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Inside cover

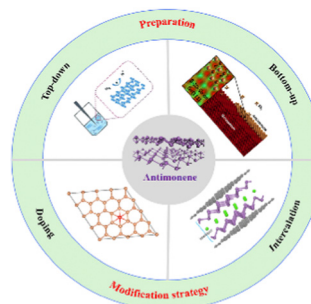
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REVIEWS

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Advances in the synthesis and modification of two-dimensional antimonene

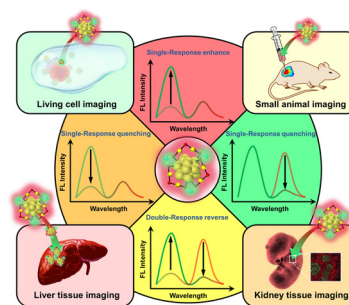
Yanjie Cheng, Zhe Li, Ye Liu, Yunhui Shi* and Mengya Zhu*



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Gold nanocluster-based fluorescent sensors for *in vitro* and *in vivo* ratiometric imaging of biomolecules

S. Santhoshkumar, Manivannan Madhu, Wei-Bin Tseng* and Wei-Lung Tseng*



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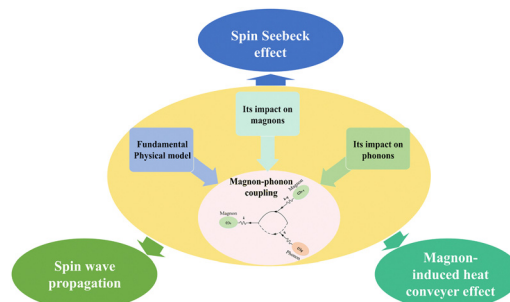


REVIEWS

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Magnon–phonon coupling: from fundamental physics to applications

Ke Wang, Kai Ren, Yinlong Hou, Yuan Cheng* and Gang Zhang*

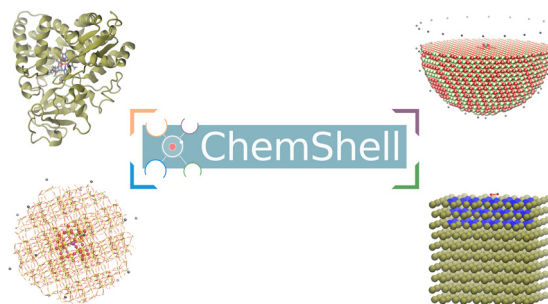


PERSPECTIVES

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Multiscale QM/MM modelling of catalytic systems with ChemShell

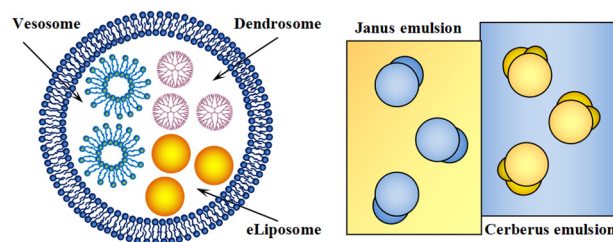
You Lu, Kakali Sen, Chin Yong, David S. D. Gunn, John A. Purton, Jingcheng Guan, Alec Desmoutier, Jamal Abdul Nasir, Xingfan Zhang, Lei Zhu, Qing Hou, Joe Jackson-Masters, Sam Watts, Rowan Hanson, Harry N. Thomas, Omal Jayawardena, Andrew J. Logsdail, Scott M. Woodley, Hans M. Senn, Paul Sherwood, C. Richard A. Catlow, Alexey A. Sokol and Thomas W. Keal*



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Multicompartment colloid systems with lipid and polymer membranes for biomedical applications

Marina Koroleva

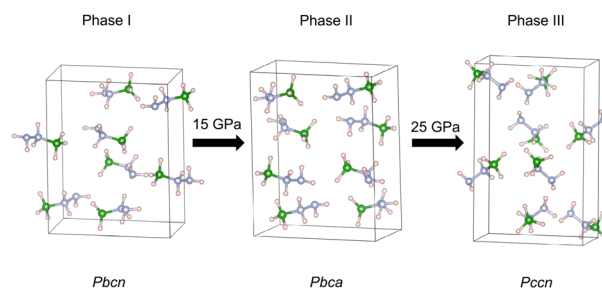


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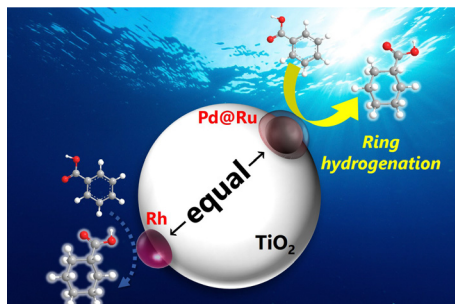
Structural stability, dihydrogen bonding, and pressure-induced polymorphic transformations in hydrazine borane

Rongfeng Guan, Pan Wang, Yujin Ji,* Youyong Li and Yang Song*



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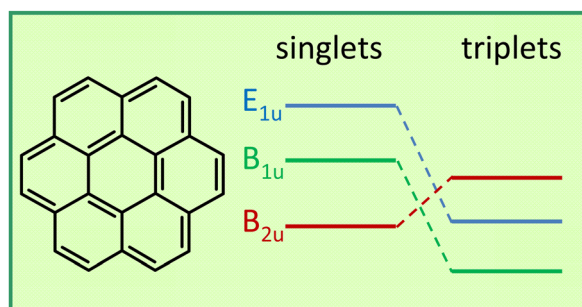
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Ruthenium and palladium bimetallic nanoparticles achieving functional parity with a rhodium cocatalyst for TiO_2 -photocatalyzed ring hydrogenation of benzoic acid

Kousuke Nakanishi, Sakae Araki, Kousuke Nomoto, Yuichi Onoue, Ryosuke Yagi, Hiroyuki Asakura, Atsuhiko Tanaka, Tsunehiro Tanaka and Hiroshi Kominami*

