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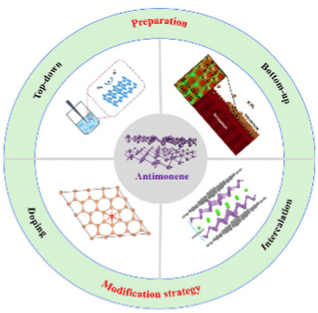
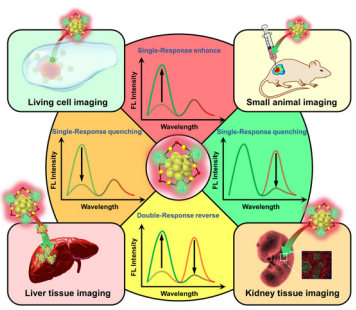
See Yujin Ji, Yang Song *et al.*, pp. 21860–21867. Image reproduced by permission of Rongfeng Guan, Pan Wang, Yujin Ji, Youyong Li and Yang Song from *Phys. Chem. Chem. Phys.*, 2023, **25**, 21860.

REVIEWS





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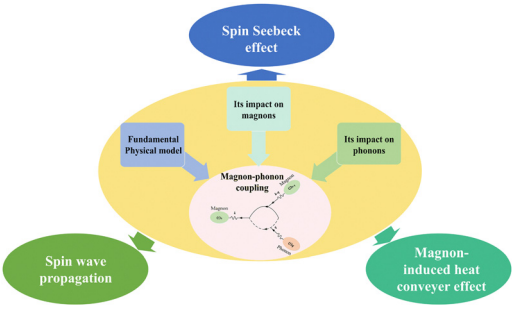

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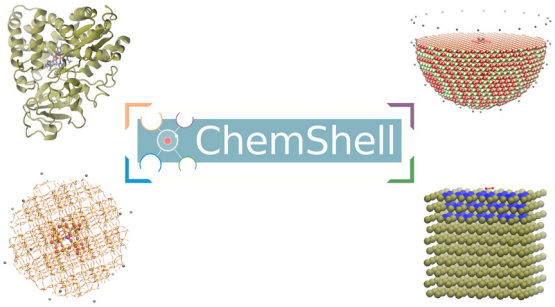

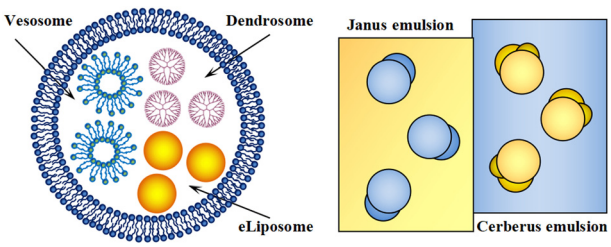

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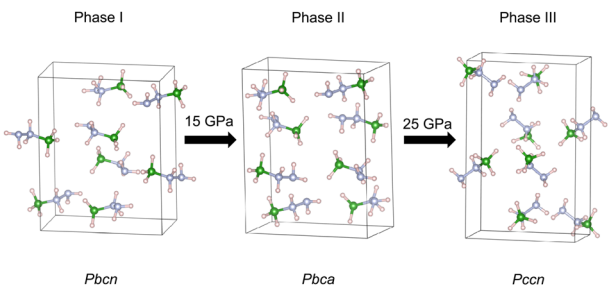

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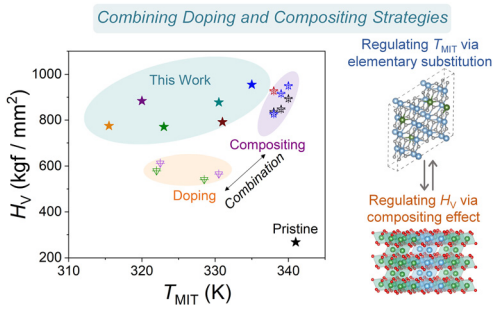
Manipulating the metal-to-insulator transitions of VO_2 by combining compositing and doping strategies

