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Cover

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Inside cover

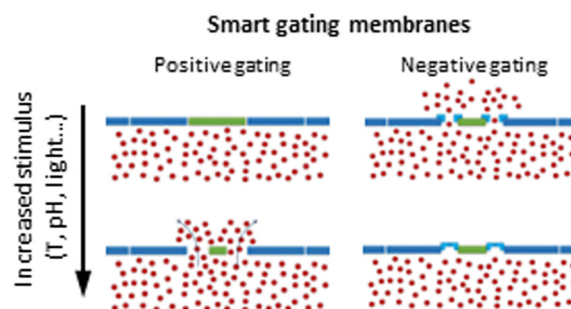
See Miriam Arak Freedman *et al.*, pp. 2887–2894. Image reproduced by permission of Danielle Zemba from *Phys. Chem. Chem. Phys.*, 2024, 26, 2887.

REVIEWS

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A review of stimuli-responsive polymer-based gating membranes

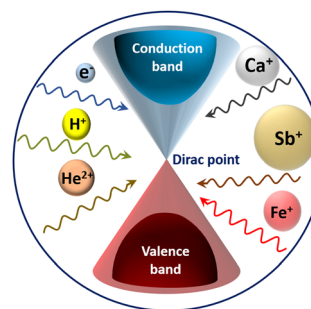
Stefanie Uredat, Aditi Gujare, Jonas Runge, Domenico Truzzolillo, Julian Oberdisse* and Thomas Hellweg*



2745

The effect of charged particle irradiation on the transport properties of bismuth chalcogenide topological insulators: a brief review

Abhirami S,* E. P. Amaladass,* S. Amirthapandian, C. David and Awadhesh Mani*



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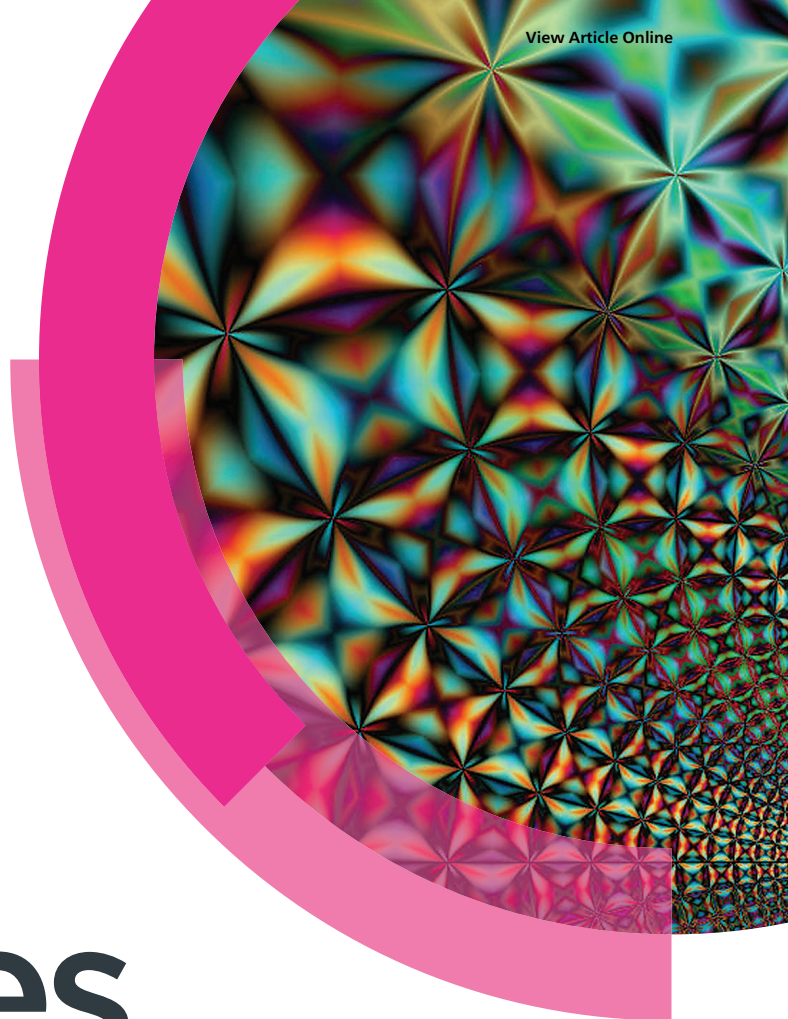


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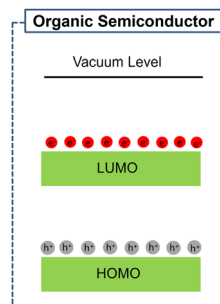
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Energy level measurement for organic semiconductors

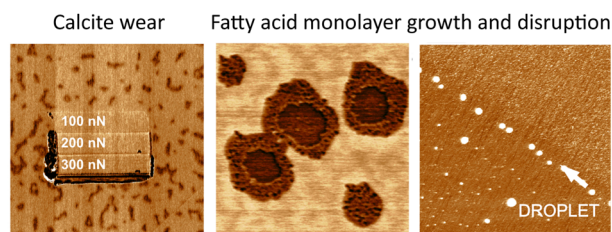
Xuehua Zhou,* Shixing Yang, Qingxia Li, Guoliang Bai, Chunhua Wang and Chao Han*



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The dynamic nature of natural and fatty acid modified calcite surfaces

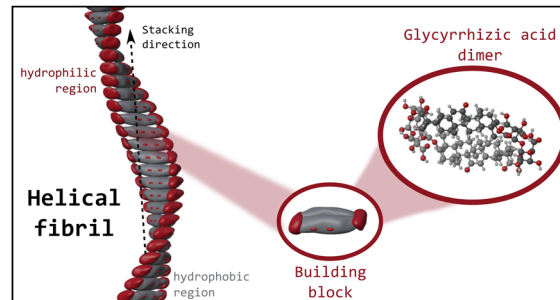
Per M. Claesson,* Natalia A. Wojas,* Robert Corkery, Andra Dedinaite, Joachim Schoelkopf and Eric Tyrode



2806

Glycyrrhizic acid aggregates seen from a synthetic surfactant perspective

Peter Fischer* and Viviane Lutz-Bueno*



2815

Natural resonance-theoretic conceptions of extreme electronic delocalization in soft materials

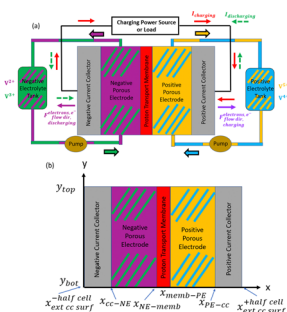
Frank Weinhold* and Eric D. Glendening

"material" type	<u>hard</u>	<u>soft</u>
nature of interaction	<u>QM</u>	<u>QM</u>
resonance bond orders	$b_{AB} \geq 1$	$b_{AB} < 1$
Lewis-structure weighting	$w_L > 50\%$	$w_L \approx 0$
e-delocalization	<u>weak</u> (perturbative)	<u>strong!</u> (network-like)



PERSPECTIVES

2823

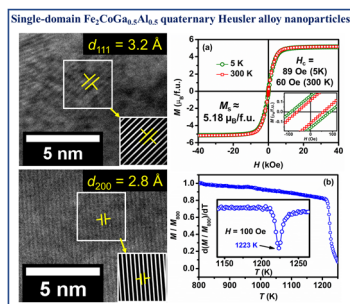


Physics, electrochemistry, chemistry, and electronics of the vanadium redox flow battery by analyzing all the governing equations

Clifford M. Krowne

COMMUNICATIONS

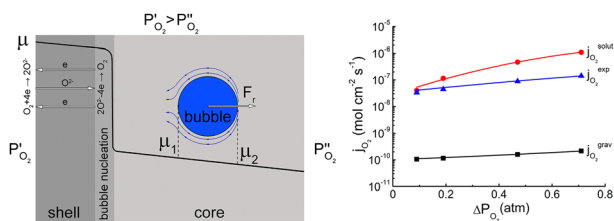
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Single-domain $\text{Fe}_2\text{CoGa}_{0.5}\text{Al}_{0.5}$ Heusler alloy nanoparticles with enhanced properties

