

## IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 26(4) 2707–3668 (2024)



### Cover

See Xiaoyu Wang, Michael J. Servis *et al.*, pp. 2877–2886. Image reproduced by permission of Argonne National Laboratory, managed and operated by UChicago Argonne, LLC, for the U.S. Department of Energy under Contract No. DE-AC02-06CH11357 from *Phys. Chem. Chem. Phys.*, 2024, 26, 2877.



### Inside cover

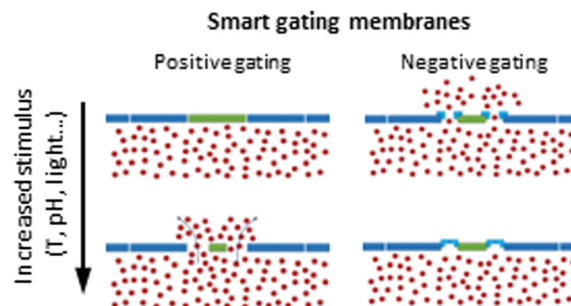
See Miriam Arak Freedman *et al.*, pp. 2887–2894. Image reproduced by permission of Danielle Zemba from *Phys. Chem. Chem. Phys.*, 2024, 26, 2887.

## REVIEWS

2732

### A review of stimuli-responsive polymer-based gating membranes

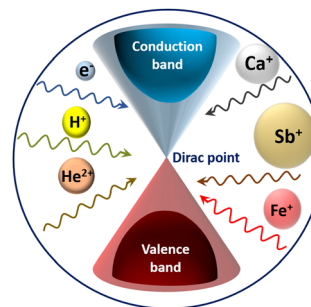
Stefanie Uredat, Aditi Gujare, Jonas Runge, Domenico Truzzolillo, Julian Oberdisse\* and Thomas Hellweg\*



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\*



# RSC Advances

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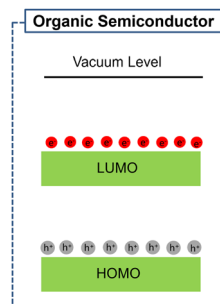
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2768

### Energy level measurement for organic semiconductors

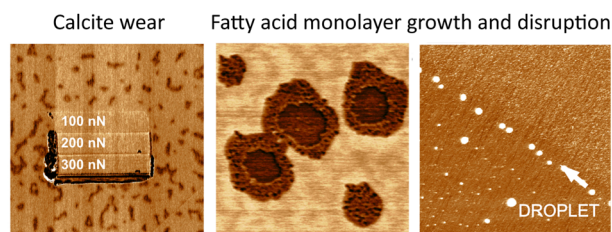
Xuehua Zhou,\* Shixing Yang, Qingxia Li,  
Guoliang Bai, Chunhua Wang and Chao Han\*



2780

### The dynamic nature of natural and fatty acid modified calcite surfaces

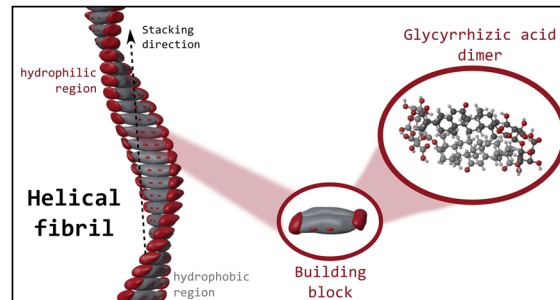
Per M. Claesson,\* Natalia A. Wojas,\* Robert Corkery,  
Andra Dedinaite, Joachim Schoelkopf and Eric Tyrode



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

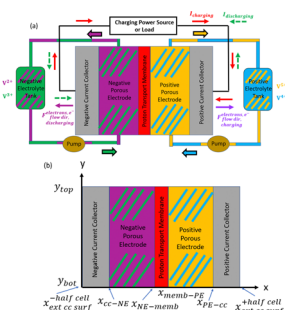
Frank Weinhold\* and Eric D. Glendening

"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

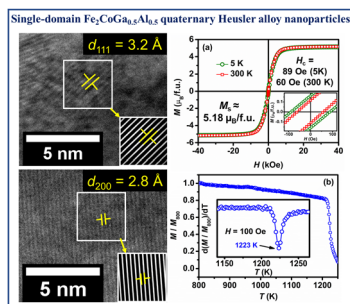


### Physics, electrochemistry, chemistry, and electronics of the vanadium redox flow battery by analyzing all the governing equations

Clifford M. Krowne

## COMMUNICATIONS

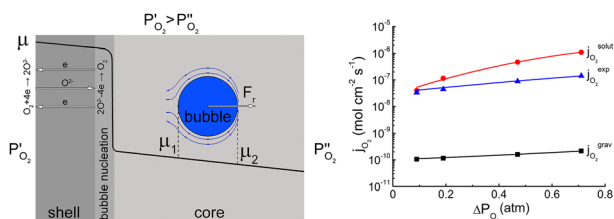
2863



### 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

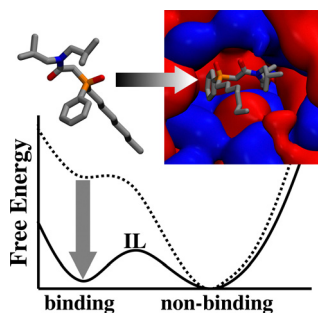


### Solutocapillary transport of oxygen bubbles in a diffusion-bubbling membrane core

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\*

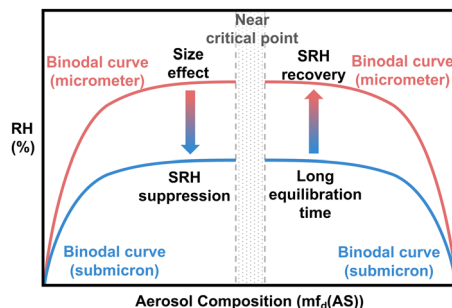


## RESEARCH PAPERS

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

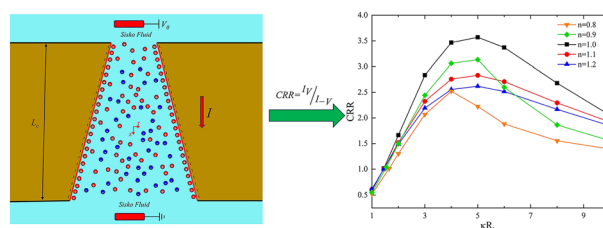
Qishen Huang, Kiran R. Pitta, Kayla Constantini, Emily-Jean E. Ott, Andreas Zuend and Miriam Arak Freedman\*