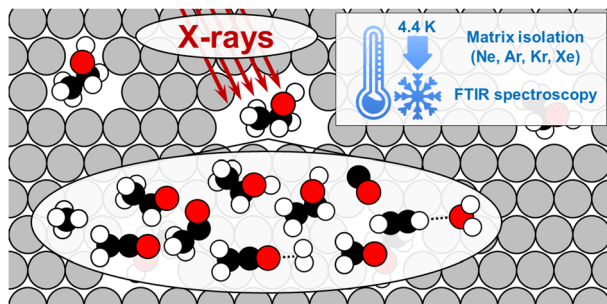
21875



Excited-state singlet–triplet inversion in hexagonal aromatic and heteroaromatic compounds

Andrzej L. Sobolewski* and Wolfgang Domcke*

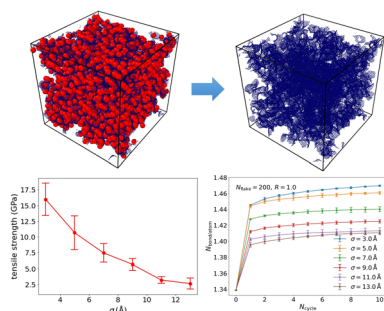
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Radiation-induced transformations of matrix-isolated ethanol molecules at cryogenic temperatures: an FTIR study

Pavel V. Zasimov, Elizaveta V. Sanochkina, Daniil A. Tyurin and Vladimir I. Feldman*

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Investigation of mechanical properties and structural integrity of graphene aerogels via molecular dynamics simulations

Bowen Zheng, Chen Liu, Zhou Li, Carlo Carraro, Roya Maboudian, Debbie G. Senesky and Grace X. Gu*

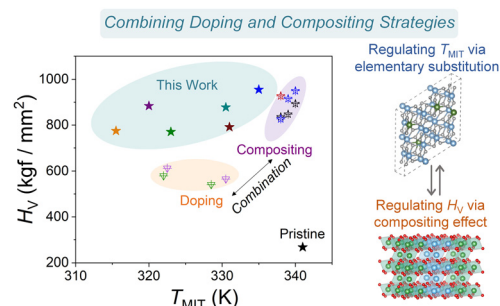


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Manipulating the metal-to-insulator transitions of VO₂ by combining compositing and doping strategies

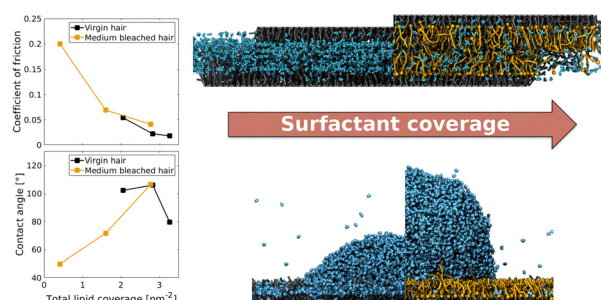
Xuanchi Zhou, Haifan Li, Yanlong Shang, Fanqi Meng, Ziang Li, Kangkang Meng, Yong Wu, Xiaoguang Xu, Yong Jiang,* Nuofu Chen* and Jikun Chen*



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

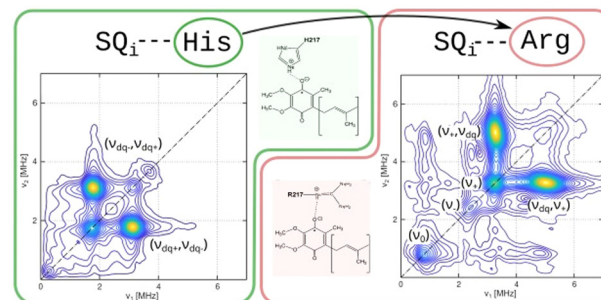
Erik Weiland,* Francisco Rodriguez-Ropero, Yuri Roiter, Peter H. Koenig, Stefano Angioletti-Uberti, Daniele Dini and James P. Ewen*



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Probing molecular interactions of semiquinone radicals at quinone reduction sites of cytochrome bc₁ by X-band HYSCORE EPR spectroscopy and quantum mechanical calculations

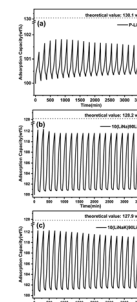
Patryk Kuleta, Rafał Pietras, Justyna Andrys-Olek, Anna Wójcik-Augustyn and Artur Osyczka*



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CO₂ capture by Li₂CaSiO₄ and enhancement with alkali carbonates

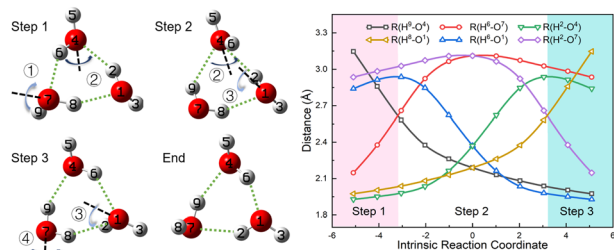
Zhen Wang, Chenteng Sun,* Qian Xu,* Xingli Zou, Hongwei Cheng and Xionggang Lu



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Sequential Flipping: a New Donor-Acceptor Exchange Mechanism

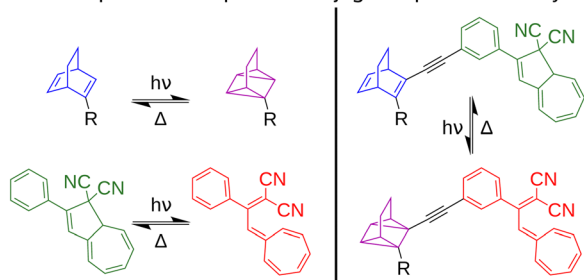


Sequential flipping: the donor–acceptor exchange mechanism in water trimers

Xinrui Yang, Rui Liu, Ruiqi Xu and Zhigang Wang*

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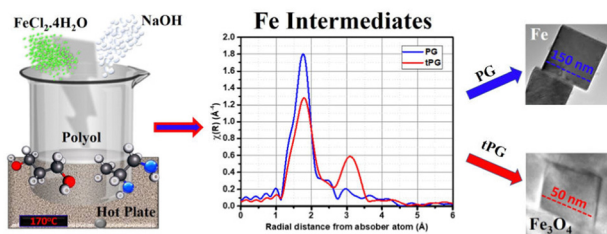
Individual photoswitch pairs vs conjugated photoswitch dyads