Manisha Srivastava, Gajendra S. Bisht and Ananthakrishnan Srinivasan*

2870

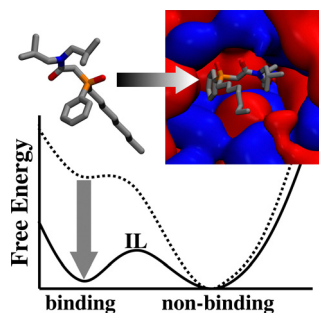


Solutocapillary transport of oxygen bubbles in a diffusion-bubbling membrane core

Valery V. Belousov* and Sergey V. Fedorov

RESEARCH PAPERS

2877



Solvent effects on extractant conformational energetics in liquid–liquid extraction: a simulation study of molecular solvents and ionic liquids

Xiaoyu Wang,* Srikanth Nayak, Richard E. Wilson, L. Soderholm and Michael J. Servis*

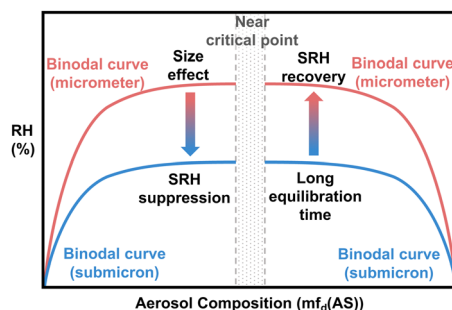


RESEARCH PAPERS

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Experimental phase diagram and its temporal evolution for submicron 2-methylglutaric acid and ammonium sulfate aerosol particles

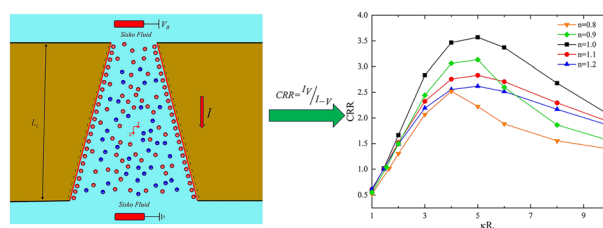
Qishen Huang, Kiran R. Pitta, Kayla Constantini, Emily-Jean E. Ott, Andreas Zuend and Miriam Arak Freedman*



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Ion current rectification properties of non-Newtonian fluids in conical nanochannels

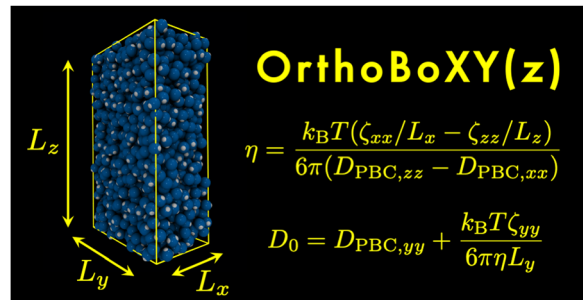
Lei Tang, Yu Hao, Li Peng, Runxin Liu, Yi Zhou and Jie Li*



2907

An OrthoBoXY-method for various alternative box geometries

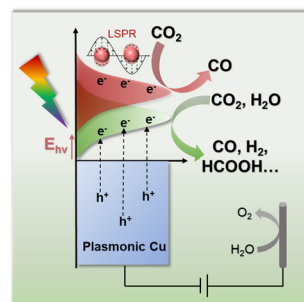
Johanna Busch and Dietmar Paschek*



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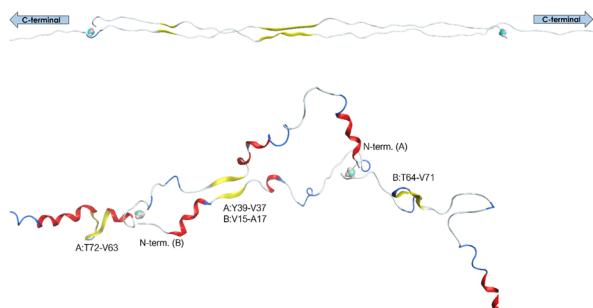
The plasmonic effect of Cu on tuning CO₂ reduction activity and selectivity

Jing Xue, Zhenlin Chen, Kun Dang, Lei Wu, Hongwei Ji, Chuncheng Chen, Yuchao Zhang* and Jincai Zhao



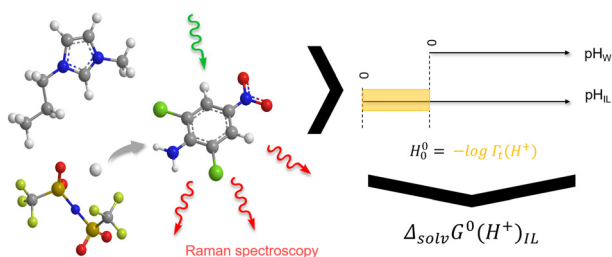
RESEARCH PAPERS

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Computational investigation of copper-mediated conformational changes in α -synuclein dimer

Loizos Savva and James A. Platts*

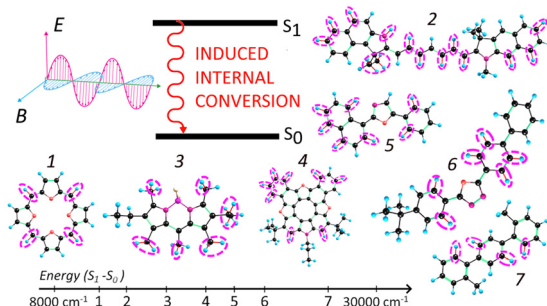
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Experimental determination of solvation free energy of protons in non-protic ionic liquids using Raman spectroscopy

Aurelie Rensonnet and Cedric Malherbe*

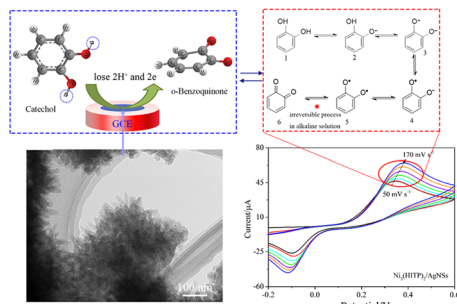
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Internal conversion induced by external electric and magnetic fields

R. R. Valiev,* R. T. Nasibullin, B. S. Merzlikin, K. Khoroshkin, V. N. Cherepanov and D. Sundholm

2951

Sensing platform for the highly sensitive detection of catechol based on composite coupling with conductive $\text{Ni}_3(\text{HITP})_2$ and nanosilvers

Yuandong Xu,* Yingying Ben, Lili Sun, Jishan Su, Hui Guo, Rongjia Zhou, Yaqing Wei, Yajun Wei, Yongjuan Lu, Yizhan Sun and Xia Zhang*

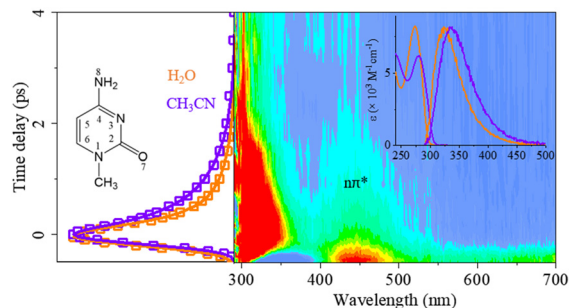


RESEARCH PAPERS

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Is 1-methylcytosine a faithful model compound for ultrafast deactivation dynamics of cytosine nucleosides in solution?