2895

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

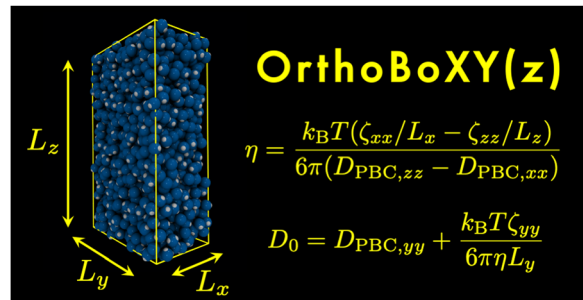
Lei Tang, Yu Hao, Li Peng, Runxin Liu, Yi Zhou and Jie Li\*



2907

### An OrthoBoXY-method for various alternative box geometries

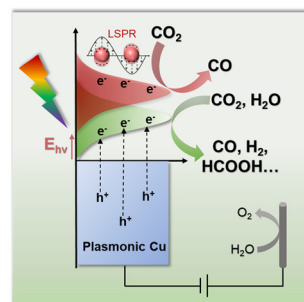
Johanna Busch and Dietmar Paschek\*



2915

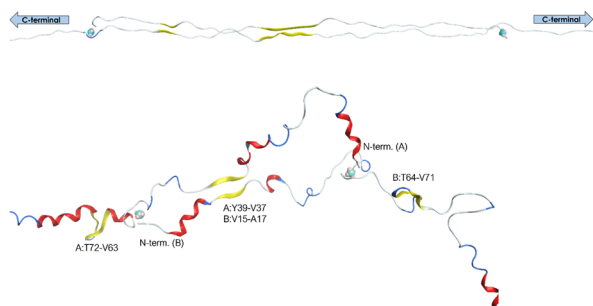
### The plasmonic effect of Cu on tuning CO<sub>2</sub> reduction activity and selectivity

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



## RESEARCH PAPERS

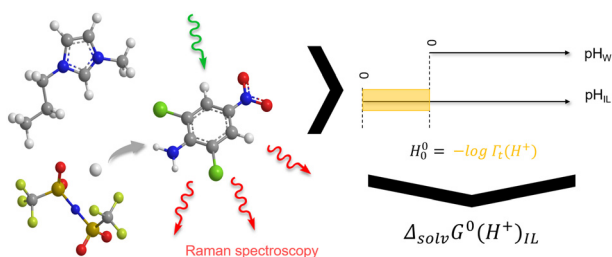
2926



### Computational investigation of copper-mediated conformational changes in $\alpha$ -synuclein dimer

Loizos Savva and James A. Platts\*

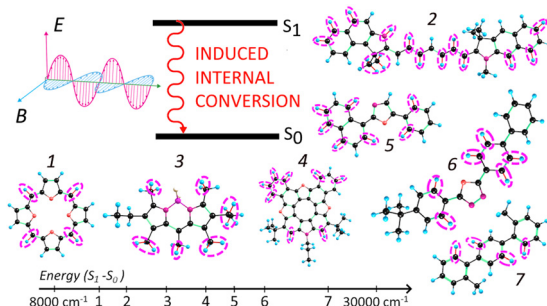
2936



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

Aurelie Rensonnet and Cedric Malherbe\*

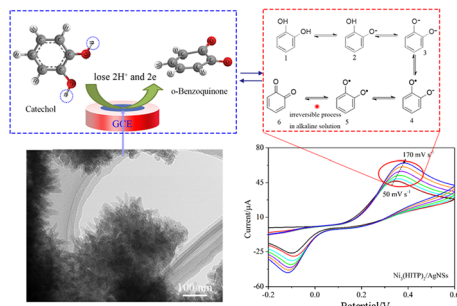
2945



### 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\*

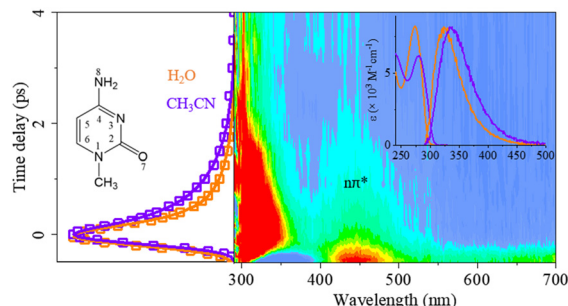


## RESEARCH PAPERS

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

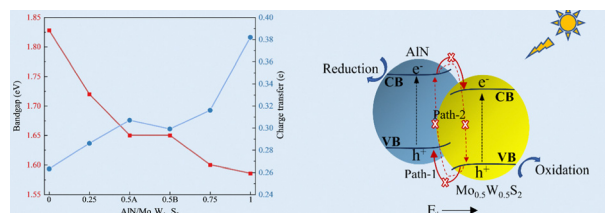
Chensheng Ma,\* Qingwu Xiong, Jingdong Lin, Xiaoyan Zeng, Mingliang Wang and Wai-Ming Kwok\*



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

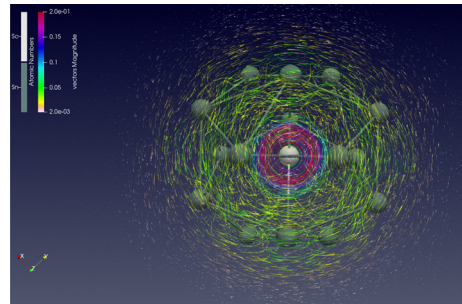
Liang Xu,\* Can Li, S. X. Xiong,\* Shuaihao Tang, Zhiqiang Xu, Lei Cao, Ji Tao, Ying Zhang, Kejun Dong\* and Ling-Ling Wang



