

IN THIS ISSUE

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Cover

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Inside cover

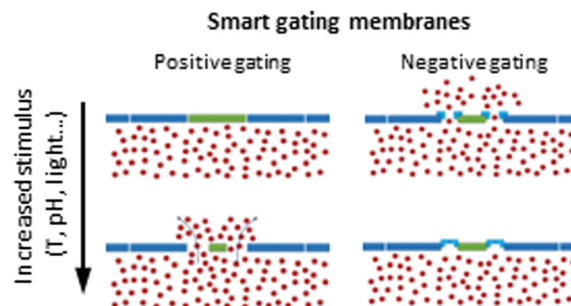
See Miriam Arak Freedman *et al.*, pp. 2887–2894. Image reproduced by permission of Danielle Zemba from *Phys. Chem. Chem. Phys.*, 2024, **26**, 2887.

REVIEWS

2732

A review of stimuli-responsive polymer-based gating membranes

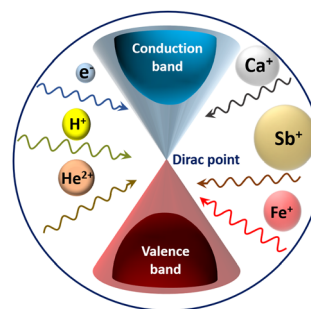
Stefanie Uredat, Aditi Gujare, Jonas Runge, Domenico Truzzolillo, Julian Oberdisse* and Thomas Hellweg*



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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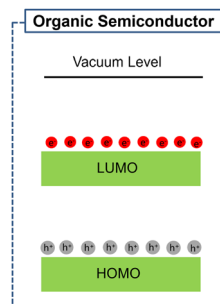
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2768

Energy level measurement for organic semiconductors

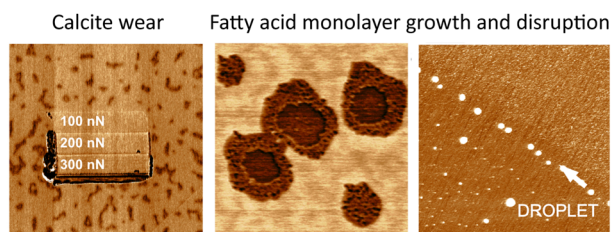
Xuehua Zhou,* Shixing Yang, Qingxia Li, Guoliang Bai, Chunhua Wang and Chao Han*



2780

The dynamic nature of natural and fatty acid modified calcite surfaces

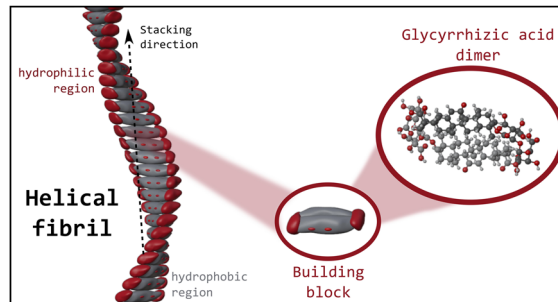
Per M. Claesson,* Natalia A. Wojas,* Robert Corkery, Andra Dedinaite, Joachim Schoelkopf and Eric Tyrode



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

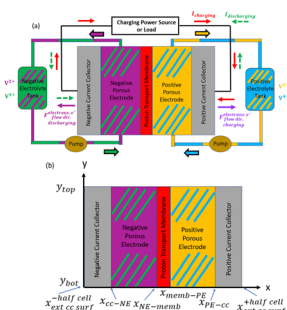
Frank Weinhold* and Eric D. Glendening

"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>	<u>strong!</u>
	(perturbative)	(network-like)



PERSPECTIVES

2823

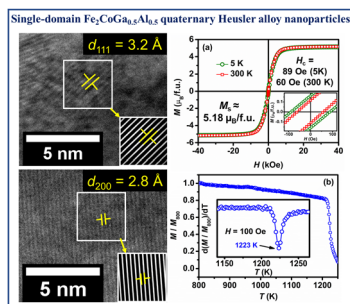


Physics, electrochemistry, chemistry, and electronics of the vanadium redox flow battery by analyzing all the governing equations

Clifford M. Krowne

COMMUNICATIONS

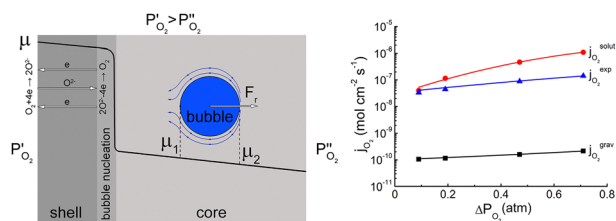
2863



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

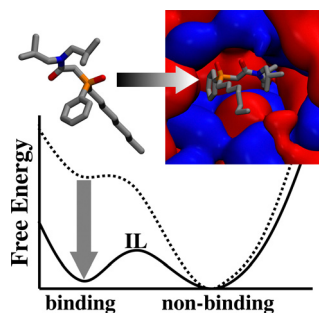


Solutocapillary transport of oxygen bubbles in a diffusion-bubbling membrane core

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*

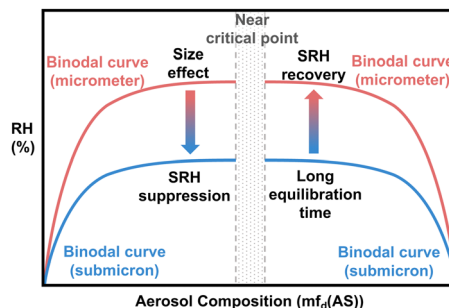


RESEARCH PAPERS

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

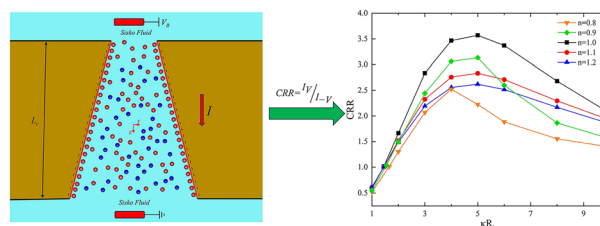
Qishen Huang, Kiran R. Pitta, Kayla Constantini, Emily-Jean E. Ott, Andreas Zuend and Miriam Arak Freedman*