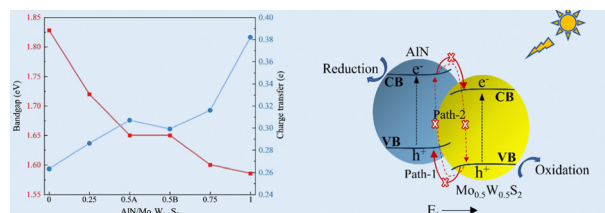
Chensheng Ma,* Qingwu Xiong, Jingdong Lin, Xiaoyan Zeng, Mingliang Wang and Wai-Ming Kwok*



2973

A bicomponent synergistic $\text{Mo}_x\text{W}_{1-x}\text{S}_2$ /aluminum nitride vdW heterojunction for enhanced photocatalytic hydrogen evolution: a first principles study

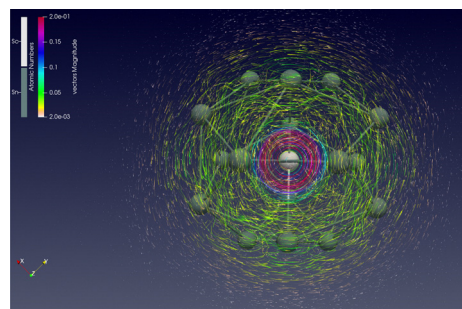
Liang Xu,* Can Li, S. X. Xiong,* Shuaihao Tang, Zhiqiang Xu, Lei Cao, Ji Tao, Ying Zhang, Kejun Dong* and Ling-Ling Wang



2986

Exploring the stability and aromaticity of rare earth doped tin cluster MSn_{16}^- ($\text{M} = \text{Sc}, \text{Y}, \text{La}$)

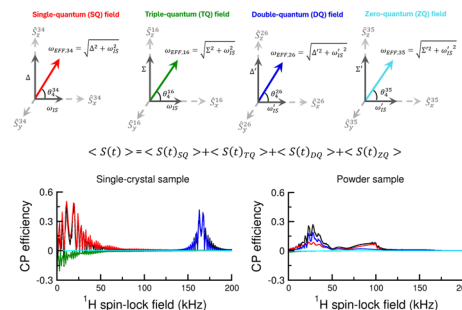
Jin-Kun Zeng, Huai-Qian Wang,* Hui-Fang Li, Hao Zheng, Jia-Ming Zhang, Xun-Jie Mei, Yong-Hang Zhang and Xun-Lei Ding



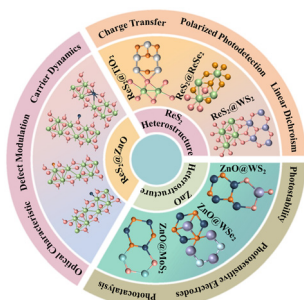
2995

Unravelling the mechanism of polarization transfer from spin-1/2 to spin-1 system in solids

Ekta Nehra and Manoj Kumar Pandey*



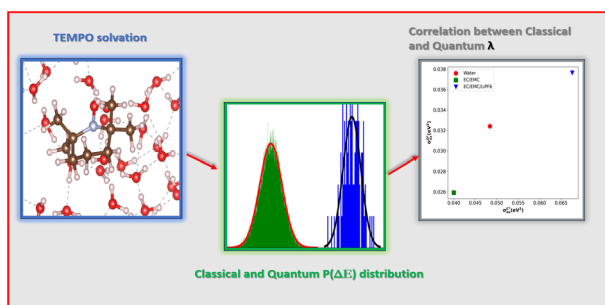
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Study on interface engineering and chemical bonding of the $\text{ReS}_2@ZnO$ heterointerface for efficient charge transfer and nonlinear optical conversion efficiency

Xin-Yu Zheng, Hong-Yu Li, Bing-Yin Shi, Hong-Xu Cao, Yu Liu and Hai-Tao Yin*

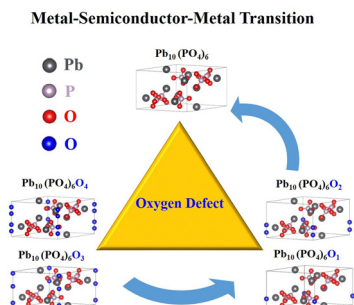
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Electron transfer reaction of TEMPO-based organic radical batteries in different solvent environments: comparing quantum and classical approaches

Souvik Mitra, Andreas Heuer and Diddo Diddens*

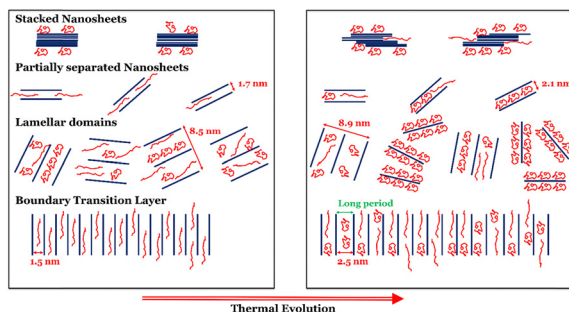
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Exceptional metal–semiconductor–metal transition of lead apatites *via* oxygen defect tuning

Zhijing Huang, Xiaojian Ni, Hao Huang, Yusong Tu,* Zonglin Gu* and Shuming Zeng*

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Thermal evolution of a polymer–nanoparticle binary mixture

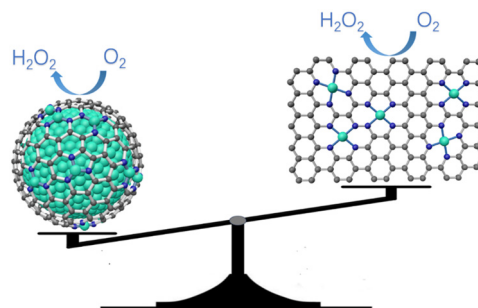
Sanjay Kumar, Sangram K. Rath, Ashwani Kushwaha, S. K. Deshpande, T. Umasankar Patro and G. Harikrishnan*



3044

Encapsulation of Co nanoparticles with single-atomic Co sites into nitrogen-doped carbon for electro-synthesis of hydrogen peroxide

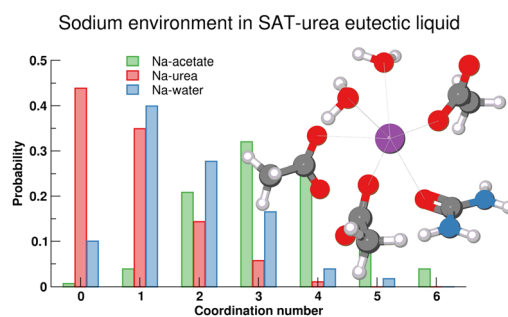
Kun Li, Yanyan Sun,* Ziwei Zhao and Ting Zhu*



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The role of urea in formation of the sodium acetate trihydrate (SAT)–urea eutectic liquid: a neutron diffraction and isotopic substitution study

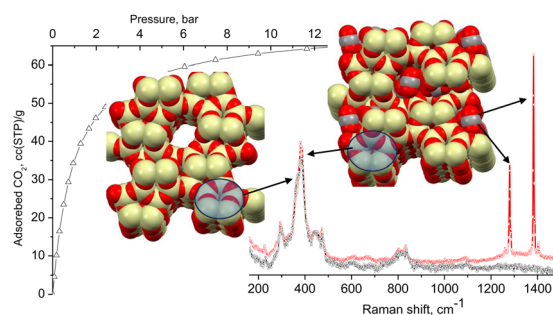
Emily L. Byrne, Sanskrita Madhukailya, Oliver L. G. Alderman, Marijana Blesic and John D. Holbrey*



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Tracking carbon dioxide adsorbate intramolecular dynamics in pure silica zeolite Silicalite-1 by *in situ* Raman scattering

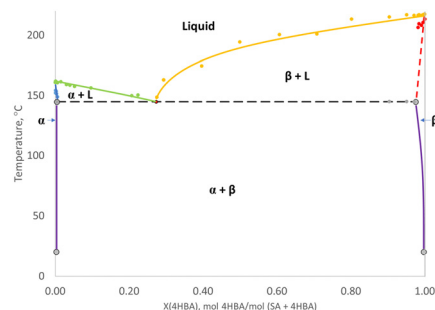
Dimitar V. Tzankov and Peter A. Georgiev*



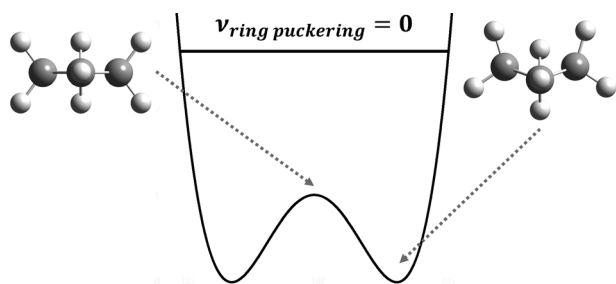
3069

Terminal crystalline solid solutions, solubility enhancements and T–X phase diagram of salicylic acid – 4-hydroxybenzoic acid