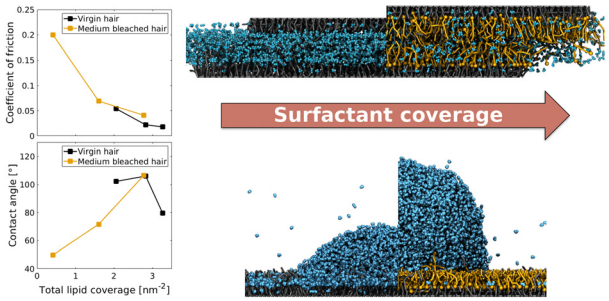
Xuanchi Zhou, Haifan Li, Yanlong Shang, Fanqi Meng, Ziang Li, Kangkang Meng, Yong Wu, Xiaoguang Xu, Yong Jiang,* Nuofu Chen* and Jikun Chen*



21916

Effects of surfactant adsorption on the wettability and friction of biomimetic surfaces

Erik Weiand,* Francisco Rodriguez-Ropero, Yuri Roiter, Peter H. Koenig, Stefano Angioletti-Uberti, Daniele Dini and James P. Ewen*



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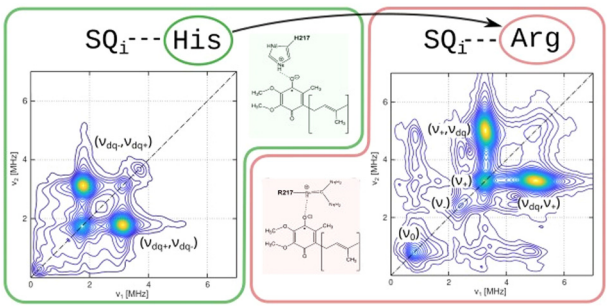
Probing molecular interactions of semiquinone radicals at quinone reduction sites of cytochrome bc_1 by X-band HYSCORE EPR spectroscopy and quantum mechanical calculations

Patryk Kuleta, Rafał Pietras, Justyna Andrys-Olek, Anna Wójcik-Augustyn and Artur Osyczka*



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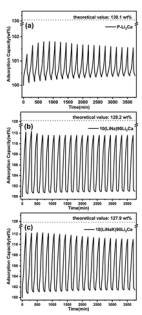
CO_2 capture by Li_2CaSiO_4 and enhancement with alkali carbonates

Zhen Wang, Chenteng Sun,* Qian Xu,* Xingli Zou, Hongwei Cheng and Xionggang Lu



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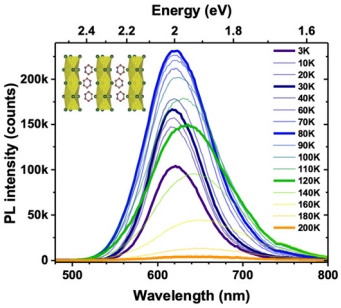