2895

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

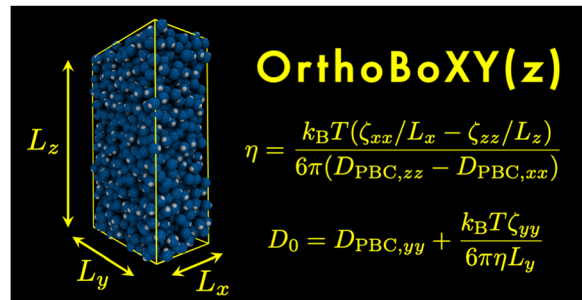
Lei Tang, Yu Hao, Li Peng, Runxin Liu, Yi Zhou and Jie Li*



2907

An OrthoBoXY-method for various alternative box geometries

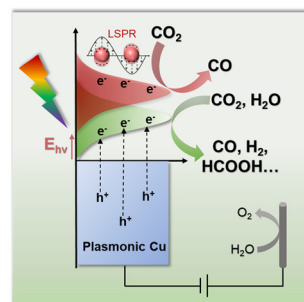
Johanna Busch and Dietmar Paschek*



2915

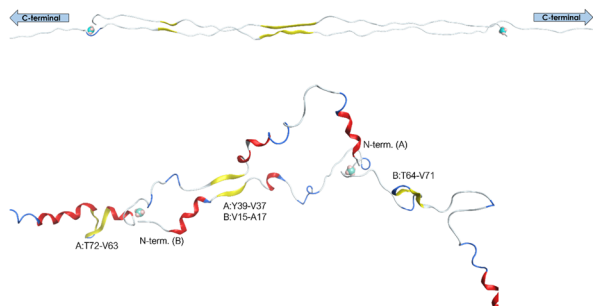
The plasmonic effect of Cu on tuning CO₂ reduction activity and selectivity

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



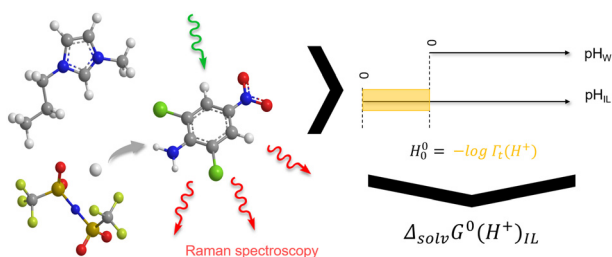
RESEARCH PAPERS

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

Loizos Savva and James A. Platts*

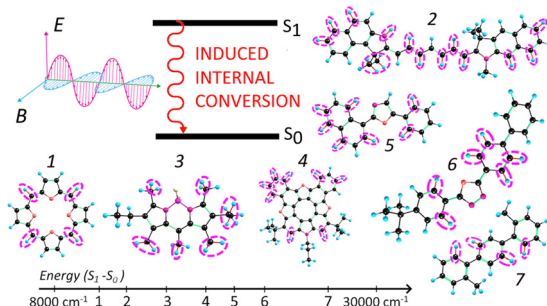
2936



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

Aurelie Rensonnet and Cedric Malherbe*

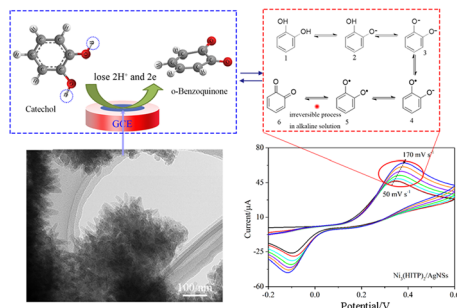
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Internal conversion induced by external electric and magnetic fields

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*

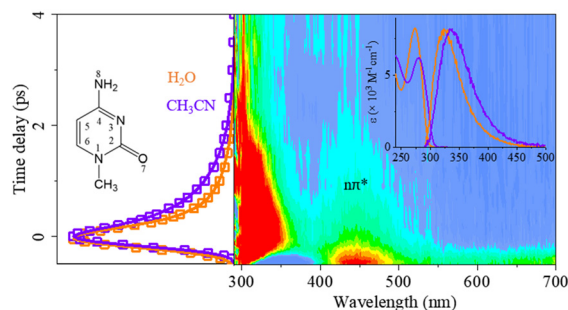


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Is 1-methylcytosine a faithful model compound for ultrafast deactivation dynamics of cytosine nucleosides in solution?

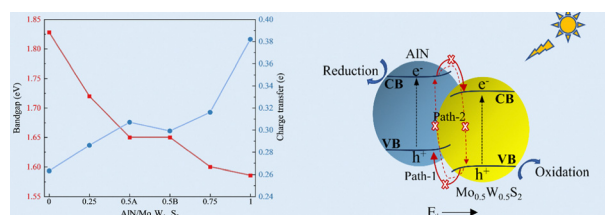
Chensheng Ma,* Qingwu Xiong, Jingdong Lin, Xiaoyan Zeng, Mingliang Wang and Wai-Ming Kwok*



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

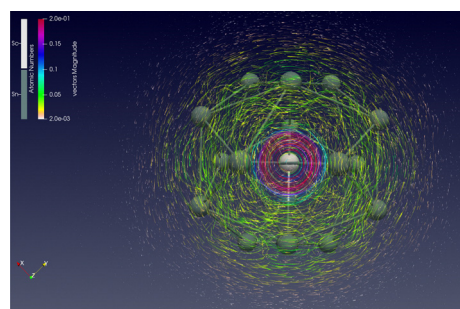
Liang Xu,* Can Li, S. X. Xiong,* Shuaihao Tang, Zhiqiang Xu, Lei Cao, Ji Tao, Ying Zhang, Kejun Dong* and Ling-Ling Wang