Computational investigation of photoswitch conjugates for molecular solar energy storage

Jacob Lyng Elholm, Zacharias Liasi, Marie Kathrine Mikkelsen, Andreas Erbs Hillers-Bendtsen and Kurt V. Mikkelsen*

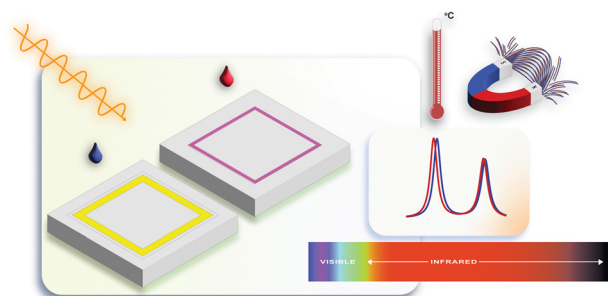
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New insights into pertinent Fe-complexes for the synthesis of iron via the instant polyol process

Sivaranjani Kottaipalayam Somasundaram, Ana Guilherme Buzanich, Franziska Emmerling,* Sangameswaran Krishnan, Kittusamy Senthilkumar and Raphael Justin Joseyphus*

21981



A dual functional asymmetric plasmonic silver nanostructure for temperature and magnetic field sensing

Simitha S, Devika Mohan, Shinto M Francis, Ajith Ramachandran, Jesly Jacob* and Vibin Ipe Thomas*

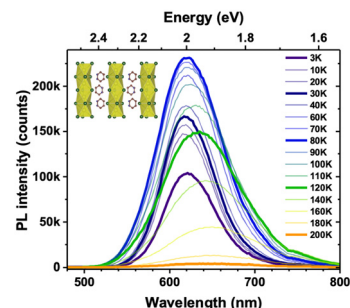


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Temperature dependence of radiative and non-radiative decay in the luminescence of one-dimensional pyridinium lead halide hybrids

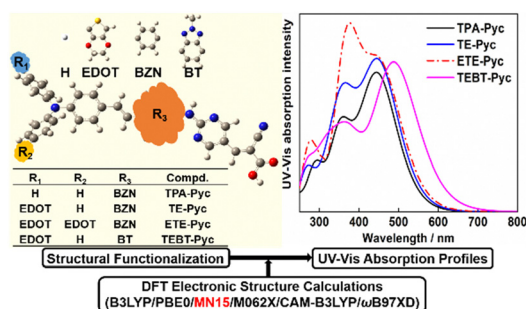
Abdulrahman M. Alfaraidi, Jonas Schaab, Eric T. McClure, Michael Kellogg, Taylor L. Hodgkins, Muazzam Idris, Stephen E. Bradforth, Brent C. Melot,* Mark E. Thompson* and Peter I. Djurovich*



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Theoretical investigation on the functional group modulation of UV-Vis absorption profiles of triphenylamine derivatives

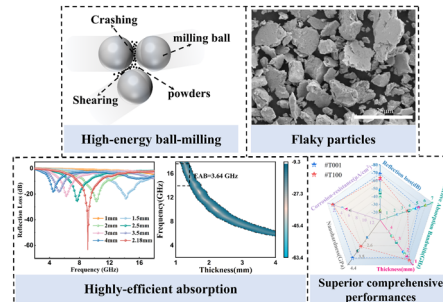
Kun Gong, Fang Xu, Zhen Zhao, Wei Li, Dongzhi Liu, Xueqin Zhou* and Lichang Wang*



22011

Multifunctional amorphous FeCoNiTi_xSi high-entropy alloys with excellent electromagnetic-wave absorption performances

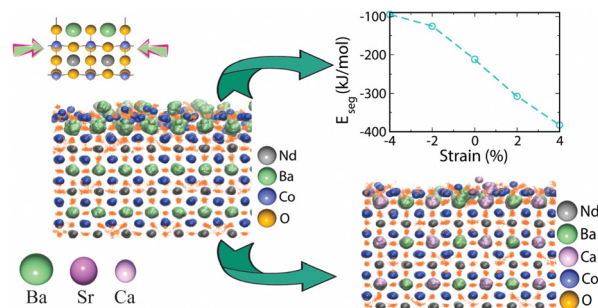
Lei Jia, Linwen Jiang,* Haoran Zhou, Siqin Yan, Anhua Wu and Xiaofeng Zhang*



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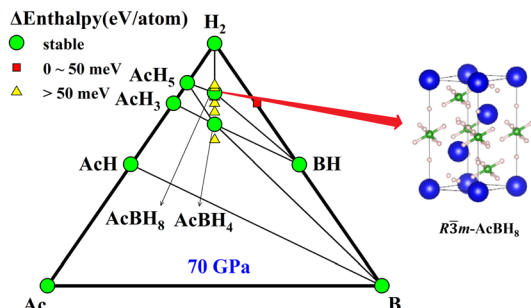
Controlling surface cation segregation in a double perovskite for oxygen anion transport in high temperature energy conversion devices

Jyotsana Kala, Uzma Anjum, B. K. Mani* and M. Ali Haider*



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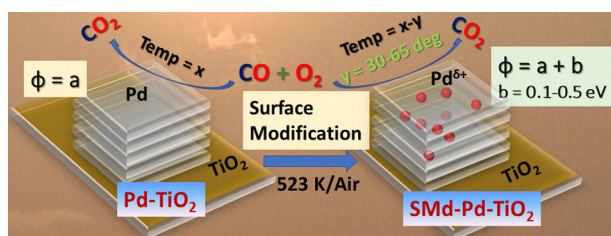
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Pressure-induced superconductivity of Ac–B–H hydrides