Yongjian Wang, Francesco Ricci, Brian Linehan and Fredrik L Nordstrom*



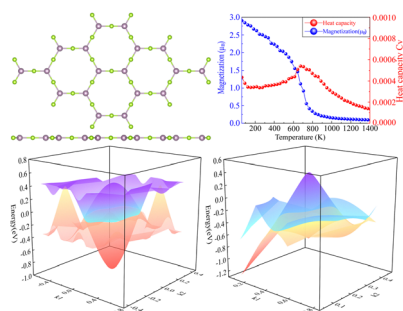
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High-resolution infrared spectroscopy of jet cooled cyclobutyl in the α -CH stretch region: large-amplitude puckering dynamics in a 4-membered ring radical

Ya-Chu Chan and David J. Nesbitt*

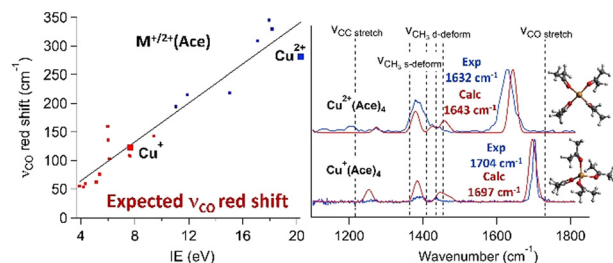
3092



Prediction of a two-dimensional high Curie temperature Weyl nodal line kagome semimetal

Jie Li, Xiao-Tian Wang, Ya-Qing Chen, Yu-Hao Wei, Hong-Kuan Yuan and Chun-Ling Tian*

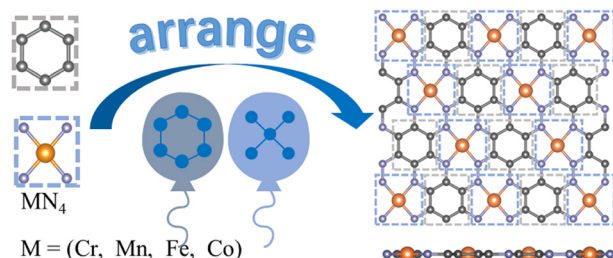
3101



How the nature and charge of metal cations affect vibrations in acetone solvent molecules

Apakorn Phasuk, Joel Lemaire, Vincent Steinmetz, Philippe Maitre and Ricardo B. Metz*

3110



Prediction of transition metal carbonitride monolayers MN_4C_6 ($M = Cr, Mn, Fe, \text{ and } Co$) made up of a benzene ring and a planar MN_4 moiety

Tong Liu, Bingxin Liu, Miao Gao, Xun-Wang Yan* and Fengjie Ma*



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Structural and electronic changes in the Ni₁₃@Ag₄₂ nanoparticle under surface oxidation: the role of silver coating

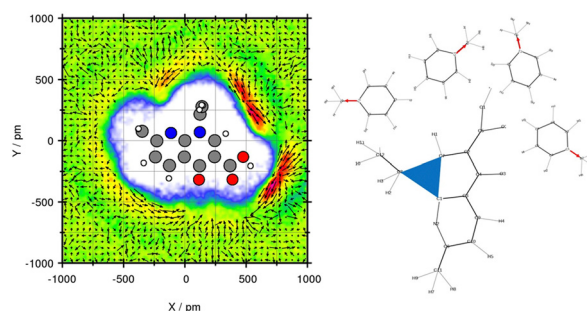
R. H. Aguilera-del-Toro,* F. Aguilera-Granja and A. Vega

Ag₄₂Ni₁₃ nanoparticle oxidation.

3126

Prediction of toluene/water partition coefficients of SAMPL9 compounds: comparison of the molecular dynamics force fields GAFF/RESP and GAFF/IPolQ-Mod + LJ-fit

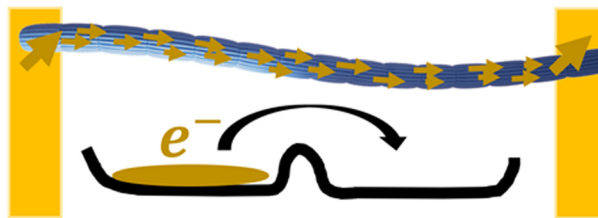
Miriam Sprick and Gabriele Raabe*



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A model analysis of centimeter-long electron transport in cable bacteria

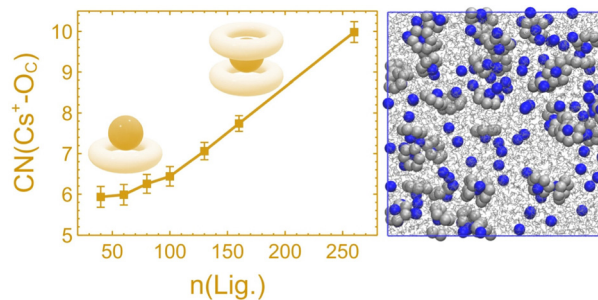
Jasper R. van der Veen,* Stephanie Valianti, Herre S. J. van der Zant, Yaroslav M. Blanter and Filip J. R. Meysman*



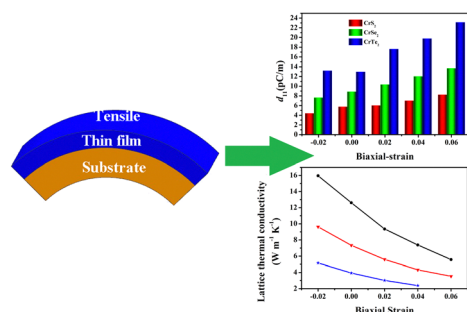
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Exclusive ion recognition using host-guest sandwich complexes

Nitesh Kumar



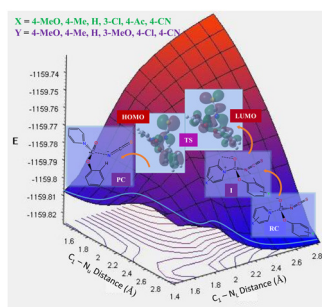
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Equibiaxial strain regulates the electronic structure and mechanical, piezoelectric, and thermal transport properties of the 2H-phase monolayers CrX_2 ($X = \text{S}, \text{Se}, \text{Te}$)

Shao-Bo Chen,* San-Dong Guo, Wan-Jun Yan, Xiang-Rong Chen* and Hua-Yun Geng

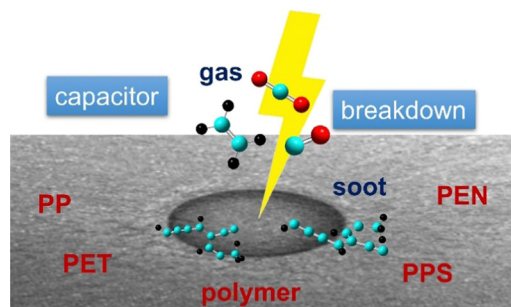
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Theoretical investigation of nucleophilic substitution reaction of phenyl carbonyl isothiocyanates with pyridines in gas and polar aprotic solvent

Keshab Kumar Adhikary,* Francis Verpoort and Philippe M. Heynderickx*

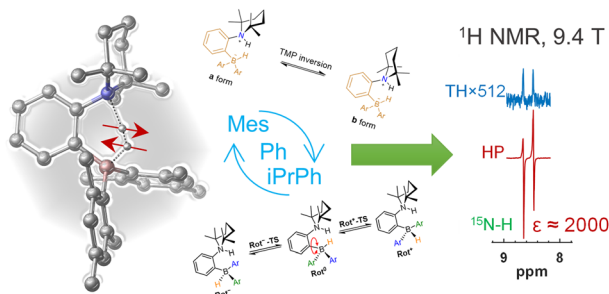
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Higher hydrogen fractions in dielectric polymers boost self-healing in electrical capacitors