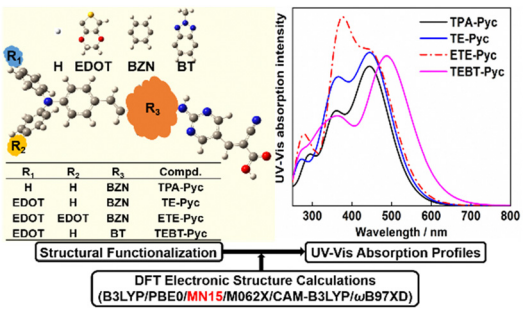

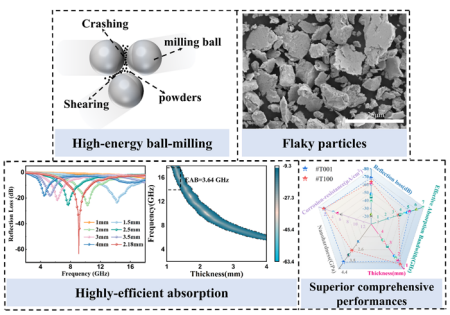

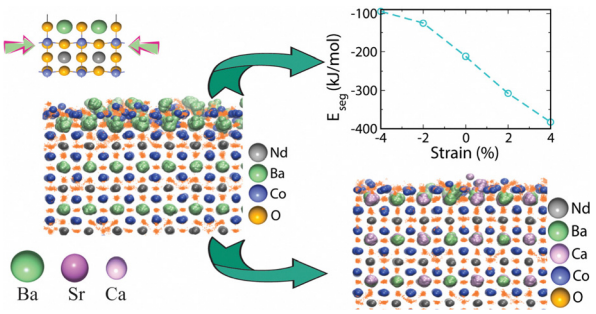

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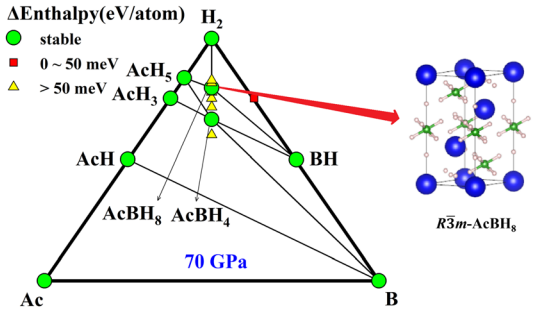

Pressure-induced superconductivity of Ac–B–H hydrides

Wen-Hua Li, Wen-Hua Yang* and Wen-Cai Lu*

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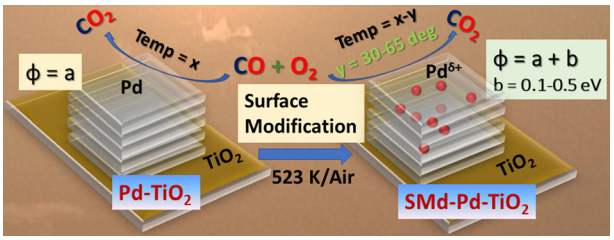

Possible handle for broadening the catalysis regime towards low temperatures: proof of concept and mechanistic studies with CO oxidation on surface modified Pd–TiO_2

Nitin B. Mhamane, Suresh Panchal, Sadhu K. Kolekar, Ravi Ranjan, Kranti N. Salgaonkar, Anand S. Burange, Naresh Nalajala, Suwarna Datar and Chinnakonda S. Gopinath*

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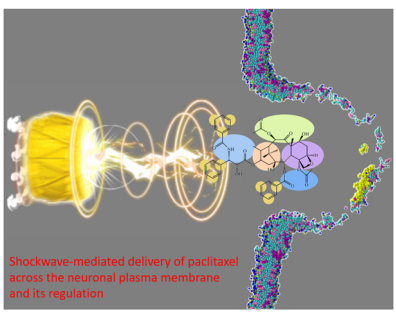

Molecular modelling of shockwave-mediated delivery of paclitaxel aggregates across the neuronal plasma membrane

Zhou Mi, Wenyu Zhou, Hong Yang, Luoxia Cao, Ming Li and Yang Zhou*

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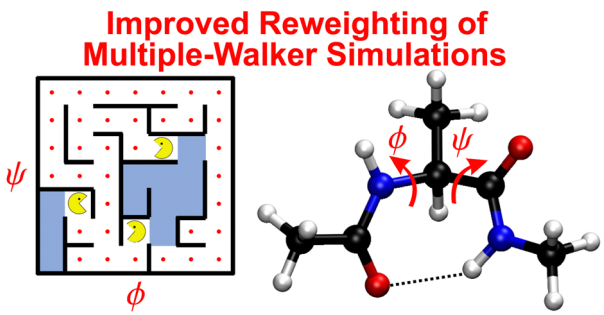

Improved reweighting protocols for variationally enhanced sampling simulations with multiple walkers

Baltzar Stevensson* and Mattias Edén*

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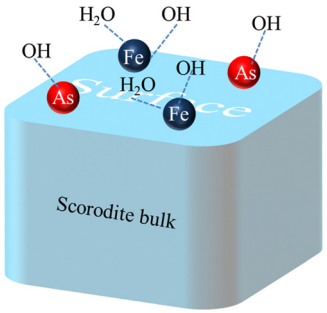