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

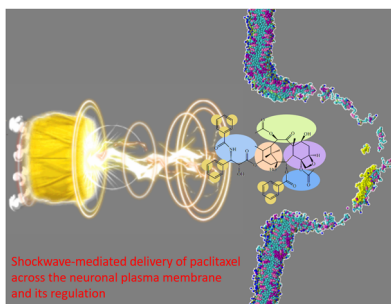
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Possible handle for broadening the catalysis regime towards low temperatures: proof of concept and mechanistic studies with CO oxidation on surface modified Pd–TiO₂

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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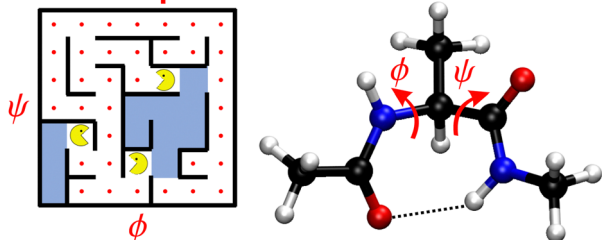


Molecular modelling of shockwave-mediated delivery of paclitaxel aggregates across the neuronal plasma membrane

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

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Improved Reweighting of Multiple-Walker Simulations



Improved reweighting protocols for variationally enhanced sampling simulations with multiple walkers

Baltzar Stevansson* and Mattias Edén*

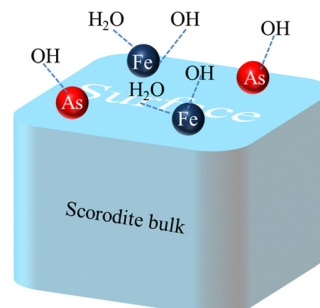


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First principles study of structural and electron properties in scorodite: the bulk and surface

Manjiao Chen,* Xinjun Hu, Xinjun Zhou, Jianping Tian, Xinqiang Yi and Xiulan Li



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The first HyDRA challenge for computational vibrational spectroscopy

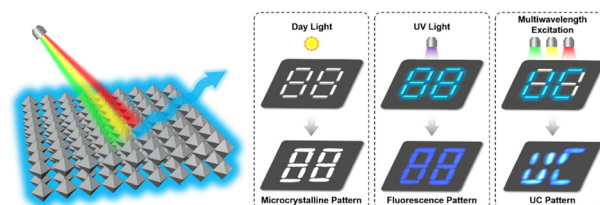
Taija L. Fischer, Margarethe Bödecker, Sophie M. Schweer, Jennifer Dupont, Valéria Lepère, Anne Zehnacker-Rentien, Martin A. Suhm, Benjamin Schröder, Tobias Henkes, Diego M. Andrada, Roman M. Balabin, Haobam Kisan Singh, Himangshu Pratim Bhattacharyya, Manabendra Sarma, Silvan Käser, Kai Töpfer, Luis I. Vazquez-Salazar, Eric D. Boittier, Markus Meuwly, Giacomo Mandelli, Cecilia Lanzi, Riccardo Conte, Michele Ceotto, Fabian Dietrich, Vicente Cisternas, Ramachandran Gnanasekaran, Michael Hippler, Mahmoud Jarraya, Majdi Hochlaf, Narasimhan Viswanathan, Thomas Nevolianis, Gabriel Rath, Wassja A. Kopp, Kai Leonhard and Ricardo A. Mata*



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Multi-wavelength excited triplet–triplet upconversion microcrystals based on hot-band excitation for optical information encryption

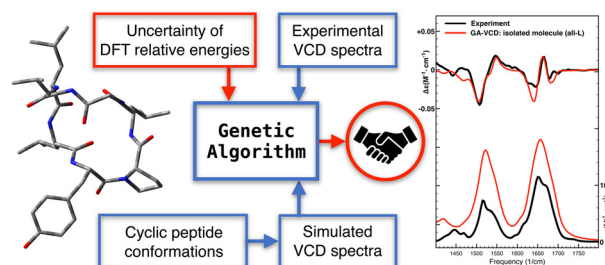
Xiaofen Gu, Shuoran Chen,* Zuoqin Liang, Xiaolei Ju, Lin Li, Xiaomei Wang and Changqing Ye*



22111

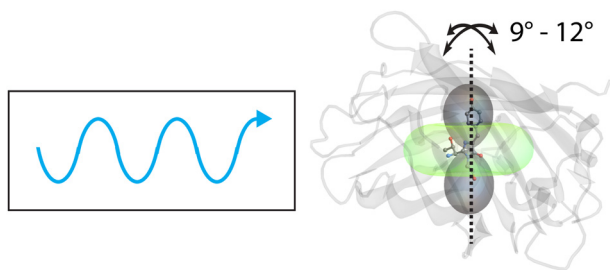
Simplified and enhanced VCD analysis of cyclic peptides guided by artificial intelligence

João M. Batista Jr.* and Valentin Paul Nicu*



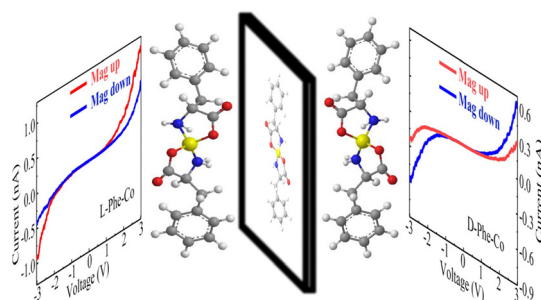
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**Dynamics of transition dipole moment orientation in representative fluorescent proteins**