2986

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

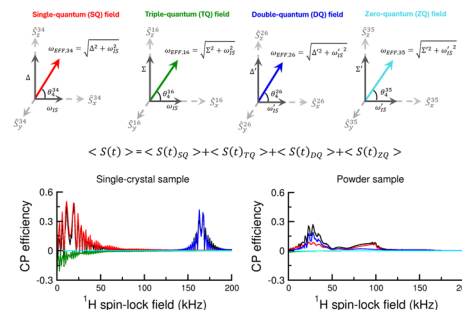
Jin-Kun Zeng, Huai-Qian Wang,\* Hui-Fang Li, Hao Zheng, Jia-Ming Zhang, Xun-Jie Mei, Yong-Hang Zhang and Xun-Lei Ding



2995

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

Ekta Nehra and Manoj Kumar Pandey\*

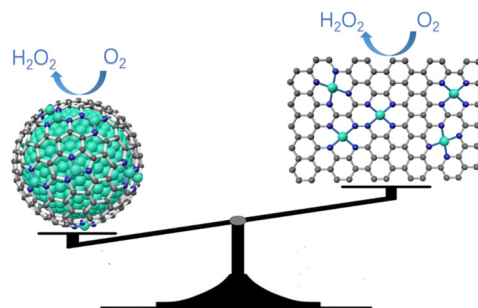




3044

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

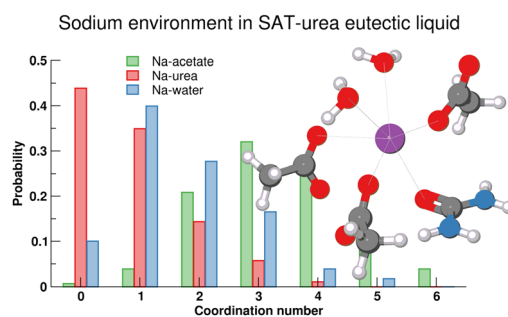
Kun Li, Yanyan Sun,\* Ziwei Zhao and Ting Zhu\*



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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

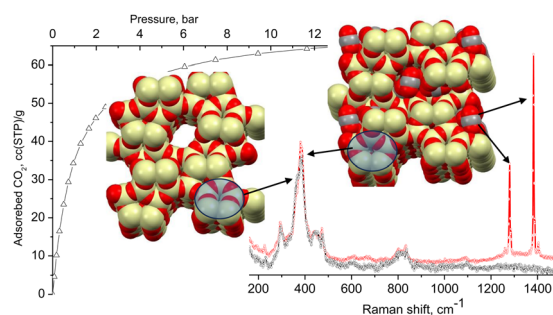
Emily L. Byrne, Sanskrita Madhukailya, Oliver L. G. Alderman, Marijana Blesic and John D. Holbrey\*



3060

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

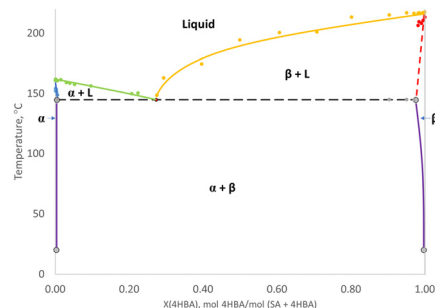
Dimitar V. Tzankov and Peter A. Georgiev\*



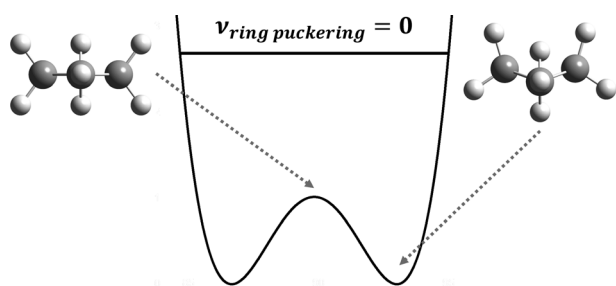
3069

### 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\*



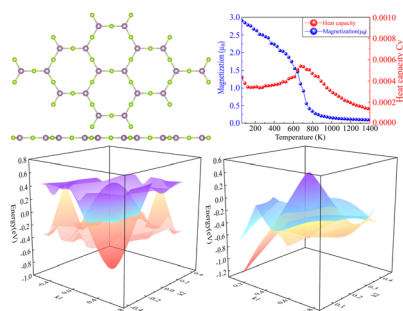
3081



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

Ya-Chu Chan and David J. Nesbitt\*

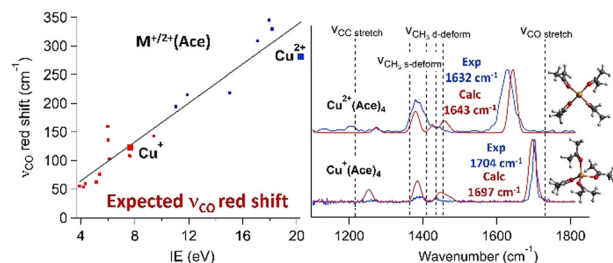
3092



### 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\*

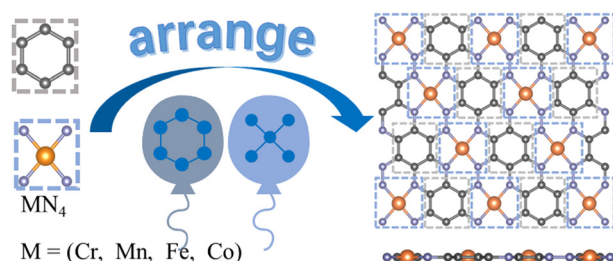
3101



### 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 Ni<sub>13</sub>@Ag<sub>42</sub> nanoparticle under surface oxidation: the role of silver coating