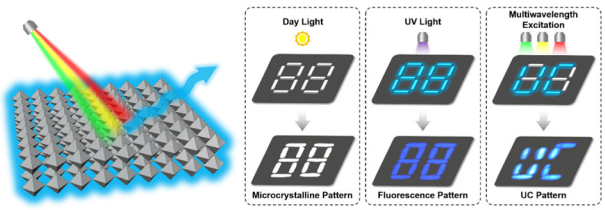

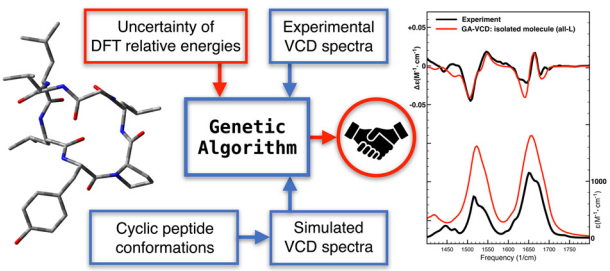

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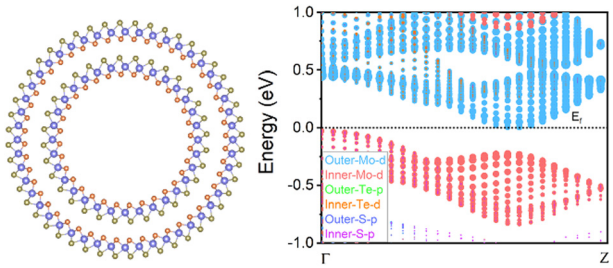

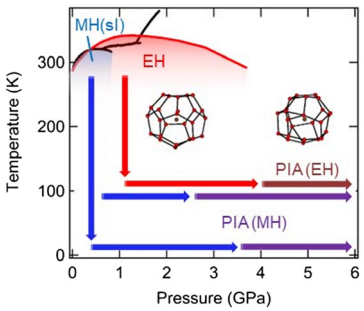

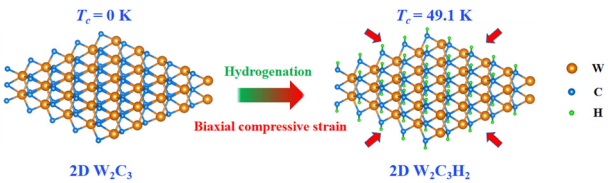

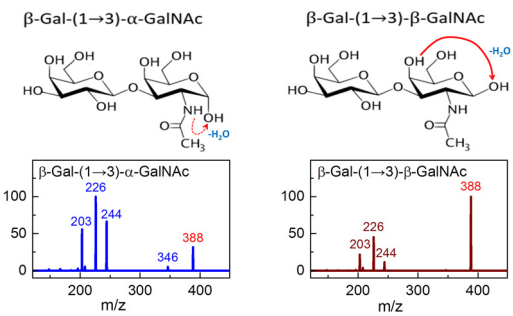

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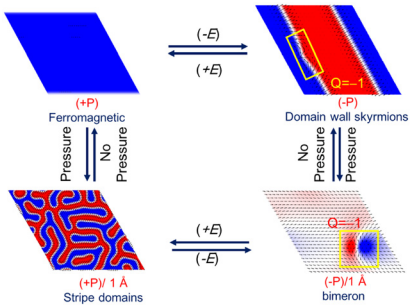

