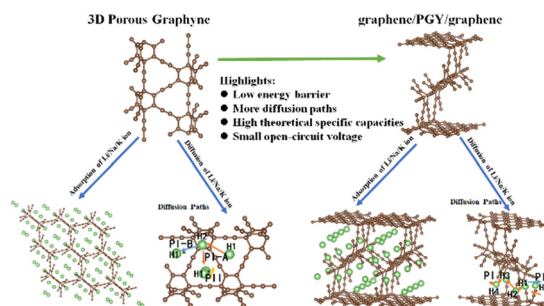
Peter L. Rodriguez-Kessler and Alvaro Muñoz-Castro*



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

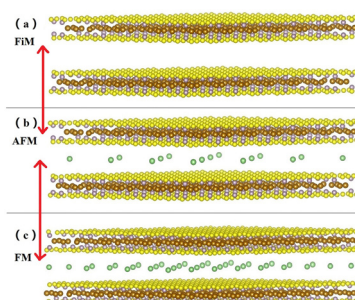
Haidong Liu, Xiaowei Li,* Haotian Chen, Jin Chen and Zixun Shi



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

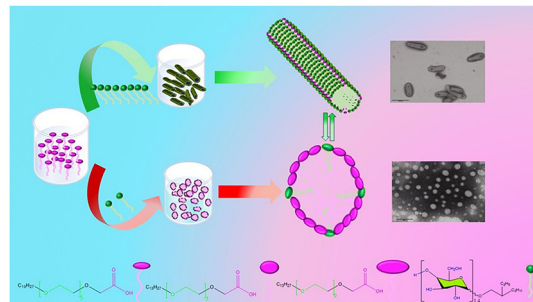
Dong Chen,* Chunlei Wang and Chengxiao Peng



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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

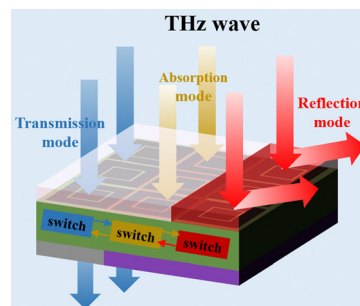
Yukai Wang, Zihui Zhang, Liang Bai,* Xiuquan Yang,* Yunqin Qi, Jiahao Li, Yuan Zhou, Zhiyu Wu and Ziyu Qin



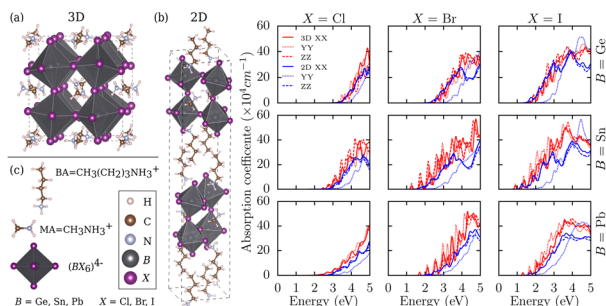
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Thermal controlled multi-functional metasurface for freely switching of absorption, reflection, and transmission

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



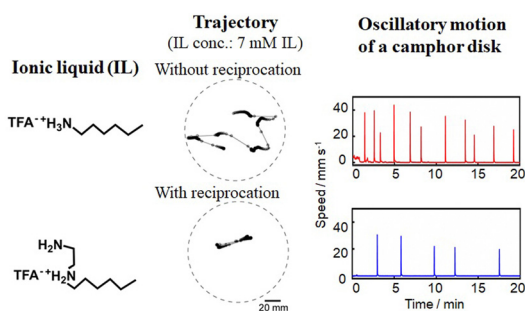
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Contrasting the stability, octahedral distortions, and optoelectronic properties of 3D MABX₃ and 2D (BA)₂(MA)B₂X₇ (B = Ge, Sn, Pb; X = Cl, Br, I) perovskites

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

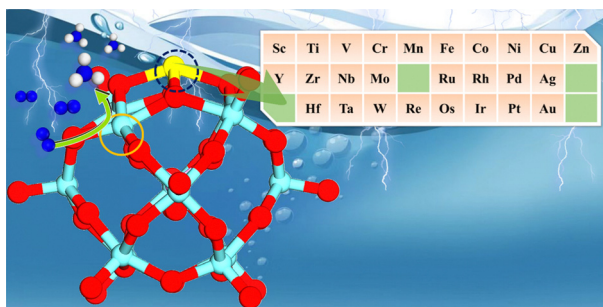
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Self-propelled motion controlled by ionic liquids

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

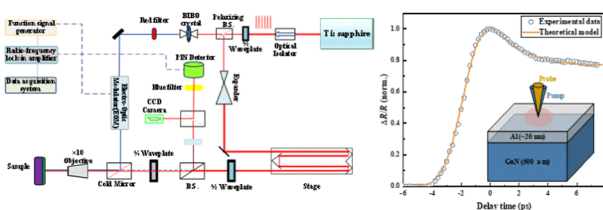
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Design of high performance nitrogen reduction electrocatalysts by doping defective polyoxometalate with a single atom promoter

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

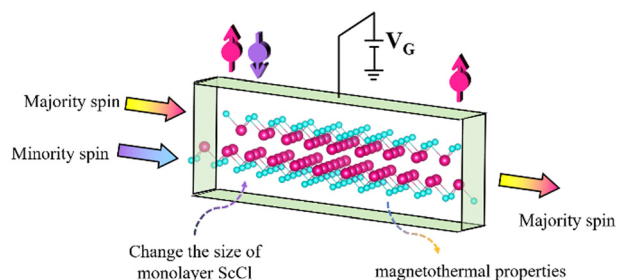


RESEARCH PAPERS

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Electronic structure and magnetothermal properties of two-dimensional ScCl

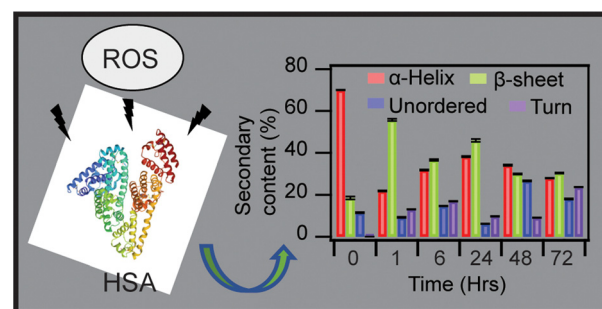
Hao-Jia Wu, Dan Wang, Hua-Yun Geng and Xiang-Rong Chen*



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Oxidative stress induced conformational changes of human serum albumin

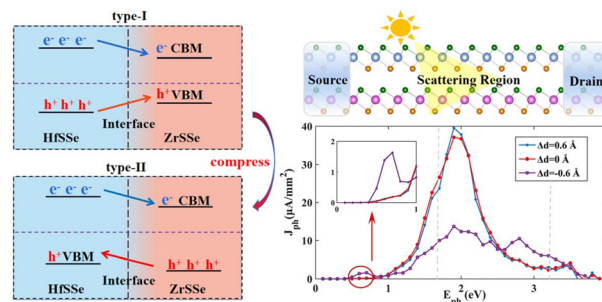
Debdip Brahma, Akshay Narayan Sarangi, Rupal Kaushik and Amar Nath Gupta*



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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*