2986

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

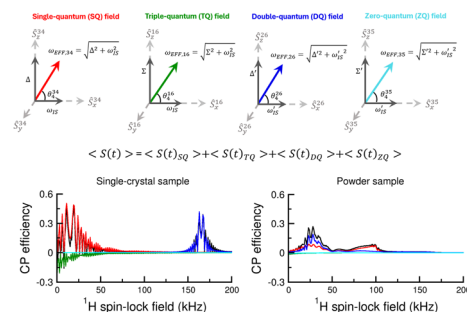
Jin-Kun Zeng, Huai-Qian Wang,* Hui-Fang Li, Hao Zheng, Jia-Ming Zhang, Xun-Jie Mei, Yong-Hang Zhang and Xun-Lei Ding



2995

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

Ekta Nehra and Manoj Kumar Pandey*

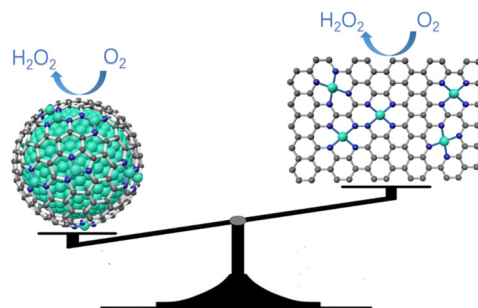


RESEARCH PAPERS

3044

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

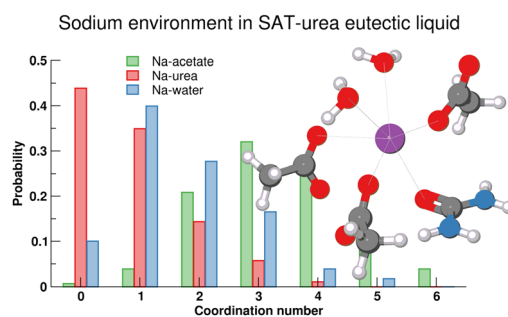
Kun Li, Yanyan Sun,* Ziwei Zhao and Ting Zhu*



3051

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

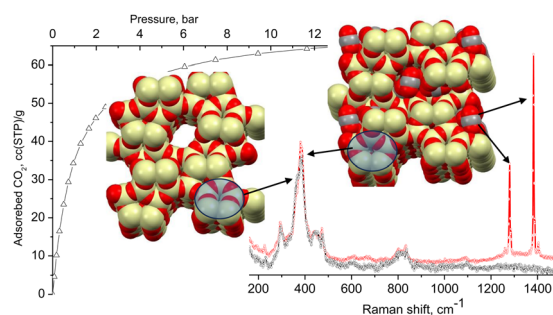
Emily L. Byrne, Sanskrita Madhukailya, Oliver L. G. Alderman, Marijana Blesic and John D. Holbrey*



3060

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

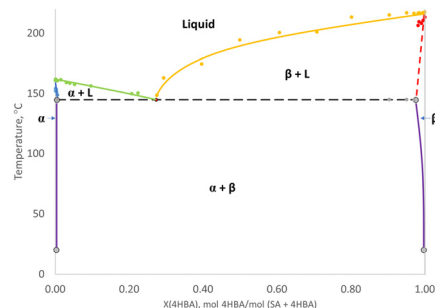
Dimitar V. Tzankov and Peter A. Georgiev*



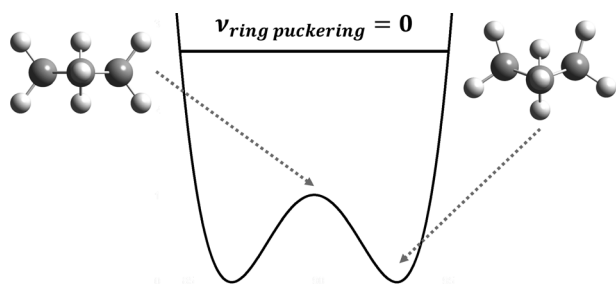
3069

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*



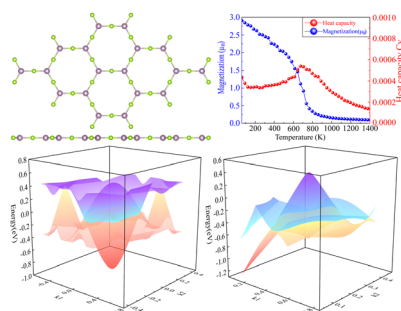
3081



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*

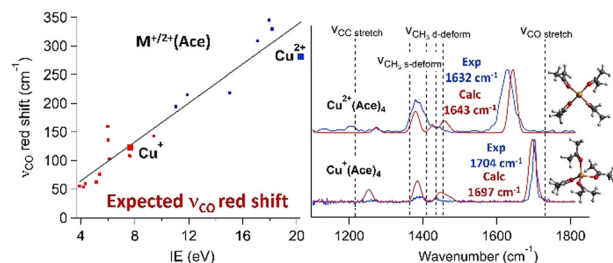
3092



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*

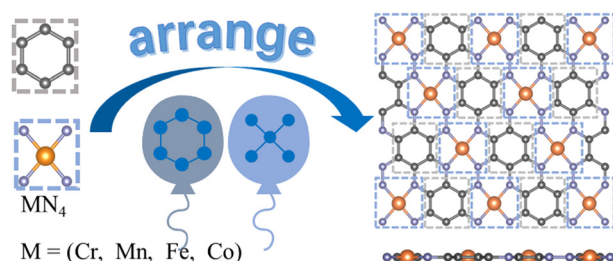
3101



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*



3117

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

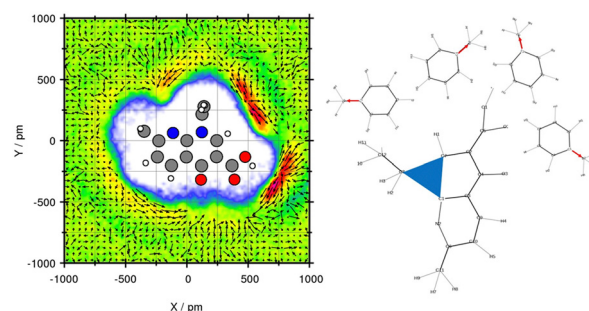
R. H. Aguilera-del-Toro,* F. Aguilera-Granja and A. Vega