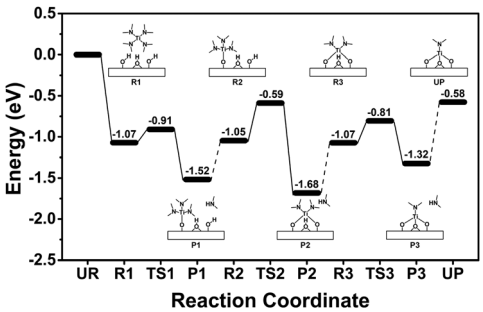

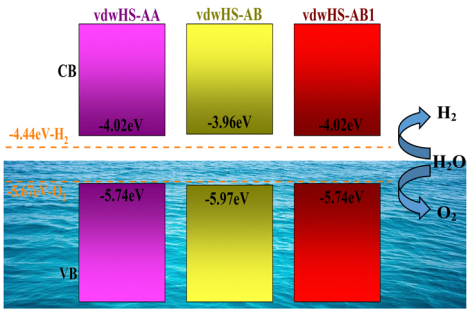

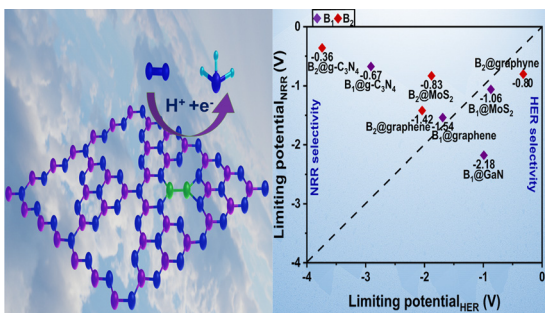

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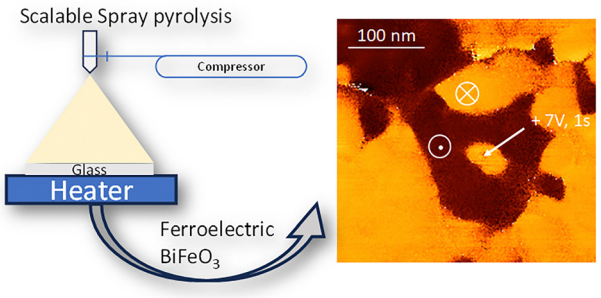

Spray pyrolysis-derived robust ferroelectric $BiFeO_3$ thin films

M. C. Nagashree, S. D. Kulkarni,* B. V. Rajendra,* J. Seidel, M. S. Murari and P. Sharma*

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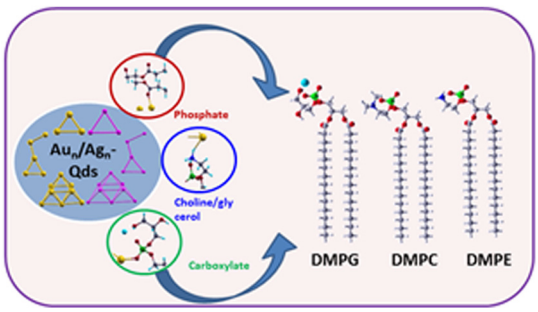

Quantum dot (Au_n/Ag_n, n = 3–8) capped single lipids: interactions and physicochemical properties

Asma H. Maneri, Shruti Suhas Varode, Ashakiran Maibam, Priyatosh Ranjan, Sailaja Krishnamurty* and Krati Joshi*

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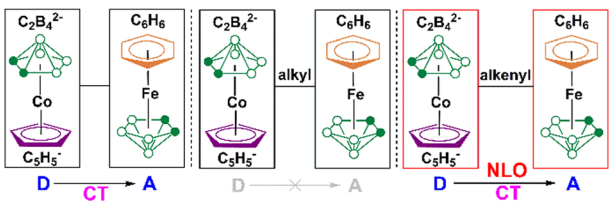

A theoretical exploration of the second-order NLO properties of linked sandwich double-layered metallacarboranes: charge transfer mediated by linker groups

Nana Ma,* Yajing Bian, Weiyi Cheng, Yameng Li, Qiongjin Wang and Shujun Li*

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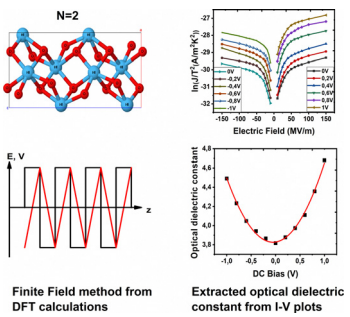

Dielectric response of high-κ hafnium oxide under finite electric field: nonlinearities from *ab initio* and experimental points of view

Othmen Khaldi,* Hanen Ferhi, Tarek Larbi, Fethi Jomni and Rached Ben Younes

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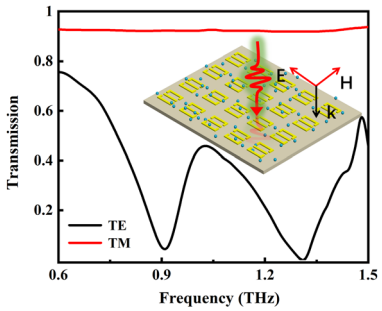