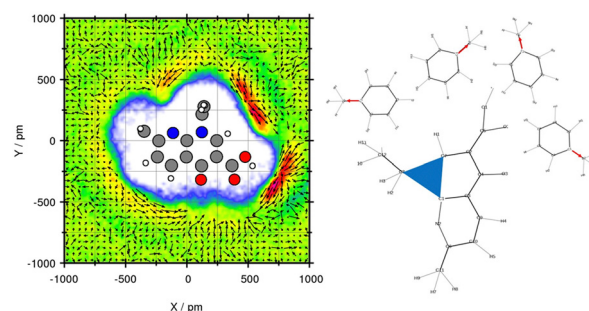
R. H. Aguilera-del-Toro,\* F. Aguilera-Granja and A. Vega

Ag<sub>42</sub>Ni<sub>13</sub> 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

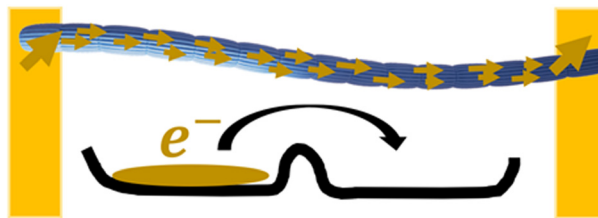
Miriam Sprick and Gabriele Raabe\*



3139

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

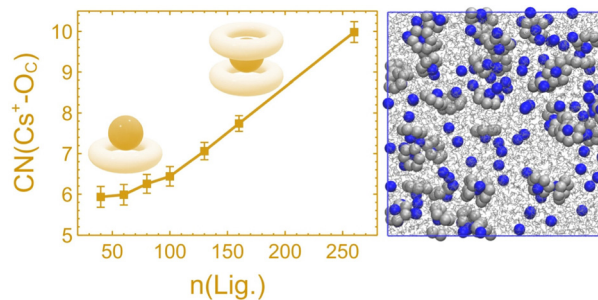
Jasper R. van der Veen,\* Stephanie Valianti, Herre S. J. van der Zant, Yaroslav M. Blanter and Filip J. R. Meysman\*



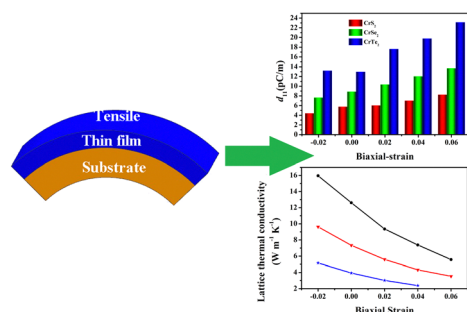
3152

### Exclusive ion recognition using host-guest sandwich complexes

Nitesh Kumar



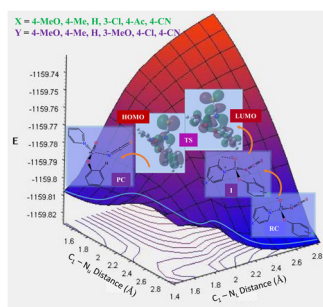
3159



Equibiaxial strain regulates the electronic structure and mechanical, piezoelectric, and thermal transport properties of the 2H-phase monolayers  $\text{CrX}_2$  ( $X = \text{S, Se, Te}$ )

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

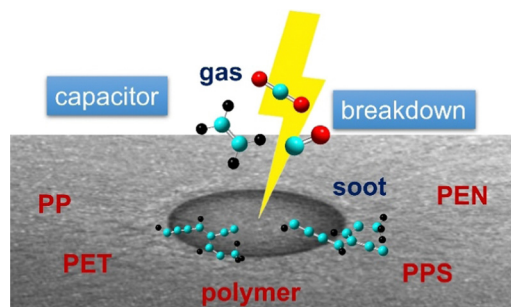
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Theoretical investigation of nucleophilic substitution reaction of phenyl carbonyl isothiocyanates with pyridines in gas and polar aprotic solvent

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

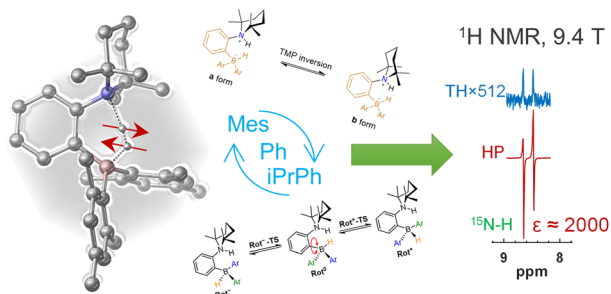
3184



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

Vitaly V. Chaban\* and Nadezhda A. Andreeva

3197



Activation of  $\text{H}_2$  using *ansa*-aminoboranes: solvent effects, dynamics, and spin hyperpolarization

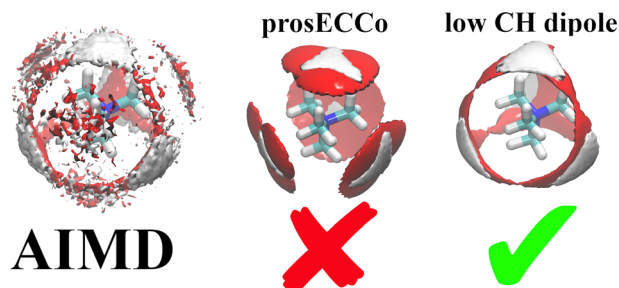
Karolina Konsewicz, Gergely Laczkó, Imre Pápai and Vladimir V. Zhivonitko\*