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

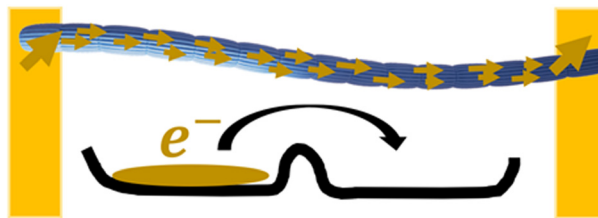
Miriam Sprick and Gabriele Raabe*



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

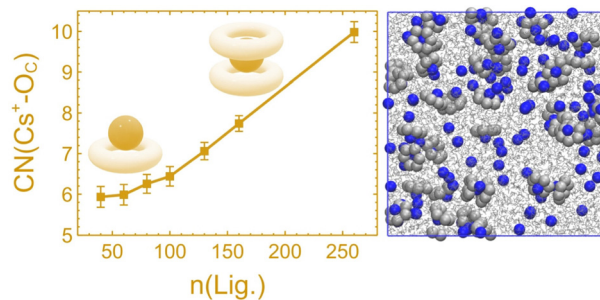
Jasper R. van der Veen,* Stephanie Valianti, Herre S. J. van der Zant, Yaroslav M. Blanter and Filip J. R. Meysman*



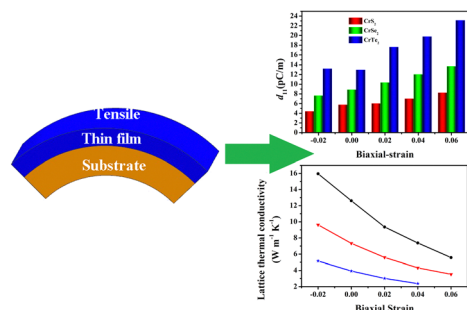
3152

Exclusive ion recognition using host-guest sandwich complexes

Nitesh Kumar



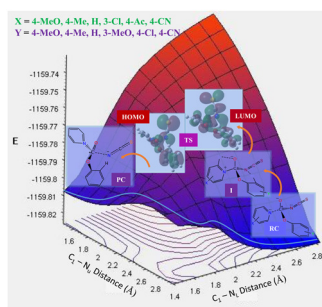
3159



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

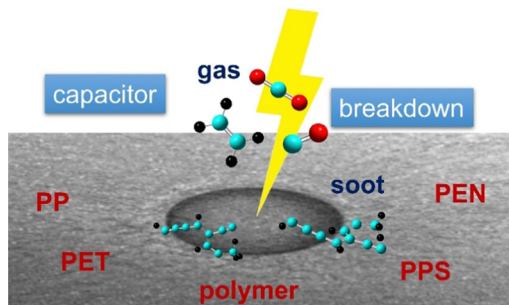
3168



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*

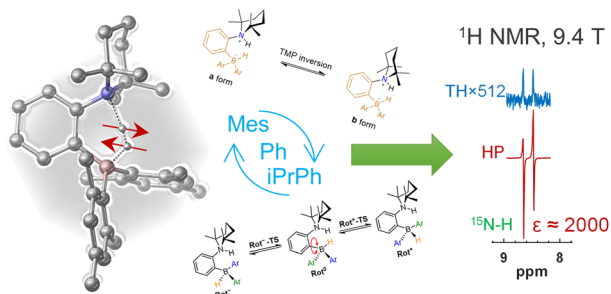
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Higher hydrogen fractions in dielectric polymers boost self-healing in electrical capacitors

Vitaly V. Chaban* and Nadezhda A. Andreeva

3197



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

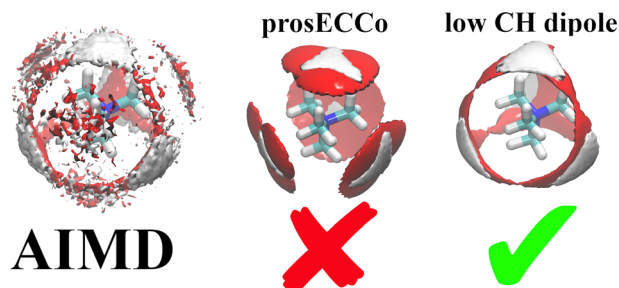
Karolina Konsewicz, Gergely Laczkó, Imre Pápai and Vladimir V. Zhivonitko*



3208

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

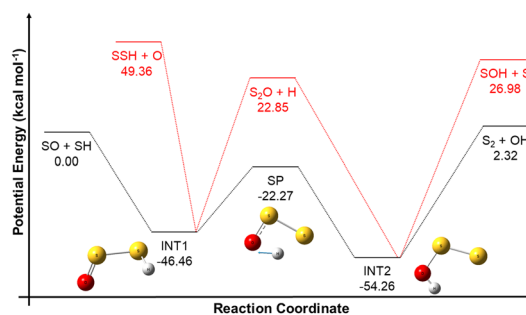
Philip E. Mason,* Tomas Martinek, Balázs Fábrián, Mario Vazdar, Pavel Jungwirth, Ondrej Tichacek, Elise Duboué-Dijon and Hector Martinez-Seara*