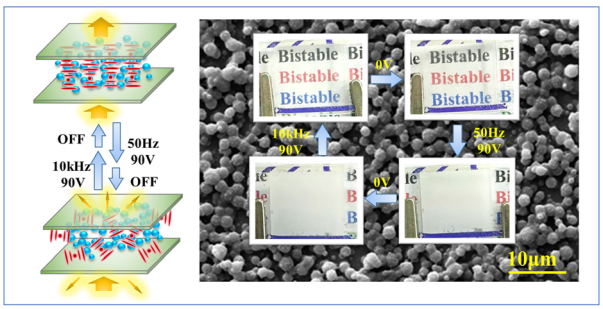

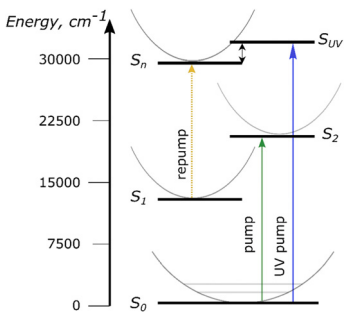

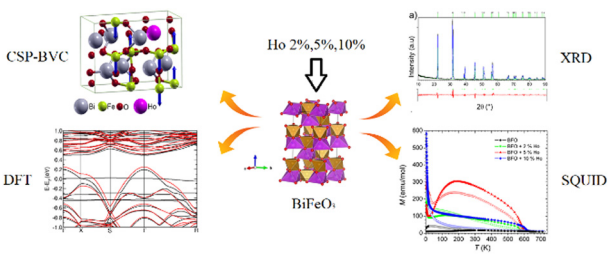

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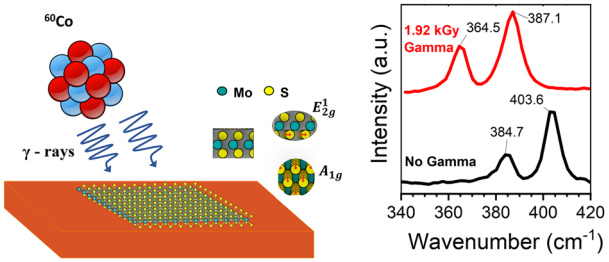

Effect of gamma irradiation on the physical properties of MoS_2 monolayer

Chintan P. Chavda, Ashok Srivastava, Erin Vaughan, Jianwei Wang, Manas Ranjan Gartia* and Georgios Veronis*

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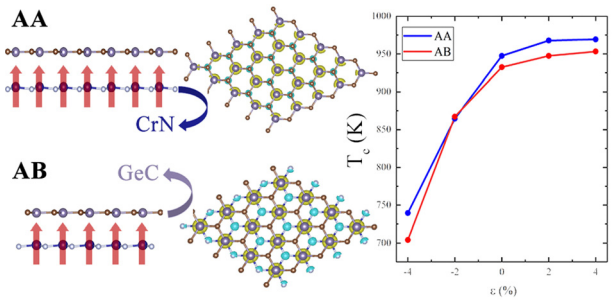

Robust ferromagnetism in two-dimensional GeC/CrN heterobilayers

Y. Ozguven, H. E. Guler, A. A. Billur, A. Mogulkoc* and M. Modarresi

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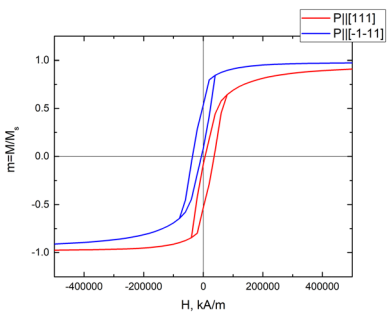

Electric field control of magnetic states in ferromagnetic–multiferroic nanostructures

Zukhra Gareeva,* Nikolai Shulga, Rurik Doroshenko and Anatoly Zvezdin*

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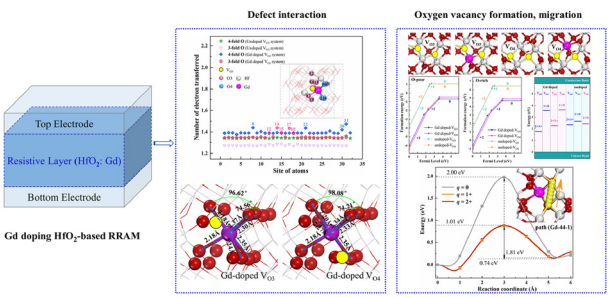

Modulating the resistive switching stability of HfO_2-based RRAM through Gd doping engineering: DFT+*U*