3208

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

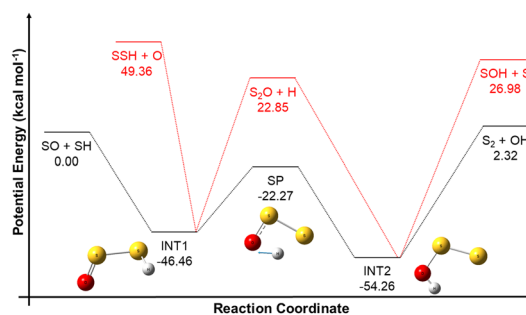
Philip E. Mason,\* Tomas Martinek, Balázs Fábrián, Mario Vazdar, Pavel Jungwirth, Ondrej Tichacek, Elise Duboué-Dijon and Hector Martinez-Seara\*



3219

### Quantum chemistry and kinetics of hydrogen sulphide oxidation

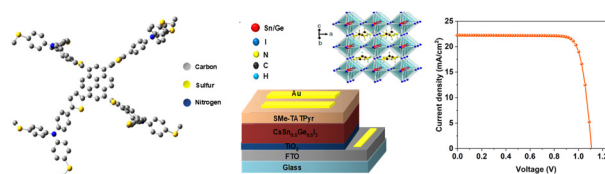
M. Monge-Palacios,\* Q. Wang,\* A. Alshaarawi, A. C. Cavazos Sepulveda and S. M. Sarathy



3229

### Improved eco-friendly CsSn<sub>0.5</sub>Ge<sub>0.5</sub>I<sub>3</sub> perovskite photovoltaic efficiency beyond 20% with SME-TATPy hole-transporting layer

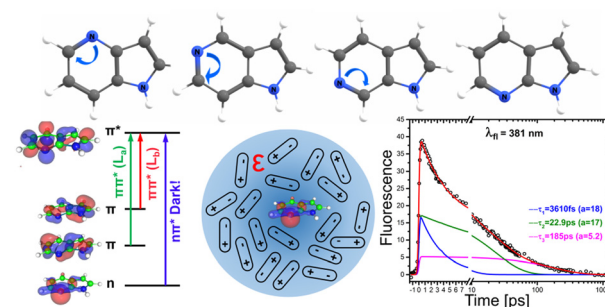
Mustafa K. A. Mohammed,\* Moaed E. Al-Gazally, Omar A. Khaleel, Ali K. Al-Mousoi, Zuhair Mohammed Ali Jeddoo, Hasan Sh. Majdi, Majid S. Jabir, M. Khalid Hossain, Mohammad Rafe Hatshan, Md. Ferdous Rahman and Davoud Dastan



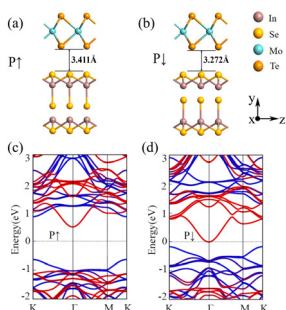
3240

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

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



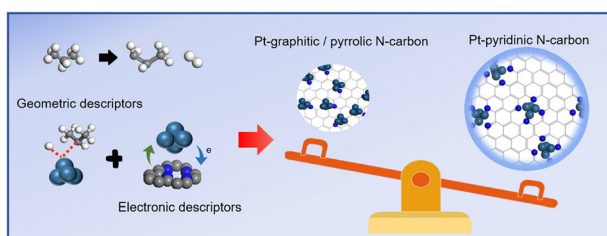
3253



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

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

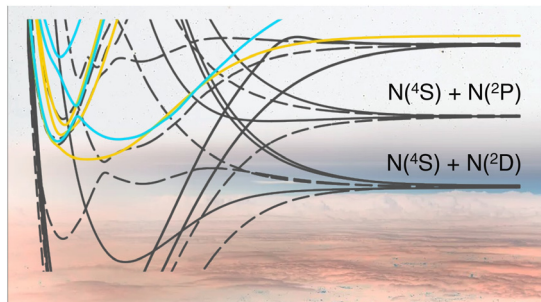
3263



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

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

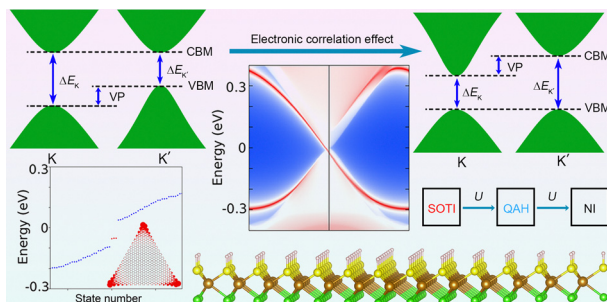
3274



### Nonadiabatic quantum dynamics explores non-monotonic photodissociation branching of $\text{N}_2$ 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

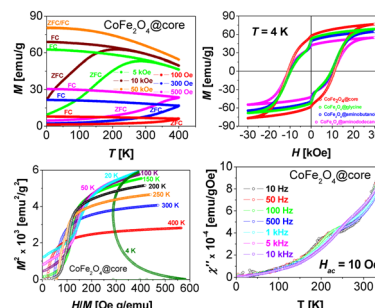
Mengteng Chen, Xiangru Kong,\* Xiao Xie, Xiaobiao Liu,  
Jia Li, François M. Peeters and Linyang Li\*



3296

### Magnetic studies of ultrafine $\text{CoFe}_2\text{O}_4$ nanoparticles with different molecular surface coatings

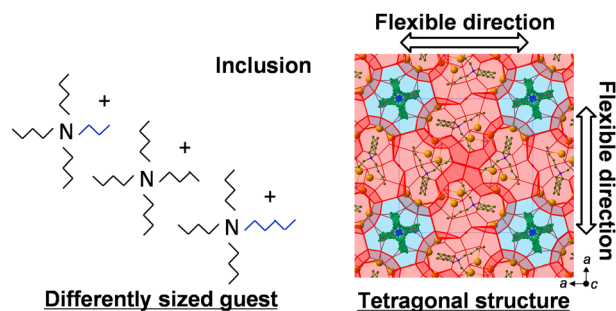
Ewa Mosiniwicz-Szablewska,\* Leandro Carlos Figueiredo, Atailson Oliveira da Silva, Marcelo Henrique Sousa and Paulo César de Morais