3219

Quantum chemistry and kinetics of hydrogen sulphide oxidation

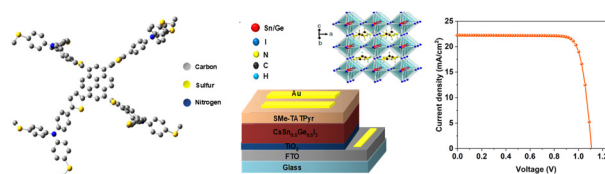
M. Monge-Palacios,* Q. Wang,* A. Alshaarawi, A. C. Cavazos Sepulveda and S. M. Sarathy



3229

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

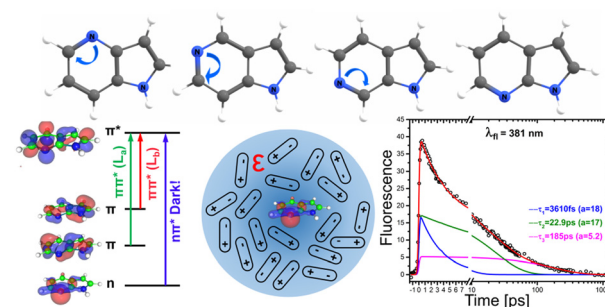
Mustafa K. A. Mohammed,* Moaed E. Al-Gazally, Omar A. Khaleel, Ali K. Al-Mousoi, Zuhair Mohammed Ali Jeddoo, Hasan Sh. Majdi, Majid S. Jabir, M. Khalid Hossain, Mohammad Rafe Hatshan, Md. Ferdous Rahman and Davoud Dastan



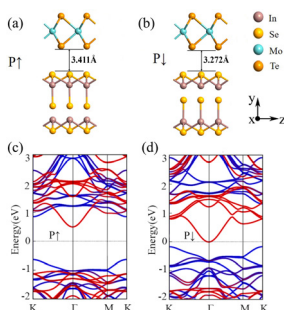
3240

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

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



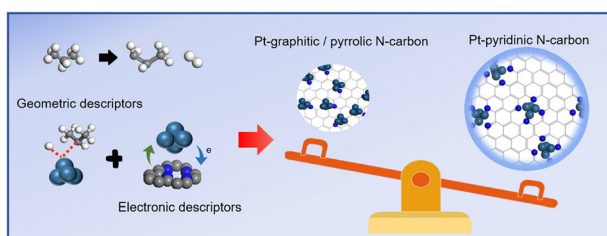
3253



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

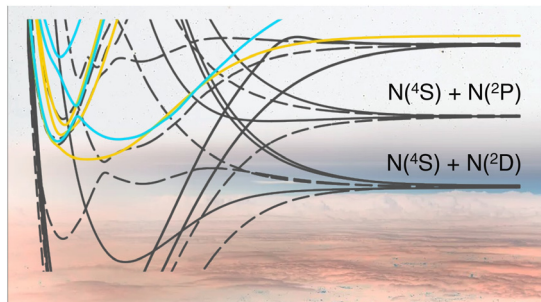
3263



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

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

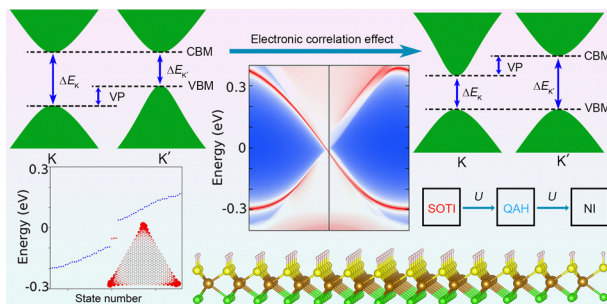
3274



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

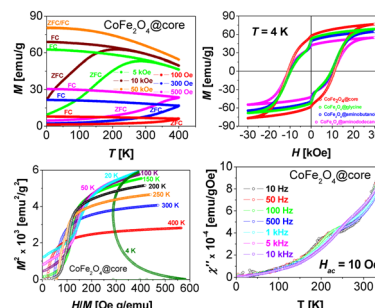
Mengteng Chen, Xiangru Kong,* Xiao Xie, Xiaobiao Liu,
Jia Li, François M. Peeters and Linyang Li*



3296

Magnetic studies of ultrafine CoFe_2O_4 nanoparticles with different molecular surface coatings

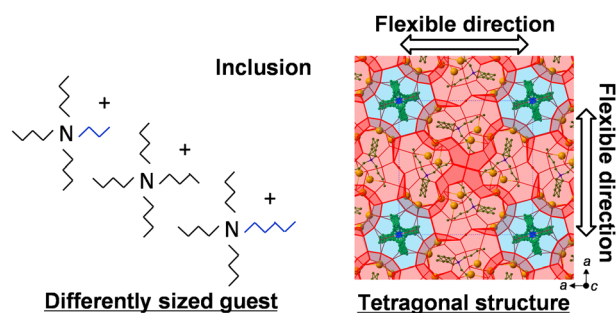
Ewa Mosiniwicz-Szablewska,* Leandro Carlos Figueiredo, Atailson Oliveira da Silva, Marcelo Henrique Sousa and Paulo César de Morais



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

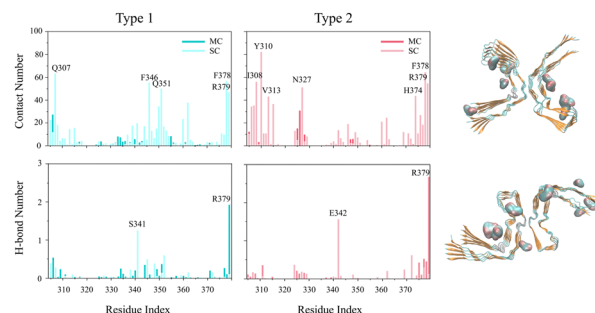
Sanehiro Muromachi* and Satoshi Takeya



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

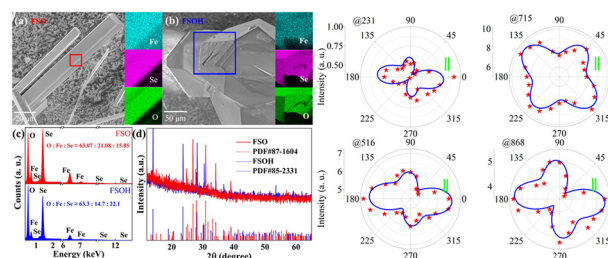
Jiaxing Tang, Ruiqing Sun, Jiaqian Wan, Yu Zou* and Qingwen Zhang*