Dong-lan Zhang, Jiong Wang,* Qing Wu and Yong Du

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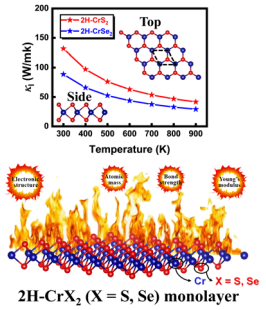
Enhancing phonon thermal transport in 2H-CrX_2 (X = S and Se) monolayers through robust bonding interactions

Shuwei Tang,* Da Wan, Shulin Bai, Shengkai Fu, Xinyu Wang, Xiaodong Li and Jingyi Zhang



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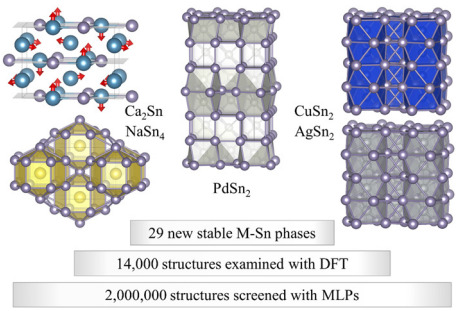
Machine learning search for stable binary Sn alloys with Na, Ca, Cu, Pd, and Ag

Aidan Thorn, Daviti Gochitashvili, Saba Kharabadze and Aleksey N. Kolmogorov*



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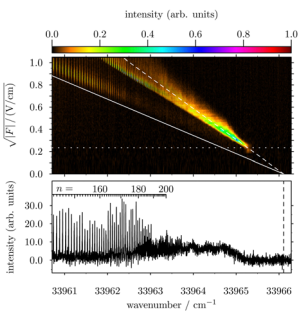
Pulsed-ramped-field-ionisation zero-kinetic-energy photoelectron spectroscopy of the metastable rare-gas atoms Ar, Kr and Xe

Holger Herburger, Vincent Wirth, Urs Hollenstein and Frédéric Merkt*



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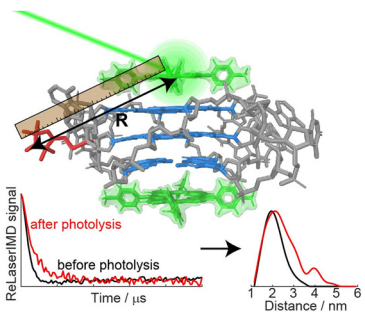
Revealing light-induced structural shifts in G-quadruplex-porphyrin complexes: a pulsed dipolar EPR study

Natalya E. Sannikova, Mikhail I. Kolokolov, Tamara A. Khlynova, Alexey S. Chubarov, Yuliya F. Polienko, Matvey V. Fedin* and Olesya A. Krumkacheva*



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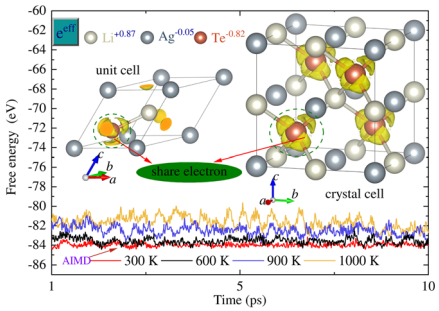

Correlation of rattlers with thermal transport and thermoelectric performance

Aixian She, Yinchang Zhao,* Jun Ni, Sheng Meng and Zhenhong Dai*

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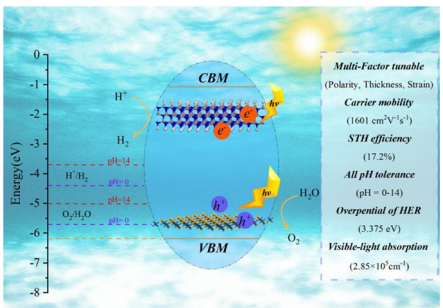
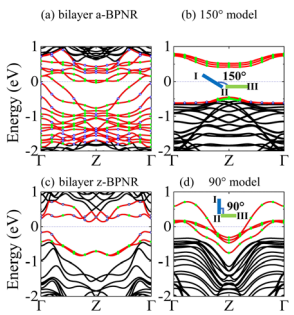


A multi-factor adjustable $PtSe_2$/GaN van der Waals heterostructure with enhanced photocatalytic performance