Vitaly V. Chaban* and Nadezhda A. Andreeva

3197



Activation of H_2 using *ansa*-aminoboranes: solvent effects, dynamics, and spin hyperpolarization

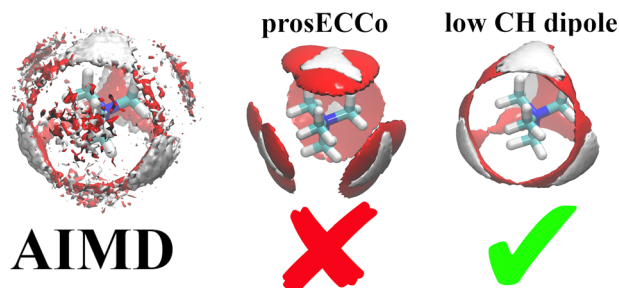
Karolina Konsewicz, Gergely Laczkó, Imre Pápai and Vladimir V. Zhivonitko*



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Hydration of biologically relevant tetramethylammonium cation by neutron scattering and molecular dynamics

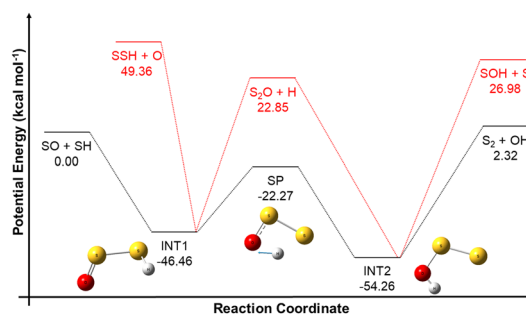
Philip E. Mason,* Tomas Martinek, Balázs Fábrián, Mario Vazdar, Pavel Jungwirth, Ondrej Tichacek, Elise Duboué-Dijon and Hector Martinez-Seara*



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Quantum chemistry and kinetics of hydrogen sulphide oxidation

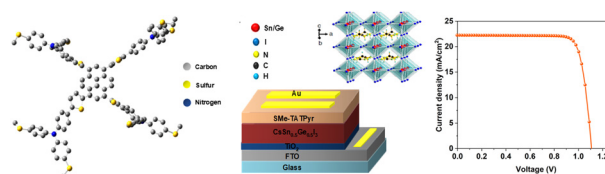
M. Monge-Palacios,* Q. Wang,* A. Alshaarawi, A. C. Cavazos Sepulveda and S. M. Sarathy



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Improved eco-friendly CsSn_{0.5}Ge_{0.5}I₃ perovskite photovoltaic efficiency beyond 20% with SMe-TATPy hole-transporting layer

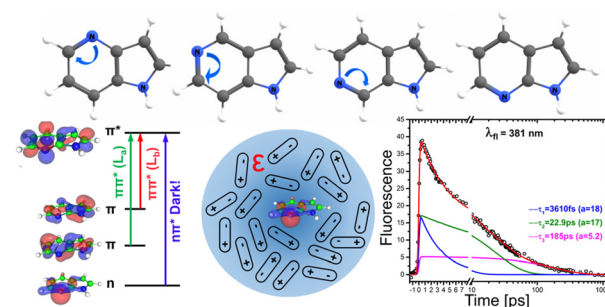
Mustafa K. A. Mohammed,* Moaed E. Al-Gazally, Omar A. Khaleel, Ali K. Al-Mousoi, Zuhair Mohammed Ali Jeddoo, Hasan Sh. Majdi, Majid S. Jabir, M. Khalid Hossain, Mohammad Rafe Hatshan, Md. Ferdous Rahman and Davoud Dastan



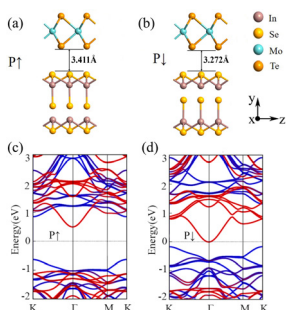
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Photodynamics of azaindoles in polar media: the influence of the environment

Iker Lamas, Raúl Montero,* Virginia Martínez-Martínez and Asier Longarte*



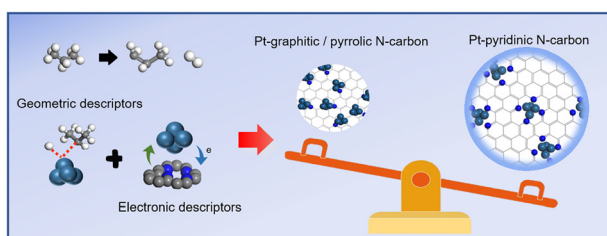
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High tunneling electroresistance in ferroelectric tunnel junctions based on two-dimensional α - $\text{In}_2\text{Se}_3/\text{MoTe}_2$ van der Waals heterostructures

Leitao Lei, Yan-Hong Zhou,* Xiaohong Zheng,*
Wenqiang Wan and Weiyang Wang

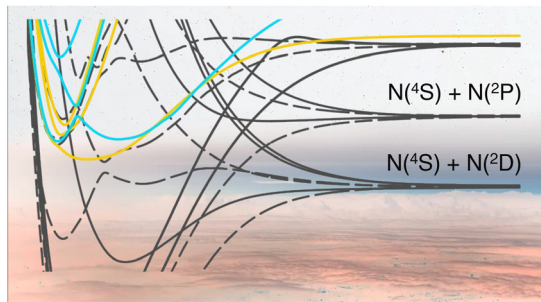
3263



Fine-tuned local coordination environment of Pt–N in nanocarbons for efficient propane dehydrogenation

Ziwei Zhai, Bofeng Zhang,* Yutong Wang and
Guozhu Liu*

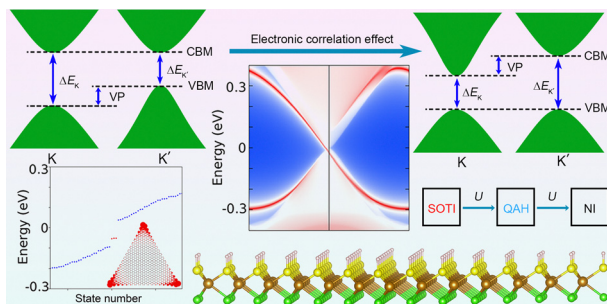
3274



Nonadiabatic quantum dynamics explores non-monotonic photodissociation branching of N_2 into the $\text{N}(^4\text{S}) + \text{N}(^2\text{D})$ and $\text{N}(^4\text{S}) + \text{N}(^2\text{P})$ product channels

Natalia Gelfand,* Ksenia Komarova, Françoise Remacle
and R. D. Levine

3285



Tunable valley polarization effect and second-order topological state in monolayer FeClSH

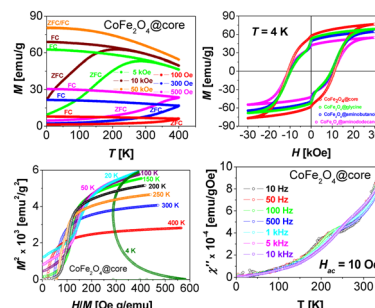
Mengteng Chen, Xiangru Kong,* Xiao Xie, Xiaobiao Liu,
Jia Li, François M. Peeters and Linyang Li*



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Magnetic studies of ultrafine CoFe_2O_4 nanoparticles with different molecular surface coatings

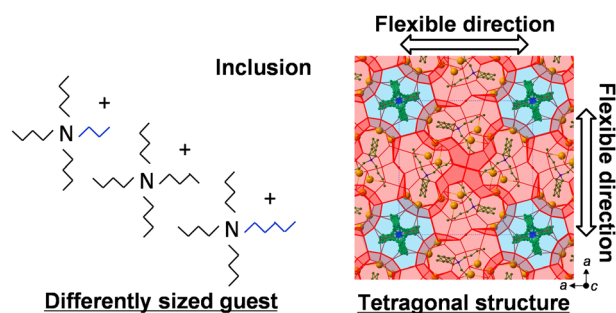
Ewa Mosiniwicz-Szablewska,* Leandro Carlos Figueiredo, Atailson Oliveira da Silva, Marcelo Henrique Sousa and Paulo César de Morais