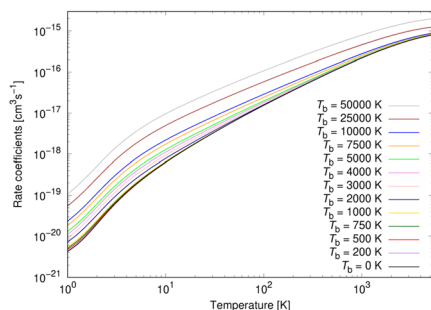
3335

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*



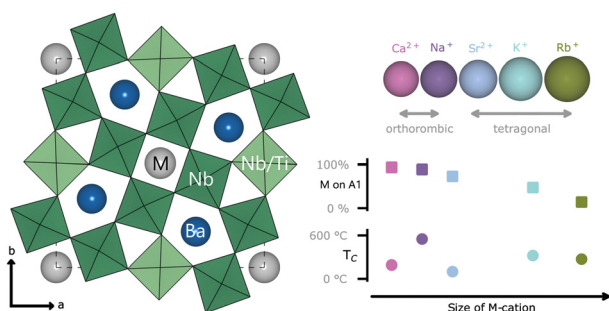
3342



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

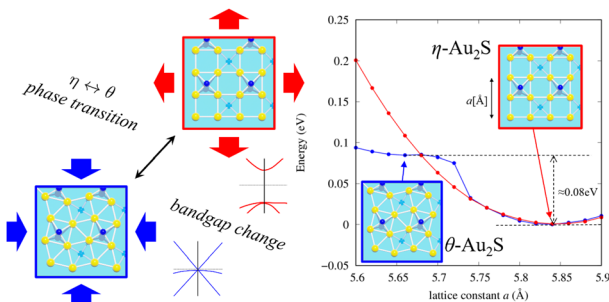
3350



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*

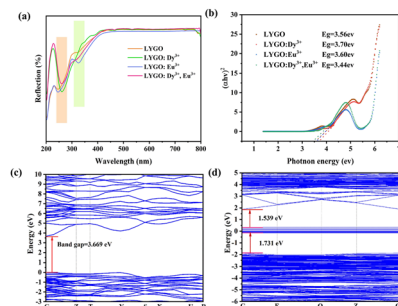
3367



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

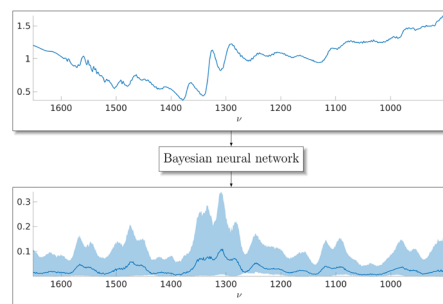
Chunyu Zuo, Rujia Chen, Xiliang Jiang, Zhuang Leng, Yimin Yang, Zhipeng Zhang, Lingbo Zhou, Chun Li,* Weiling Yang,* Hai Lin, Lina Liu, Shasha Li, Fanming Zeng* and Zhongmin Su



3389

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

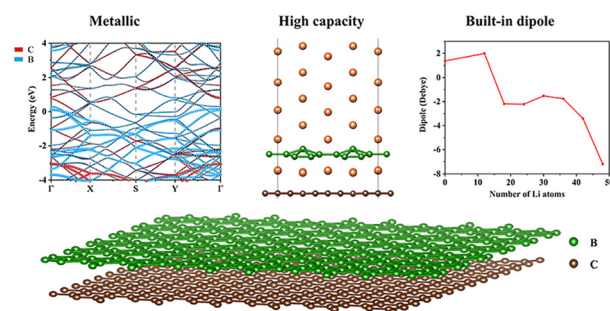
Teemu Härkönen,* Erik M. Vartiainen, Lasse Lensu, Matthew T. Moores and Lassi Roininen



3400

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

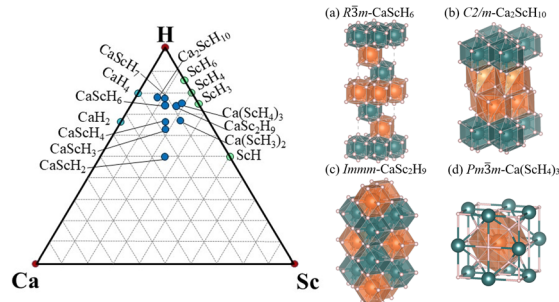
Xiaowei Jiang, Wenjun Tang, Xiaobin Niu and Haiyuan Chen*



3408

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

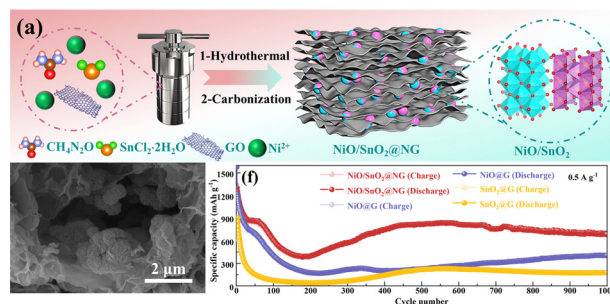
Wenjie Yuan, Xu Yang, Shichang Li,* Chunbao Feng, Bole Chen, Ying Chang and Dengfeng Li*