Qihao Zhang, Hua Zhu, Xiaodong Yang, Liang Chen and Yang Shen*

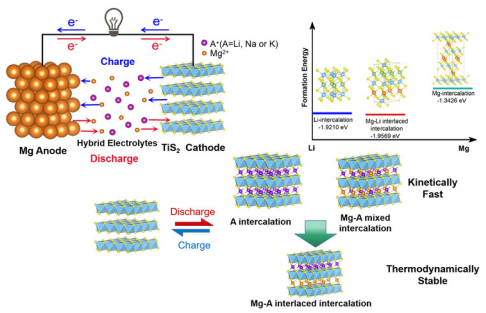
22487



Electronic structures, transport properties, and optical absorption of bilayer blue phosphorene nanoribbons

L. J. Gong, H. L. Shi, J. Yang,* Q. Z. Han,* Y. H. Ren, S. Y. He, Y. H. Zhao and Z. T. Jiang*

22497



Thermodynamics and kinetics of Mg^{2+}/Li^{+} and Mg^{2+}/Na^{+} co-intercalation into layered titanium disulfide

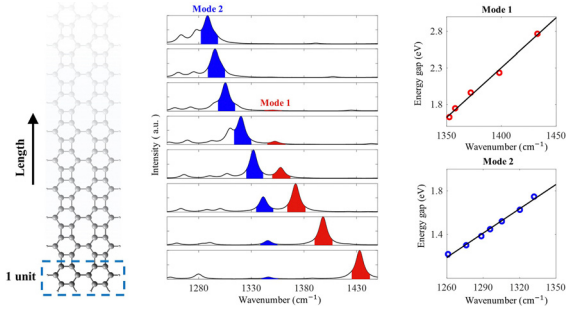
Yudi Tang, Donggang Tao, Yuliang Cao and Fei Xu*

RESEARCH PAPERS

22505

Localized vibrational characteristics of biphenylene strips resulting in length-dependent Raman spectra

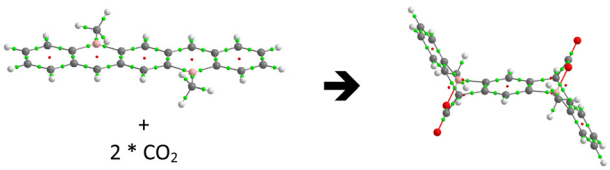
Yirui Lu, Lei Yan,* Sichen Huang, Xilin Zhou, Min Zhang, Ruhai Du and Zhenglong Zhang*



22512

A theoretical study of the reaction of borata derivatives of benzene, anthracene and pentacene with CO_2

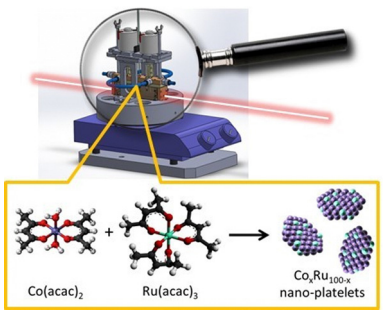
Maxime Ferrer, Ibon Alkorta,* José Elguero and Josep M. Oliva-Enrich



22523

Mechanism of formation of Co–Ru nanoalloys: the key role of Ru in the reduction pathway of Co

Brandon Azeredo, Tayssir Ben Ghzaiel, Ning Huang, Sophie Nowak, Jennifer Peron, Marion Giraud, Jeyadevan Balachandran, Olivier Taché, Laurent Barthe, Jean-Yves Piquemal,* Valérie Briois and Lorette Sicard*



CORRECTIONS

22535

Correction: Benchmark and performance of long-range corrected time-dependent density functional tight binding (LC-TD-DFTB) on rhodopsins and light-harvesting complexes

Beatrix M. Bold, Monja Sokolov, Sayan Maity, Marius Wanko, Philipp M. Dohmen, Julian J. Kranz, Ulrich Kleinekathöfer, Sebastian Höfener and Marcus Elstner*

CORRECTIONS

22538

Correction: Photoelectron angular distributions as sensitive probes of surfactant layer structure at the liquid–vapor interface

Rémi Dupuy, Jakob Filser, Clemens Richter, Robert Seidel, Florian Trinter, Tillmann Buttersack, Christophe Nicolas, John Bozek, Uwe Hergenhahn, Harald Oberhofer, Bernd Winter, Karsten Reuter* and Hendrik Bluhm*