3315

Guest size effects on a robust structure of semicathrate hydrates and their thermophysical properties

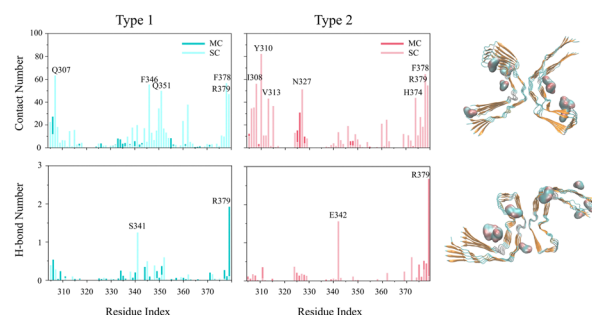
Sanehiro Muromachi* and Satoshi Takeya



3322

Molecular mechanisms involved in the destabilization of two types of R3–R4 tau fibrils associated with chronic traumatic encephalopathy by Fisetin

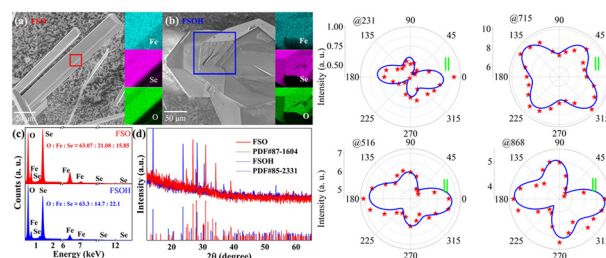
Jiaxing Tang, Ruiqing Sun, Jiaqian Wan, Yu Zou* and Qingwen Zhang*



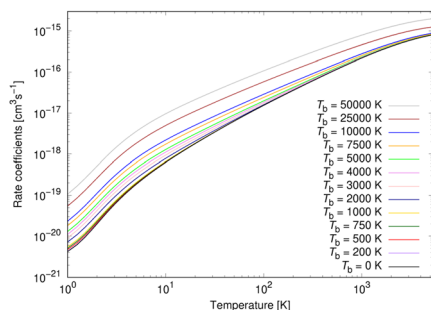
3335

Optical properties of ferroic $\text{Fe}_2\text{O}(\text{SeO}_3)_2$ and $\text{Fe}_2(\text{SeO}_3)_3 \cdot 3\text{H}_2\text{O}$

Shuai Yang, Bing Yu, Rui Ge, Beituo Liu, Ruijuan Qi, Lin Sun, Qingbiao Zhao* and Fangyu Yue*



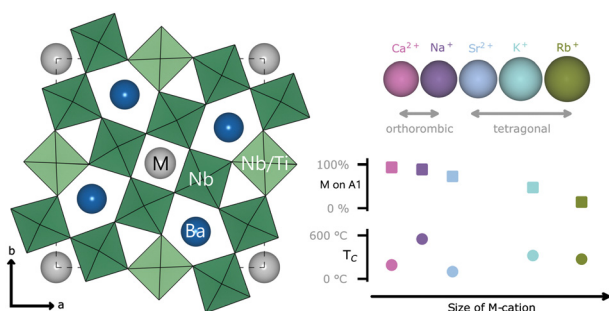
3342



Stimulated radiative association of sodium and chlorine atoms and their ions in a coupled channel treatment

Martina Šimsová née Zámečnicková,* Magnus Gustafsson, Gunnar Nyman and Pavel Soldán

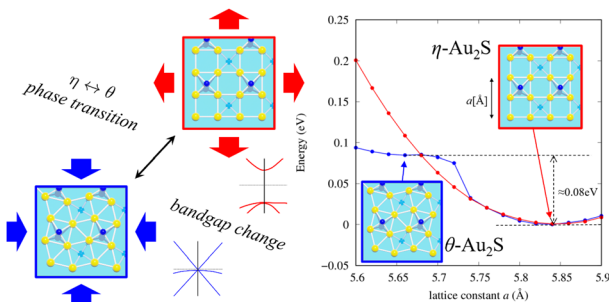
3350



The effect of cation size on structure and properties of Ba-based tungsten bronzes $\text{Ba}_4\text{M}_2\text{Nb}_{10}\text{O}_{30}$ ($\text{M} = \text{Na}, \text{K}$ or Rb) and $\text{Ba}_4\text{M}_2\text{Nb}_8\text{Ti}_2\text{O}_{30}$ ($\text{M} = \text{Ca}$ or Sr)

Nora Statle Løndal, Benjamin Albert Dobson Williamson, Julian Walker, Mari-Ann Einarsrud and Tor Grande*

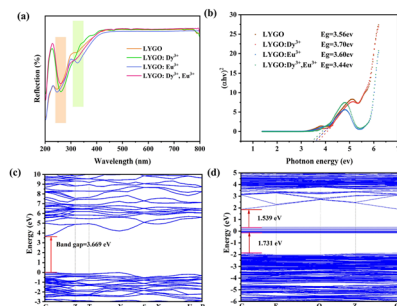
3367



Electronic band structure change with structural transition of buckled Au_2X monolayers induced by strain

Masahiro Fukuda* and Taisuke Ozaki

3375



A novel single-phase color tunable $\text{LiYGeO}_4:\text{Dy}^{3+}$, Eu^{3+} phosphor exhibiting warm white light and excellent thermal stability

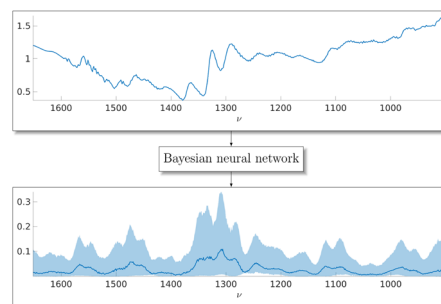
Chunyu Zuo, Rujia Chen, Xiliang Jiang, Zhuang Leng, Yimin Yang, Zhipeng Zhang, Lingbo Zhou, Chun Li,* Weiling Yang,* Hai Lin, Lina Liu, Shasha Li, Fanming Zeng* and Zhongmin Su



3389

Log-Gaussian gamma processes for training Bayesian neural networks in Raman and CARS spectroscopies

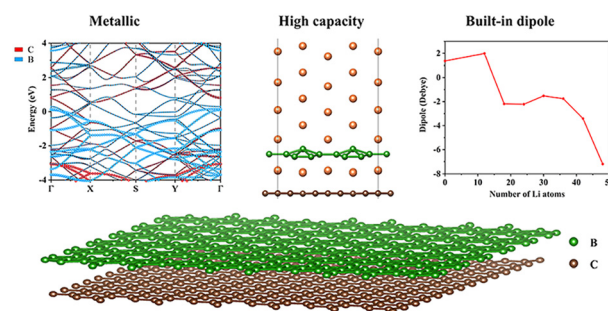
Teemu Härkönen,* Erik M. Vartiainen, Lasse Lensu, Matthew T. Moores and Lassi Roininen



3400

Enhancement of multilayer lithium storage in a β_{12} -borophene/graphene heterostructure with built-in dipoles

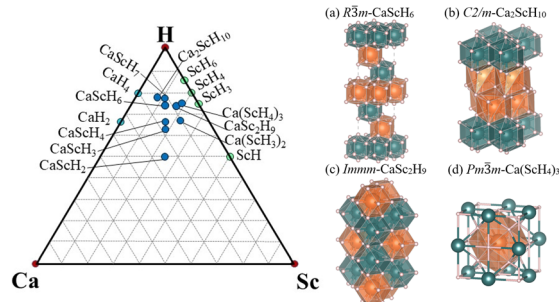
Xiaowei Jiang, Wenjun Tang, Xiaobin Niu and Haiyuan Chen*



3408

A systematic study on the phase diagram and superconductivity of ternary clathrate Ca–Sc–H at high pressures