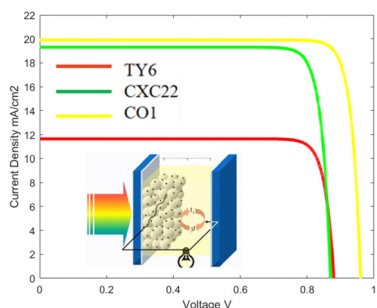
3415

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



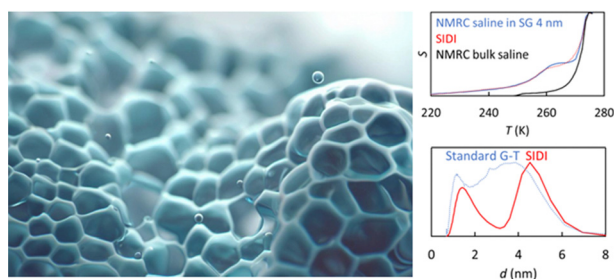
3424



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*

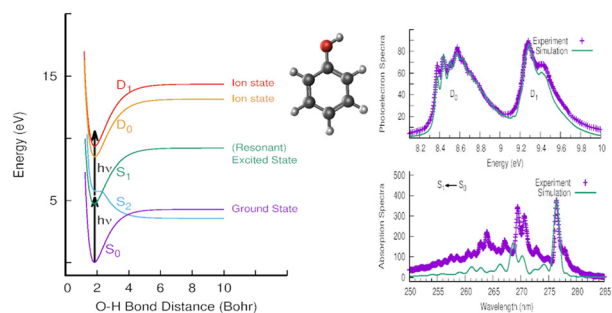
3441



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

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

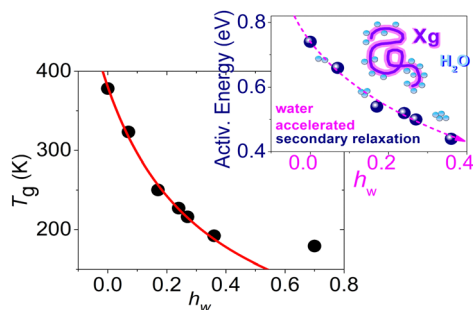
3451



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

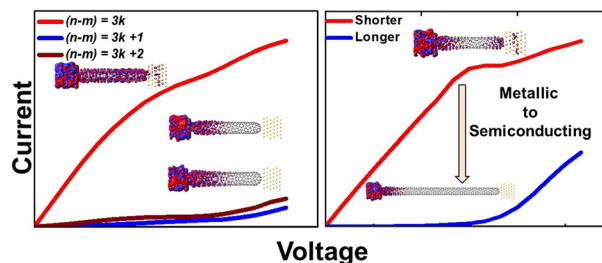
Sokratis N. Tegopoulos, Aristeidis Papagiannopoulos and Apostolos Kyritsis*



3474

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

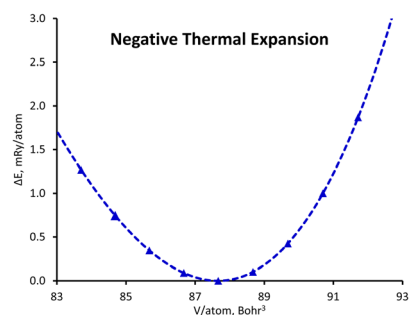
Ameet Kumar, Sudip Sarkar* and Daeheum Cho*



3482

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

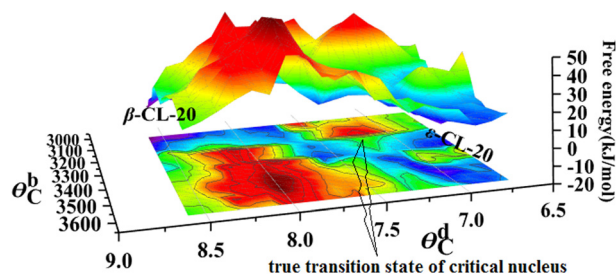
Dmitry Vasilyev



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

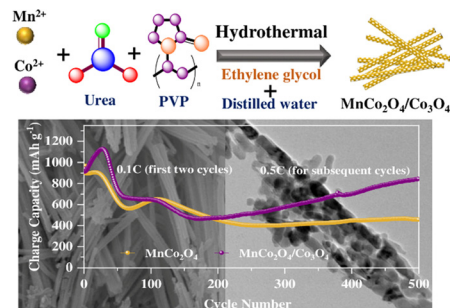
Fu-de Ren,* Ying-Zhe Liu, Ke-wei Ding, Ling-ling Chang, Duan-lin Cao and Shubin Liu*



3516

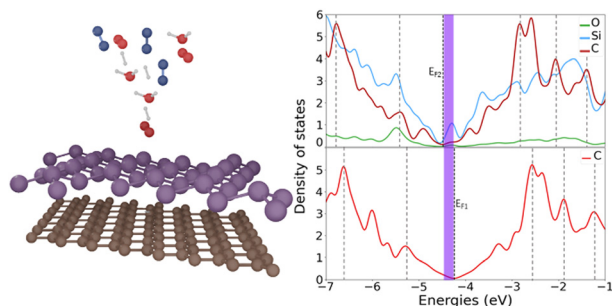
Boosting the high-rate performance of lithium-ion battery anodes using $\text{MnCo}_2\text{O}_4/\text{Co}_3\text{O}_4$ nanocomposite interfaces

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



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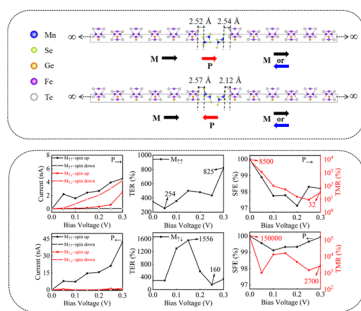
3525