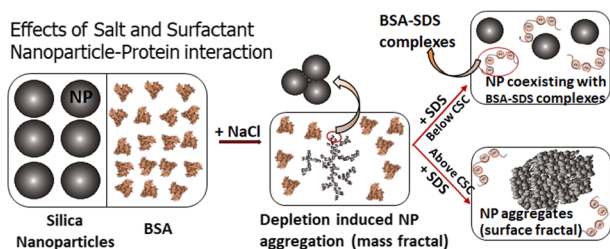
Petro Khoroshyy, Hector Martinez-Seara, Jitka Myšková and Josef Lazar*

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**Spin-induced electron transmission through metal–organic chiral crystals**

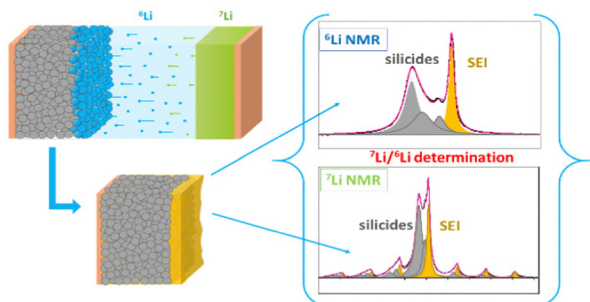
Tapan Kumar Das, Amit Kumar Mondal, Om Shanker Tiwari, Pandeewar Makam, Gregory Leitus, Ehud Gazit, Fontanesi Claudio and Ron Naaman*

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**Competitive effects of salt and surfactant on the structure of nanoparticles in a binary system of nanoparticle and protein**

Debasish Saha, Sugam Kumar,* Jitendra P. Mata, Andrew E. Whitten and Vinod K. Aswal*

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**Lithium isotope tracing in silicon-based electrodes using solid-state MAS NMR: a powerful comprehensive tool for the characterization of lithium batteries**

Manon Berthault, Anton Buzlukov,* Lionel Dubois, Pierre-Alain Bayle, Willy Porcher, Thibaut Gutel, Eric De Vito and Michel Bardet*

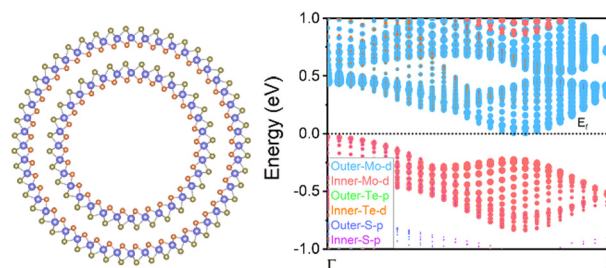


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Structural and electronic properties of double wall MoS₂ nanotubes

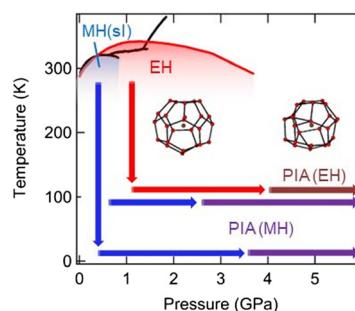
Zhenyun Lan,* Theresa Isabelle Manguerra Kapunan, Tejs Vegge and Ivano E. Castelli*



22161

Direct observation of pressure-induced amorphization of methane/ethane hydrates using Raman and infrared spectroscopy

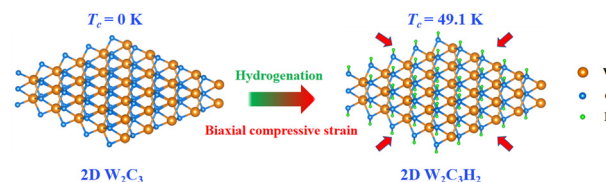
Naoki Noguchi,* Yui Shiraishi, Maho Kageyama, Yuu Yokoi, Saki Kurohama, Natsuki Okada and Hidekazu Okamura



22171

Hydrogenation induced high-temperature superconductivity in two-dimensional W₂C₃

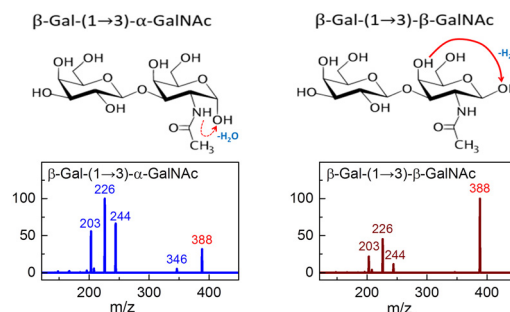
Hao Wang, Xin-Zhu Yin, Yang Liu, Ya-Ping Li, Mei-Yan Ni, Na Jiao,* Hong-Yan Lu* and Ping Zhang*

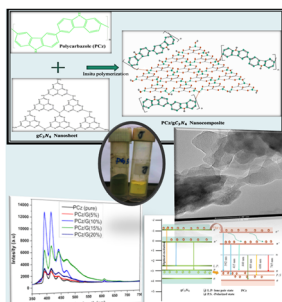


22179

The collision-induced dissociation mechanism of sodiated Hex–HexNAc disaccharides

Hock-Seng Nguan, Shang-Ting Tsai, Chia Yen Liew, N. Sivakumar Reddy, Shang-Cheng Hung and Chi-Kung Ni*





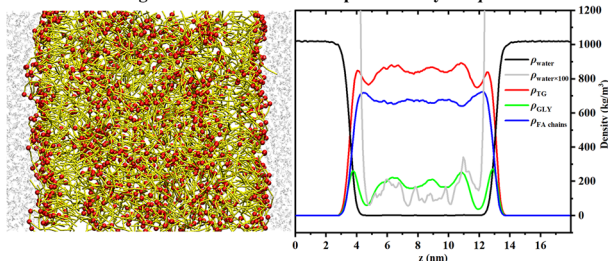
Jayanta Bauri and Ram Bilash Choudhary*

Diagram illustrating the Freedom of Design in machine learning for materials science. The diagram shows two molecular structures with their corresponding energy levels (E_L and E_H) and HOMOs. A central box labeled "Freedom of Design" is connected to a graph of "functional groups" and "atom types" via a dashed line labeled "no correlation" and " α ". The graph also shows "#atoms".