3315

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

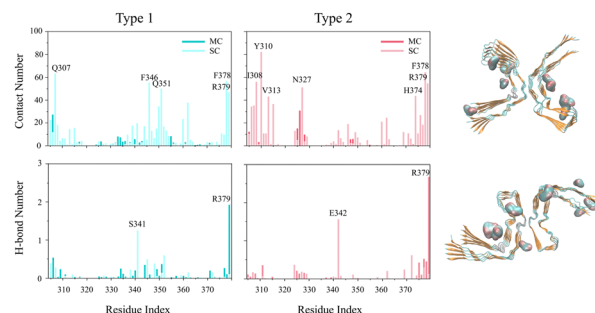
Sanehiro Muromachi\* and Satoshi Takeya



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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

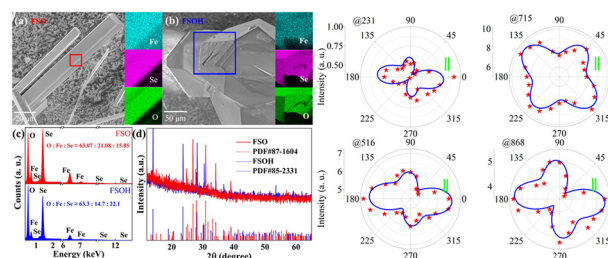
Jiaxing Tang, Ruiqing Sun, Jiaqian Wan, Yu Zou\* and Qingwen Zhang\*



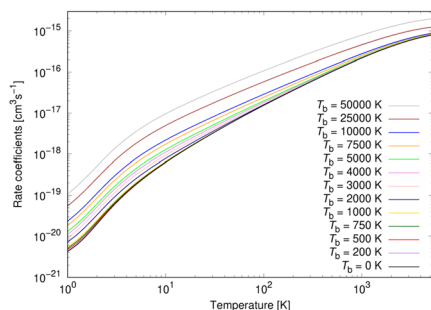
3335

### 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\*



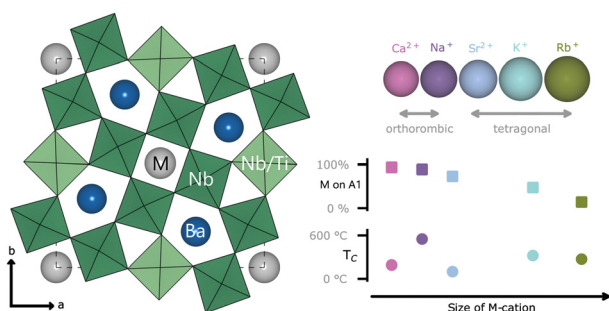
3342



### 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

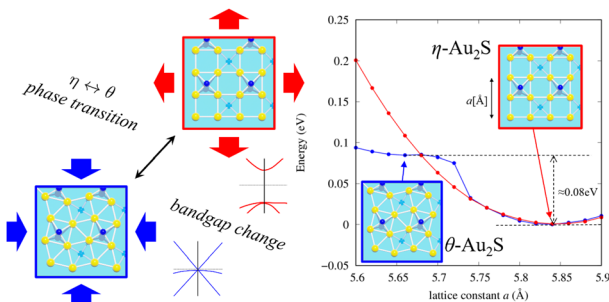
3350



### 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 $\text{Rb}$ ) and $\text{Ba}_4\text{M}_2\text{Nb}_8\text{Ti}_2\text{O}_{30}$ ( $\text{M} = \text{Ca}$ or $\text{Sr}$ )

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

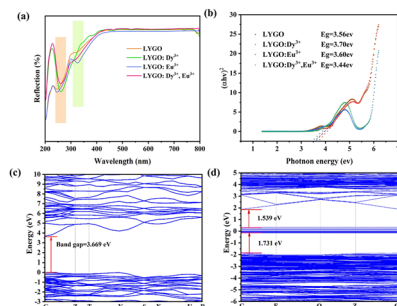
3367



### Electronic band structure change with structural transition of buckled $\text{Au}_2\text{X}$ monolayers induced by strain

Masahiro Fukuda\* and Taisuke Ozaki

3375



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

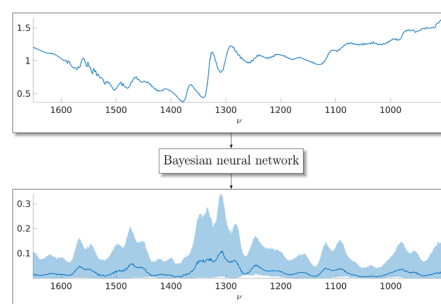
Chunyu Zuo, Rujia Chen, Xiliang Jiang, Zhuang Leng, Yimin Yang, Zhipeng Zhang, Lingbo Zhou, Chun Li,\* Weiling Yang,\* Hai Lin, Lina Liu, Shasha Li, Fanming Zeng\* and Zhongmin Su



3389

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

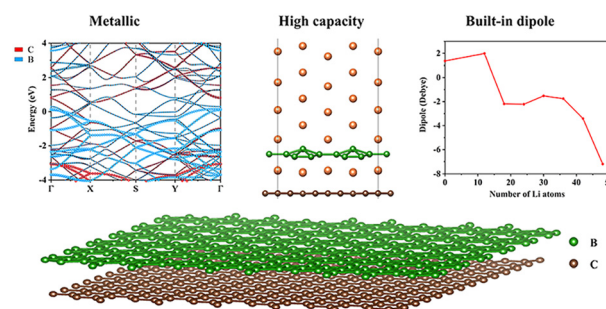
Teemu Härkönen,\* Erik M. Vartiainen, Lasse Lensu, Matthew T. Moores and Lassi Roininen