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*

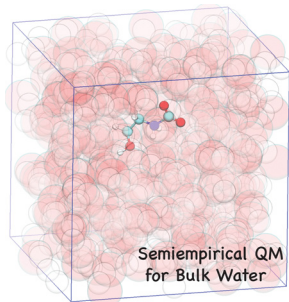
3531



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

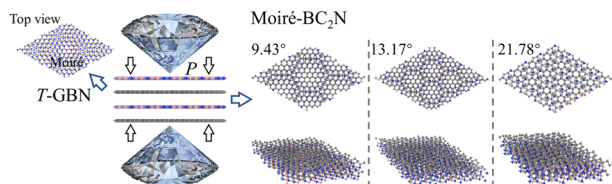
3540



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

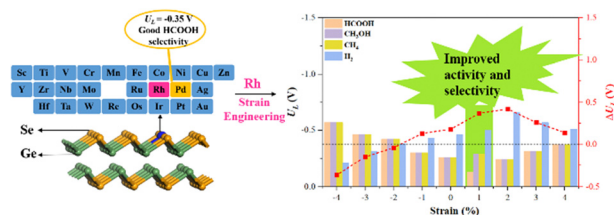
Yaomin Li and Bin Zhang*



3560

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

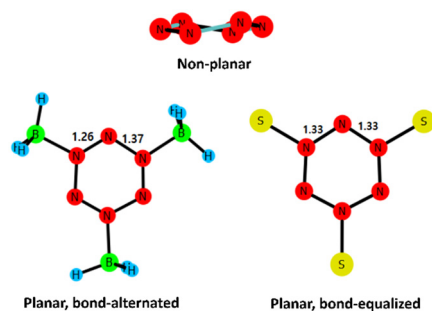
Yu-wang Sun, Lei Liu and Jing-yao Liu*



3569

Bond-alternated and bond-equalized hexazine derivatives

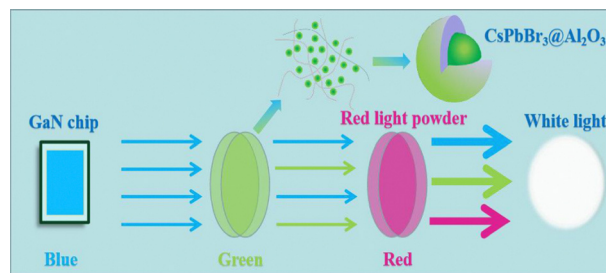
Kunnumma Chelladath Krishnapriya, Ashith Thayyil, Mithu Kumari and Priyakumari Chakkingal Parambil*



3578

Enhanced stability of CsPbBr₃ nanocrystals through Al₂O₃ and polymer coating

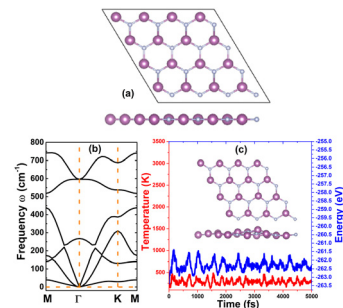
Sheng Huang,* Ce Bian, Wenjie Xu, Hui Zhang, Shasha Gao, Yue Wang* and Yuling Wang*



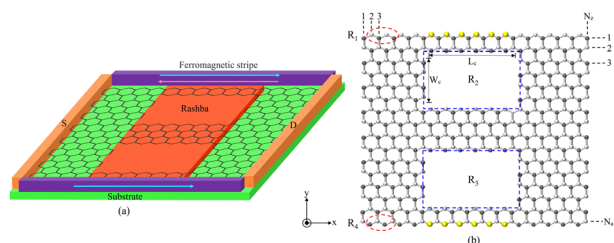
3587

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*



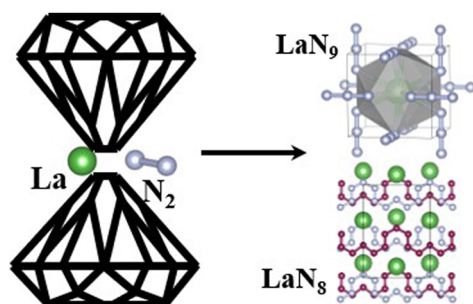
3597



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

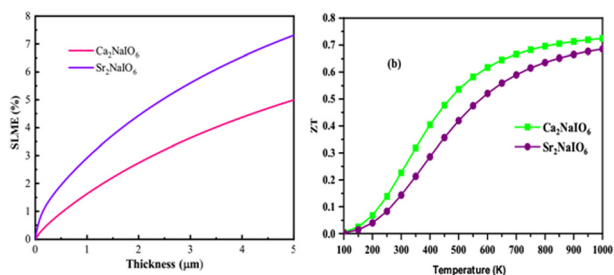
3605



Lanthanium 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

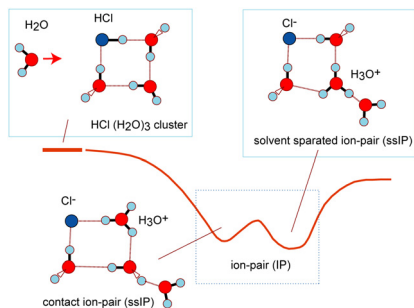
3614



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

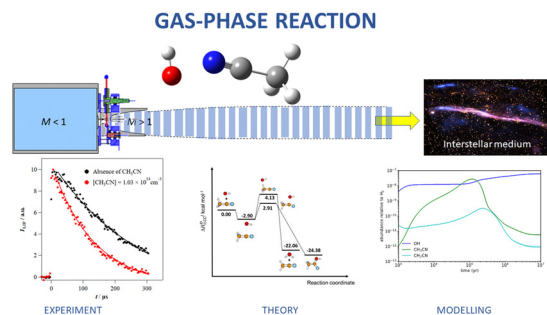
Hiroto Tachikawa



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