Szabolcs Góger, Leonardo Medrano Sandonas,
Carolin Müller and Alexandre Tkatchenko*

Balachandar Vijayakumar, Masanobu Takatsuka,
Kaito Sasaki, Rio Kita, Naoki Shinyashiki,* Shin Yagihara
and Sampathkumar Rathnasabapathy*

Percolating network of TG in water predicted by CG *p*-OMFF



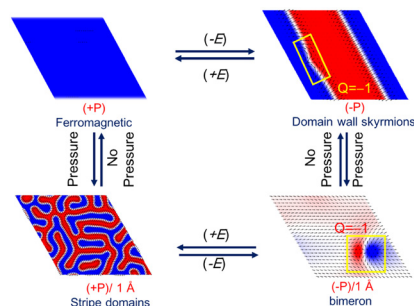
Ming Ma, Junjie Song, Yi Dong, Weihai Fang and
Lianghui Gao*

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22244

Manipulating two-dimensional magnetic states via electric field and pressure

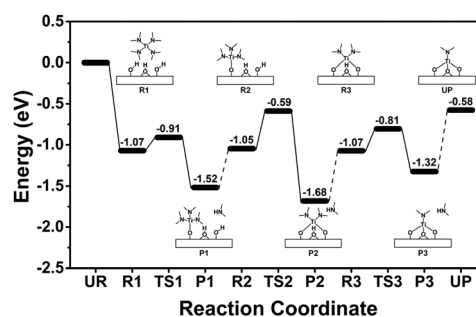
Hengxing Bao, Hao Tian,* Xu Li, Xingyue Ma, Changsong Xu, Yurong Yang* and Di Wu*



22250

A theoretical study on the surface reaction of tetrakis(dimethylamino)titanium on titanium oxide

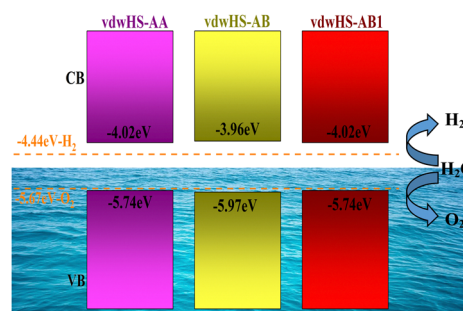
Hye-Lee Kim, Romel Hidayat, Khabib Khumaini and Won-Jun Lee*



22258

Enhanced photocatalytic performance of a stable type-II PtSe₂/GaSe van der Waals heterostructure

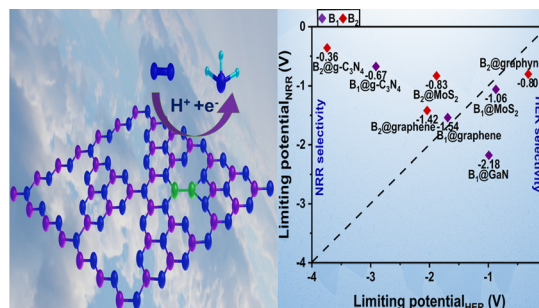
P. R. Parmar, S. J. Khengar, Yogesh Sonvane* and P. B. Thakor



22275

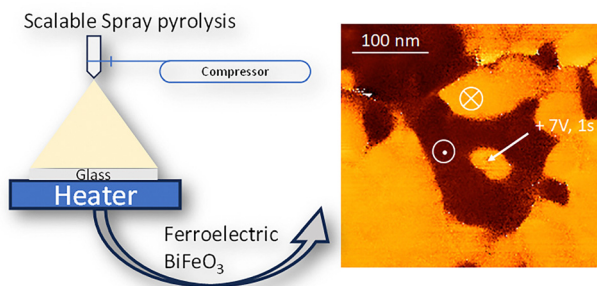
Optimizing the NRR activity of single and double boron atom catalysts using a suitable support: a first principles investigation

Anjumun Rasool, Insha Anis, Sajad Ahmad Bhat and Manzoor Ahmad Dar*



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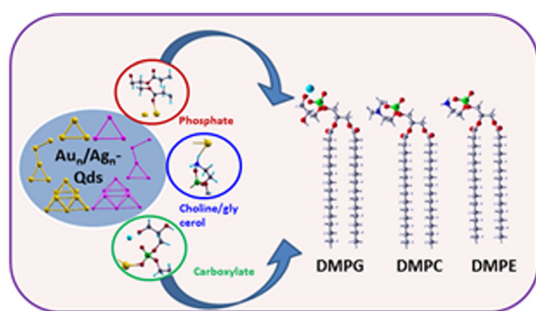
22286



Spray pyrolysis-derived robust ferroelectric BiFeO₃ thin films

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

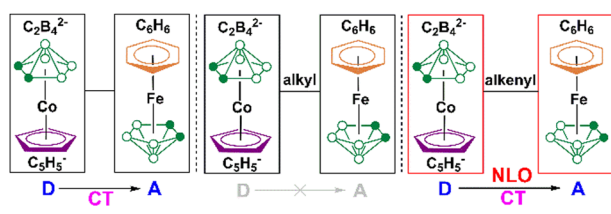
22294



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 Krishnamurthy* and Krati Joshi*

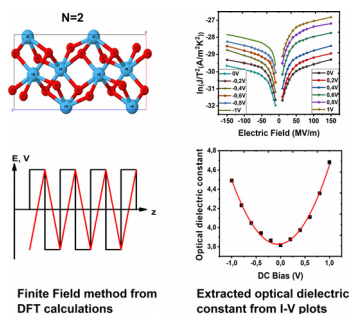
22304



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*

22310



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

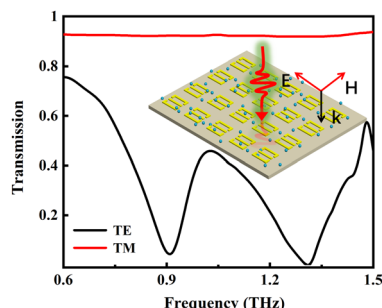


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22319

The bound state in the continuum in flexible terahertz metasurfaces enabled sensitive biosensing