3400

### Enhancement of multilayer lithium storage in a $\beta$ -12-borophene/graphene heterostructure with built-in dipoles

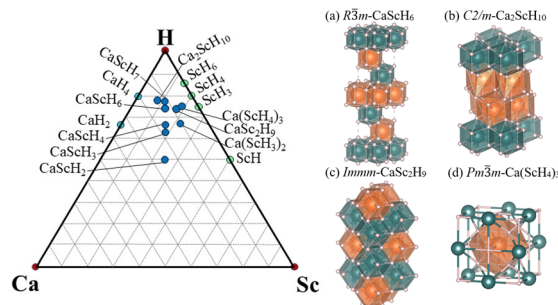
Xiaowei Jiang, Wenjun Tang, Xiaobin Niu and Haiyuan Chen\*



3408

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

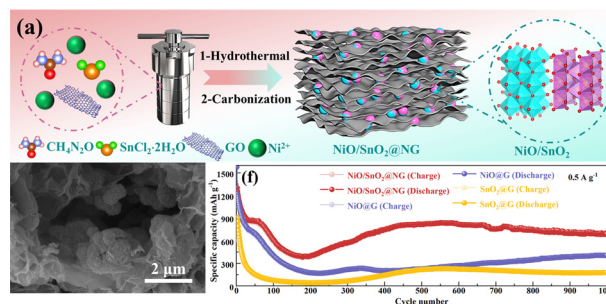
Wenjie Yuan, Xu Yang, Shichang Li,\* Chunbao Feng, Bole Chen, Ying Chang and Dengfeng Li\*



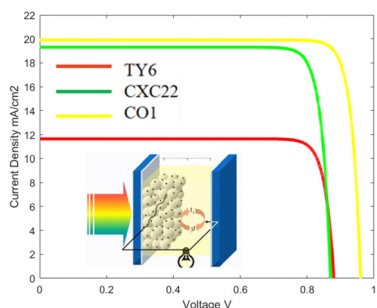
3415

### Synthesis of heterointerfaces in NiO/SnO<sub>2</sub> coated nitrogen-doped graphene for efficient lithium storage

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



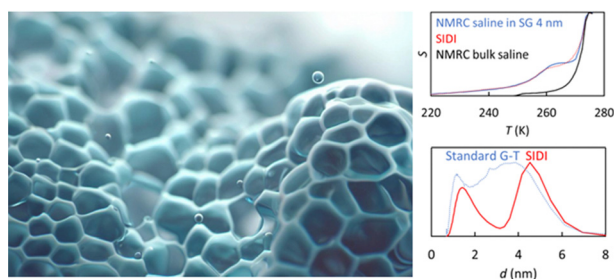
3424



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

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

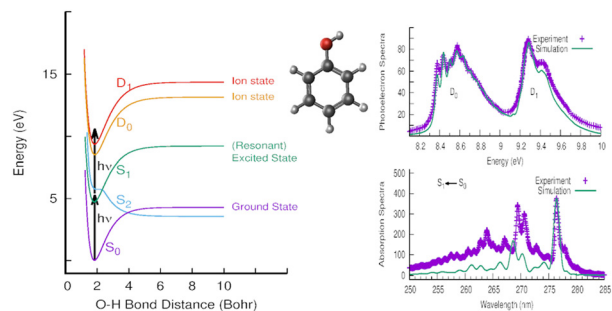
3441



### 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\*

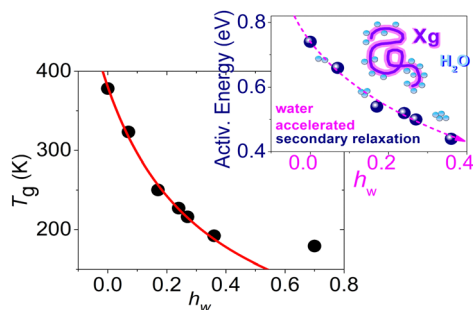
3451



### 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

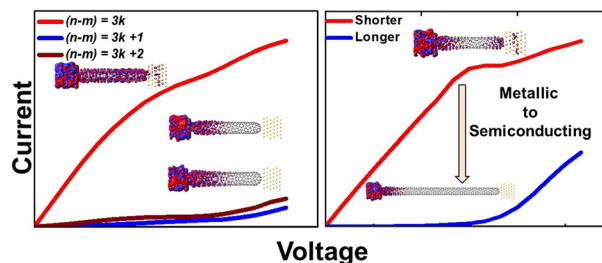
Sokratis N. Tegopoulos, Aristeidis Papagiannopoulos and Apostolos Kyritsis\*



3474

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

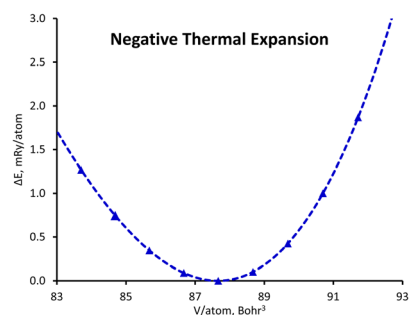
Ameet Kumar, Sudip Sarkar\* and Daeheum Cho\*



3482

### Thermal expansion anisotropy of $\text{Fe}_{23}\text{Mo}_{16}$ and $\text{Fe}_7\text{Mo}_6$ $\mu$ -phases predicted using first-principles calculations

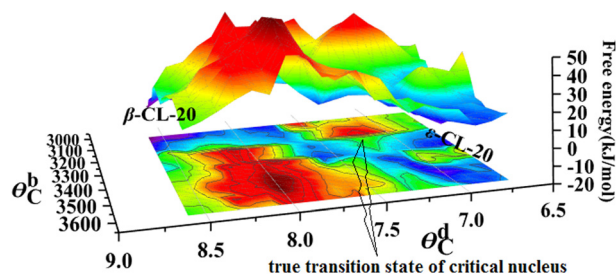
Dmitry Vasilyev



3500

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

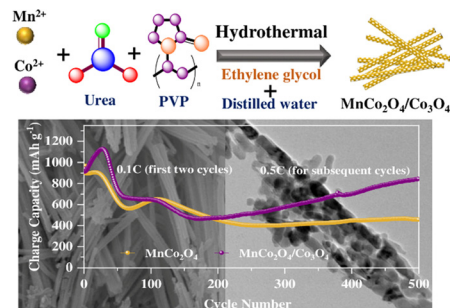
Fu-de Ren,\* Ying-Zhe Liu, Ke-wei Ding, Ling-ling Chang, Duan-lin Cao and Shubin Liu\*