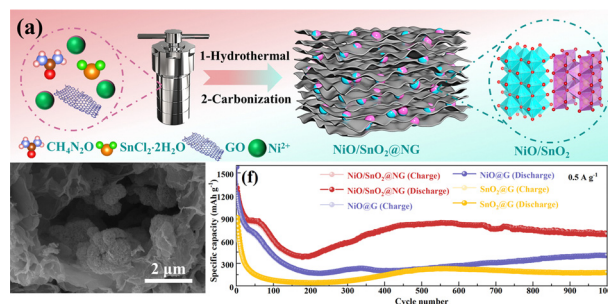
Wenjie Yuan, Xu Yang, Shichang Li,* Chunbao Feng, Bole Chen, Ying Chang and Dengfeng Li*



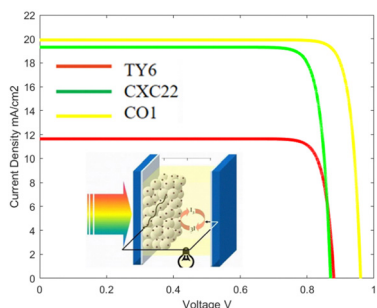
3415

Synthesis of heterointerfaces in NiO/SnO₂ coated nitrogen-doped graphene for efficient lithium storage

Shujuan Yin, Xueqian Zhang,* Dongdong Liu, Xiaoxiao Huang,* Yishan Wang* and Guangwu Wen



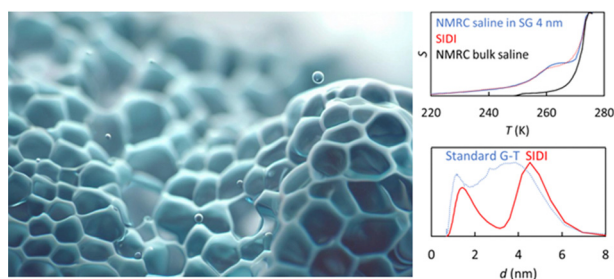
3424



Study of the microscopic mechanism of stepwise charge injection in co-sensitive DSSCs in the framework of a D- π -A dye and chlorophyll

Tao Liu, Canpu Yang, Peng Song,* Fengcai Ma and Yuanzuo Li*

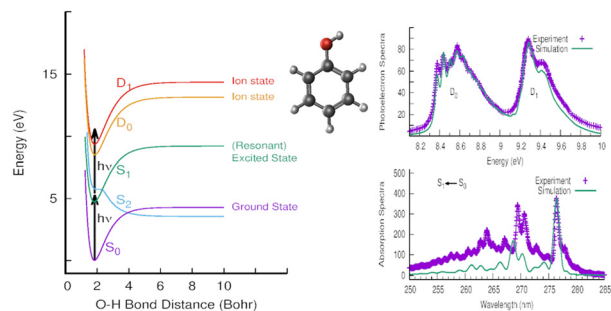
3441



Melting of aqueous NaCl solutions in porous materials: shifted phase transition distribution (SIDI) approach for determining NMR cryoporometry pore size distributions

Sarah E. Mailhot,* Katja Tolkkinen, Henning Henschel, Jiří Mareš, Matti Hanni, Miika T. Nieminen and Ville-Veikko Telkki*

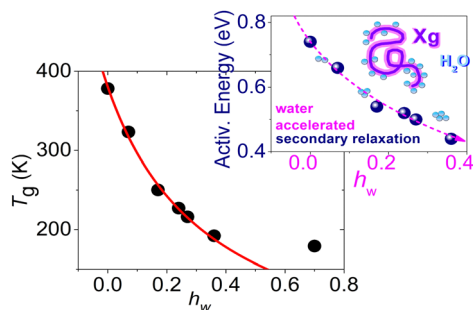
3451



On the multiphoton ionisation photoelectron spectra of phenol

Diptesh Dey,* Joanne L. Woodhouse, Marcus P. Taylor, Helen H. Fielding and Graham A. Worth*

3462



Hydration effects on thermal transitions and molecular mobility in Xanthan gum polysaccharides

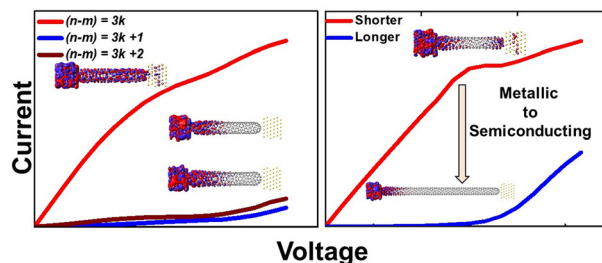
Sokratis N. Tegopoulos, Aristeidis Papagiannopoulos and Apostolos Kyritsis*



3474

Chirality and length-dependent electron transmission of fullerene-capped chiral carbon nanotubes sandwiched in gold electrodes

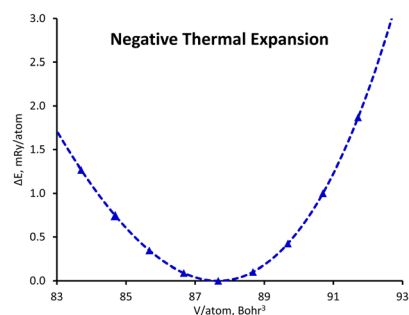
Ameet Kumar, Sudip Sarkar* and Daeheum Cho*



3482

Thermal expansion anisotropy of $\text{Fe}_{23}\text{Mo}_{16}$ and Fe_7Mo_6 μ -phases predicted using first-principles calculations

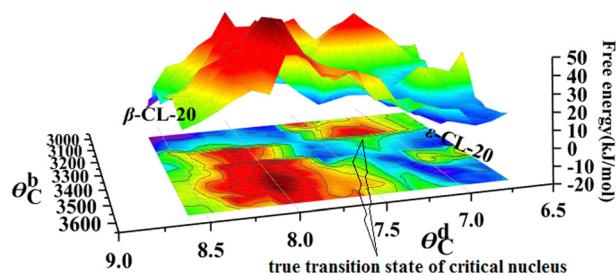
Dmitry Vasilyev



3500

Finite temperature string by *K*-means clustering sampling with order parameters as collective variables for molecular crystals: application to polymorphic transformation between β -CL-20 and ϵ -CL-20

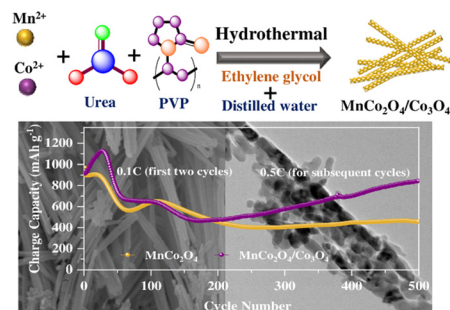
Fu-de Ren,* Ying-Zhe Liu, Ke-wei Ding, Ling-ling Chang, Duan-lin Cao and Shubin Liu*



3516

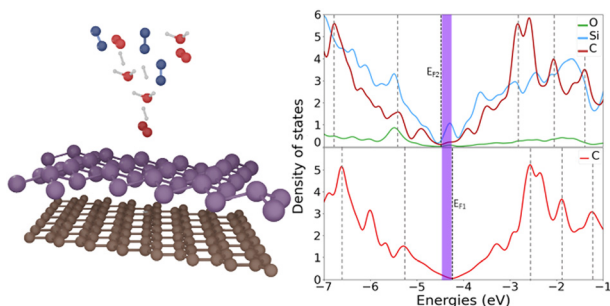
Boosting the high-rate performance of lithium-ion battery anodes using $\text{MnCo}_2\text{O}_4/\text{Co}_3\text{O}_4$ nanocomposite interfaces

Anubha Tomar, Chirag Vankani, Satendra Pal Singh, Martin Winter and Alok Kumar Rai*



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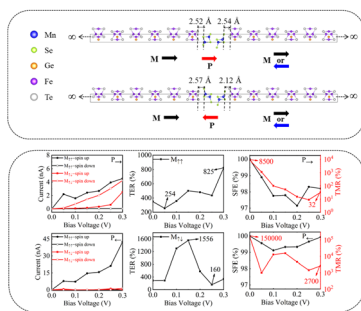
3525



A weakened Fermi level pinning induced adsorption energy non-charge-transfer mechanism during O₂ adsorption in silicene/graphene heterojunctions