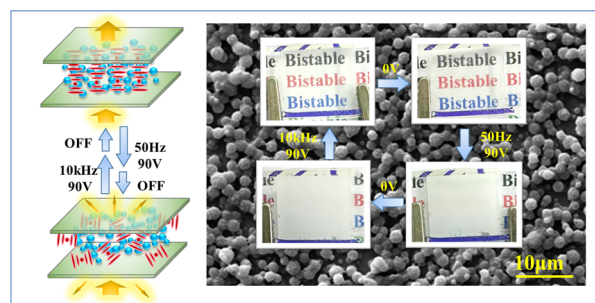
Dan Qiu, Shuai Sun,* Xuelan Cheng, Xiaoyu Jin, Yutong Qiao, Wei Zhang, Dexing Yang,* Xianzhong Chen, Zeren Li, Jia Li* and Jianquan Yao



22325

A bistable cholesteric liquid crystal film stabilized by a liquid-crystalline epoxy/thiol compound-based polymer

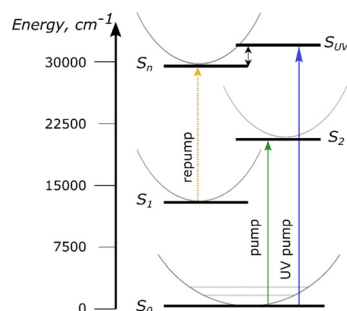
Huimin Zhang, Fei Li, Junqin Li, Zemin He, Jianjing Gao, Lifan Wen, Yuzhen Zhao and Zongcheng Miao*



22336

Relaxation dynamics of high-energy excited states of carotenoids studied by UV excitation and pump–repump–probe transient absorption spectroscopy

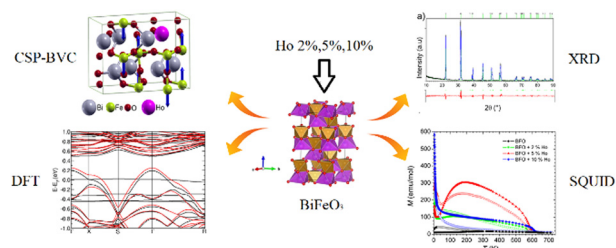
Valentyna Kuznetsova,* Marcel Fuciman and Tomáš Polívka



22345

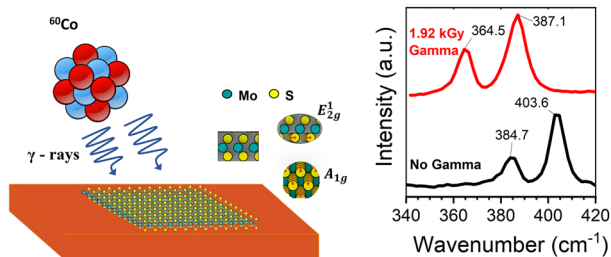
Enhancement of weak ferromagnetism, exotic structure prediction and diverse electronic properties in holmium substituted multiferroic bismuth ferrite

Maria Čebela,* Dejan Zagorac,* Igor Popov,* Filip Torić, Teodoro Klaser, Željko Skoko and Damir Pajić*



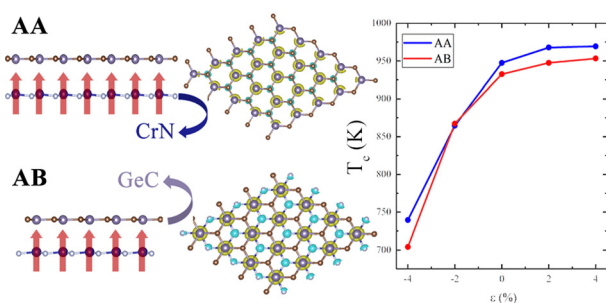
RESEARCH PAPERS

22359

Effect of gamma irradiation on the physical properties of MoS₂ monolayer

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

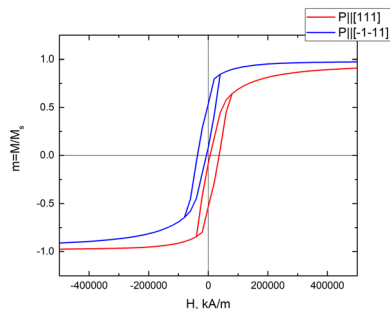
22370



Robust ferromagnetism in two-dimensional GeC/CrN heterobilayers

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

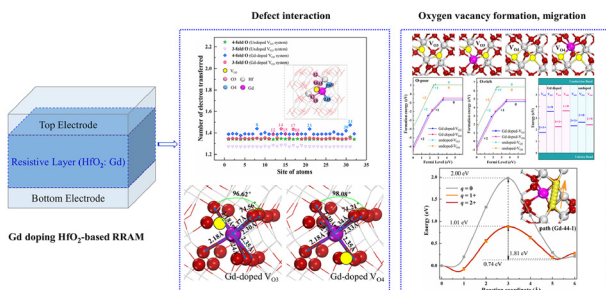
22380



Electric field control of magnetic states in ferromagnetic–multiferroic nanostructures

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

22388

Modulating the resistive switching stability of HfO₂-based RRAM through Gd doping engineering: DFT+U

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

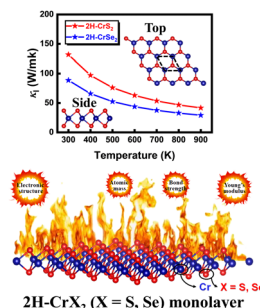


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22401

Enhancing phonon thermal transport in 2H-CrX₂ (X = S and Se) monolayers through robust bonding interactions