Xuhong Zhao, Haiyuan Chen, Jianwei Wang* and Xiaobin Niu*

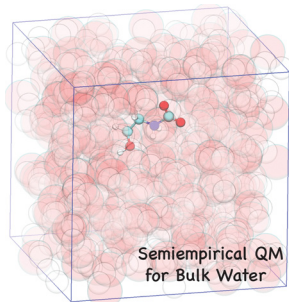
3531



Tunable multiple nonvolatile resistance states in a MnSe-based van der Waals multiferroic tunnel junction

Xiao-Hui Guo, Lin Zhu,* Zeng-Lin Cao and Kai-Lun Yao

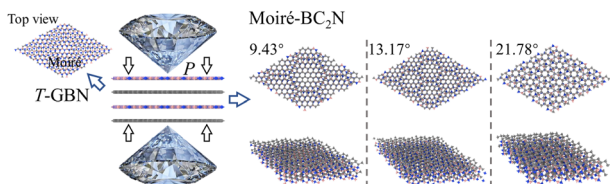
3540



Developing semi-empirical water model for efficiently simulating temperature-dependent chemisorption of CO₂ in amine solvents

Binquan Luan* and James L. McDonagh

3548



Moiré-of-Moiré phases formed in twisted graphene/hexagonal boron nitride heterostructures under high pressure

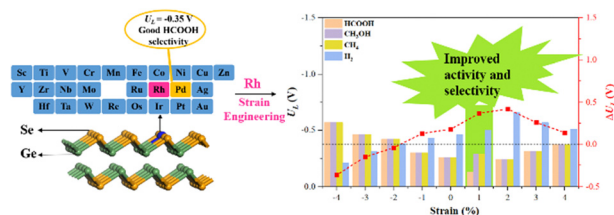
Yaomin Li and Bin Zhang*



3560

Enhancing CO₂ electroreduction performance through transition metal atom doping and strain engineering in γ -GeSe: a first-principles study

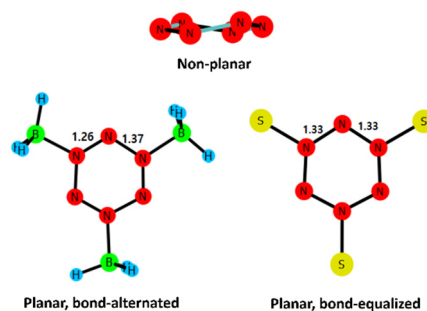
Yu-wang Sun, Lei Liu and Jing-yao Liu*



3569

Bond-alternated and bond-equalized hexazine derivatives

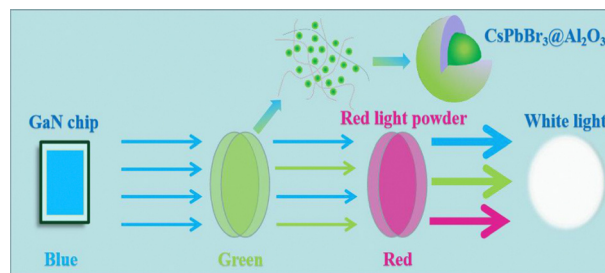
Kunnumma Chelladath Krishnapriya, Ashith Thayyil, Mithu Kumari and Priyakumari Chakkingal Parambil*



3578

Enhanced stability of CsPbBr₃ nanocrystals through Al₂O₃ and polymer coating

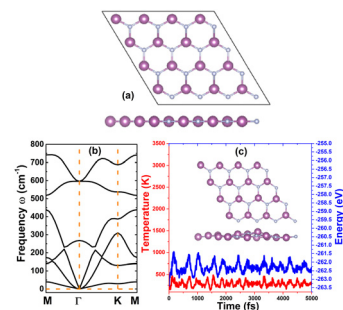
Sheng Huang,* Ce Bian, Wenjie Xu, Hui Zhang, Shasha Gao, Yue Wang* and Yuling Wang*



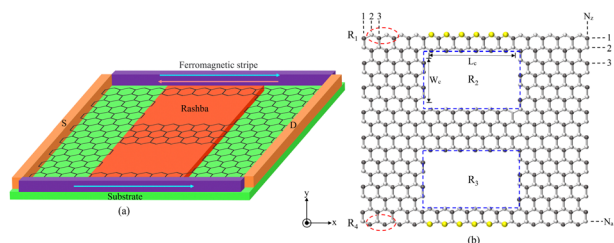
3587

Modifying the electronic and magnetic properties of the scandium nitride semiconductor monolayer via vacancies and doping

Vo Van On, J. Guerrero-Sanchez and D. M. Hoat*



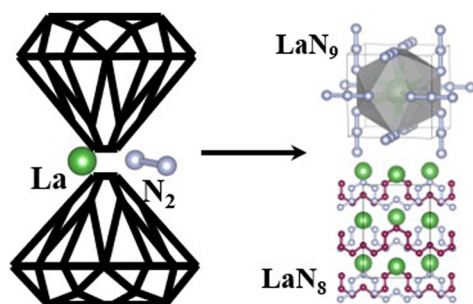
3597



Controlling the spin current around the rectangular cavities in two-dimensional topological insulators

Xiang Gao, Cheng Ma, Lei Li,* Xiaowei Zhang, Zhihong Deng, Xu Li and Zigang Zhou

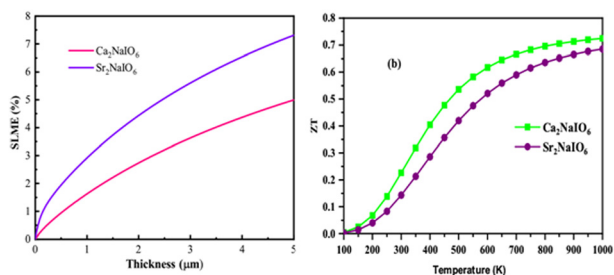
3605



Lanthanum nitride LaN_9 featuring azide units: the first metal nine-nitride as a high-energy-density material

Shuyi Lin, Jingyan Chen, Bi Zhang, Jian Hao,* Meiling Xu* and Yinwei Li

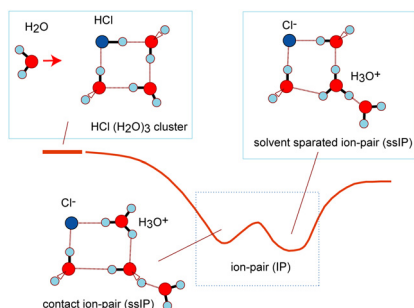
3614



Optoelectronic and thermoelectric properties of novel stable lead-free cubic double perovskites A_2NaIO_6 ($\text{A} = \text{Ca}, \text{Sr}$) for renewable energy applications

Malak Azmat Ali,* Asma A. Alothman, Mohammed Mushab and Muhammad Faizan

3623



Mechanism of ionic dissociation of HCl in the smallest water clusters

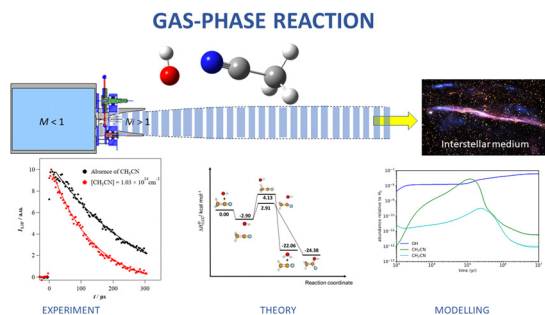
Hiroto Tachikawa



3632

Effect of temperature on the gas-phase reaction of CH₃CN with OH radicals: experimental ($T = 11.7$ – 177.5 K) and computational ($T = 10$ – 400 K) kinetic study

Daniel González, André Canosa, Emilio Martínez-Núñez, Antonio Fernández-Ramos,* Bernabé Ballesteros, Marcelino Agúndez, José Cernicharo and Elena Jiménez*



3647

A single resonance Regge pole dominates the forward-angle scattering of the state-to-state $F + H_2 \rightarrow FH + H$ reaction at $E_{\text{trans}} = 62.09$ meV

Chengkui Xiahou, J. N. L. Connor,* Dario De Fazio and Dmitri Sokolovski