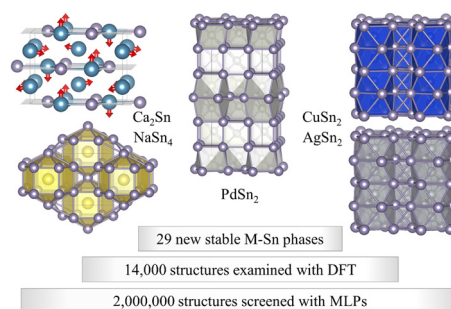
Shuwei Tang,* Da Wan, Shulin Bai, Shengkai Fu, Xinyu Wang, Xiaodong Li and Jingyi Zhang



22415

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

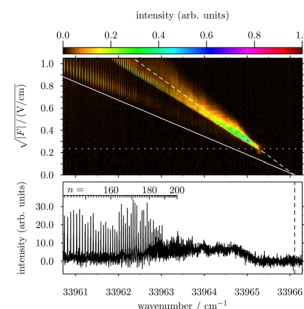
Aidan Thorn, Daviti Gochitashvili, Saba Kharabadze and Aleksey N. Kolmogorov*



22437

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

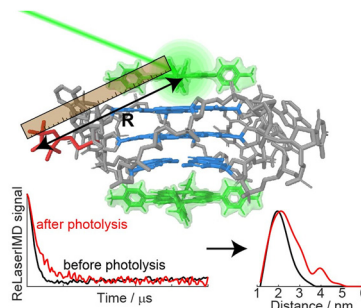
Holger Herburger, Vincent Wirth, Urs Hollenstein and Frédéric Merkt*



22455

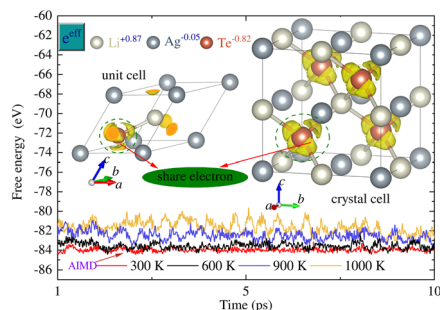
Revealing light-induced structural shifts in G-quadruplex-porphyrin complexes: a pulsed dipolar EPR study

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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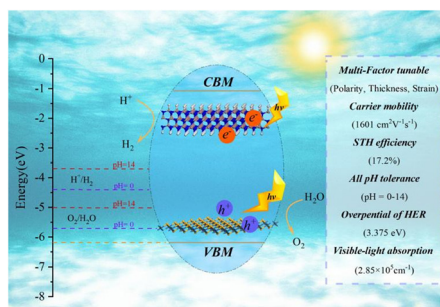
22467



Correlation of rattlers with thermal transport and thermoelectric performance

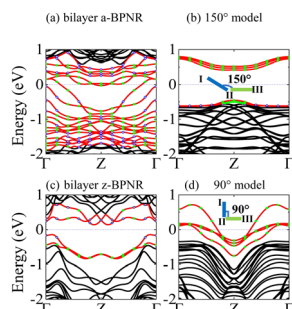
Aixian She, Yinchang Zhao,* Jun Ni, Sheng Meng and Zhenhong Dai*

22477

A multi-factor adjustable PtSe₂/GaN van der Waals heterostructure with enhanced photocatalytic performance

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

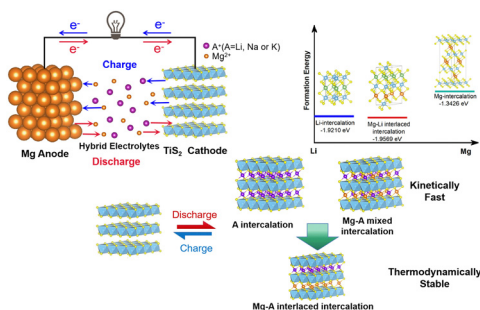
22487



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 Mg²⁺/Li⁺ and Mg²⁺/Na⁺ co-intercalation into layered titanium disulfide

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

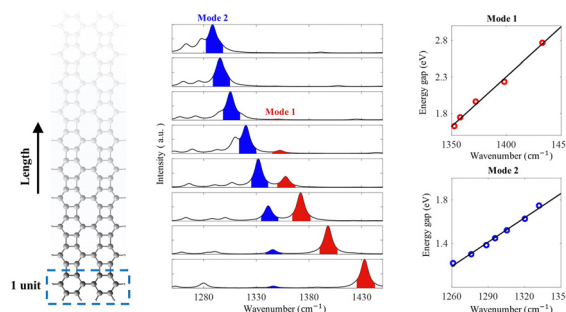


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22505

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

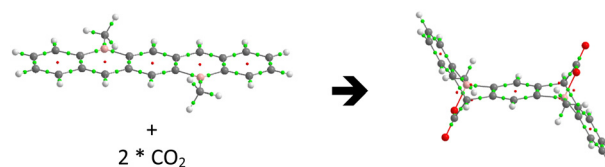
Yirui Lu, Lei Yan,* Sichen Huang, Xilin Zhou, Min Zhang, Ruhai Du and Zhenglong Zhang*



22512

A theoretical study of the reaction of borata derivatives of benzene, anthracene and pentacene with CO₂

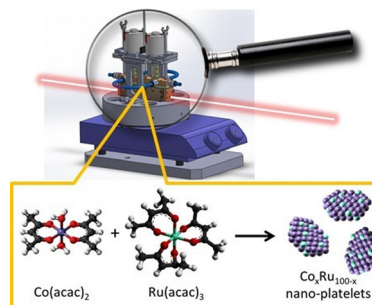
Maxime Ferrer, Ibon Alkorta,* José Elguero and Josep M. Oliva-Enrich



22523

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

Brandon Azeredo, Tayssir Ben Ghzaïel, 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 Hergenrohn, Harald Oberhofer, Bernd Winter, Karsten Reuter* and Hendrik Bluhm*