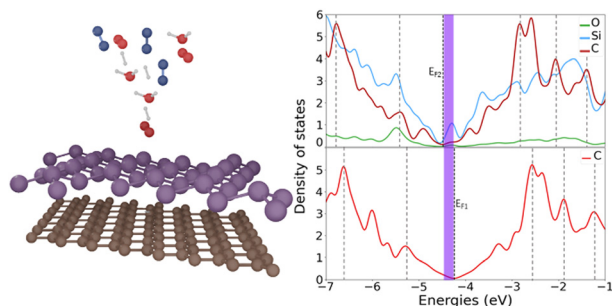
3516

### 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\*



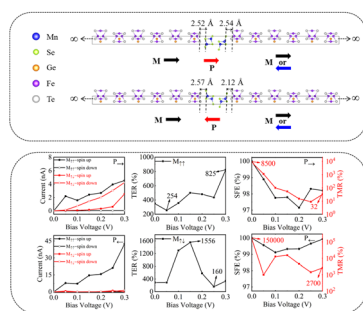
3525



### A weakened Fermi level pinning induced adsorption energy non-charge-transfer mechanism during O<sub>2</sub> adsorption in silicene/graphene heterojunctions

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

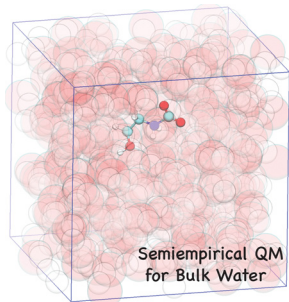
3531



### 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

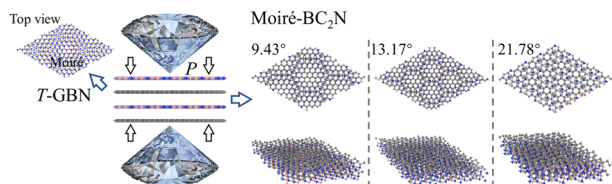
3540



### Developing semi-empirical water model for efficiently simulating temperature-dependent chemisorption of CO<sub>2</sub> 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

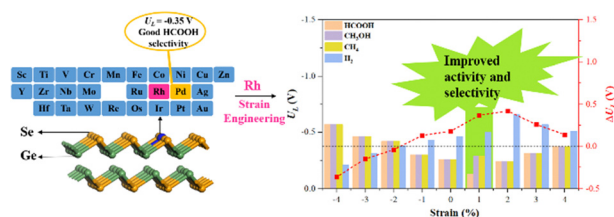
Yaomin Li and Bin Zhang\*



3560

## Enhancing CO<sub>2</sub> electroreduction performance through transition metal atom doping and strain engineering in $\gamma$ -GeSe: a first-principles study

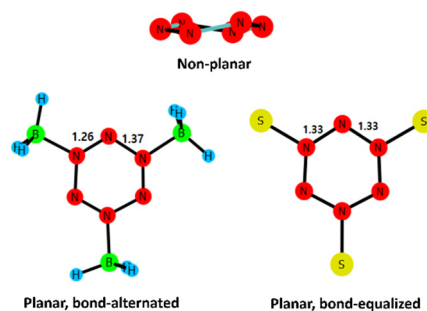
Yu-wang Sun, Lei Liu and Jing-yao Liu\*



3569

## Bond-alternated and bond-equalized hexazine derivatives

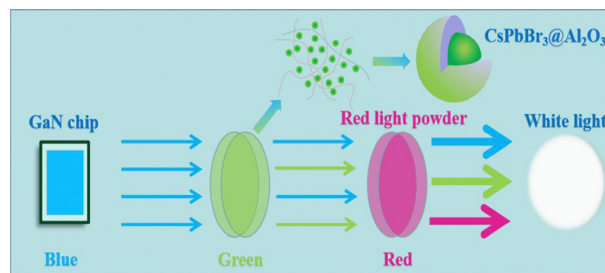
Kunnumma Chelladath Krishnapriya, Ashith Thayyil, Mithu Kumari and Priyakumari Chakkingal Parambil\*



3578

## Enhanced stability of CsPbBr<sub>3</sub> nanocrystals through Al<sub>2</sub>O<sub>3</sub> and polymer coating

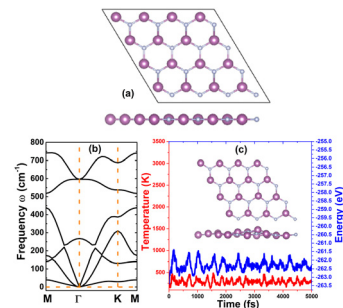
Sheng Huang,\* Ce Bian, Wenjie Xu, Hui Zhang, Shasha Gao, Yue Wang\* and Yuling Wang\*



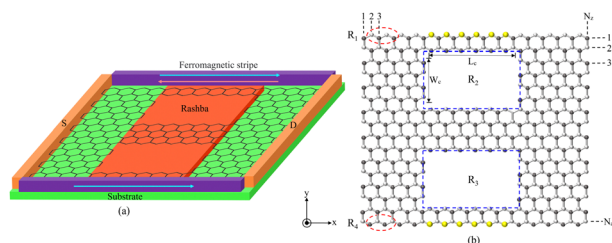
3587

## 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\*



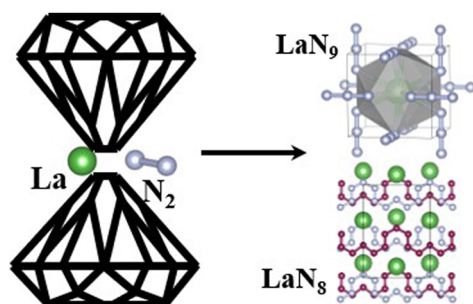
3597



### 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

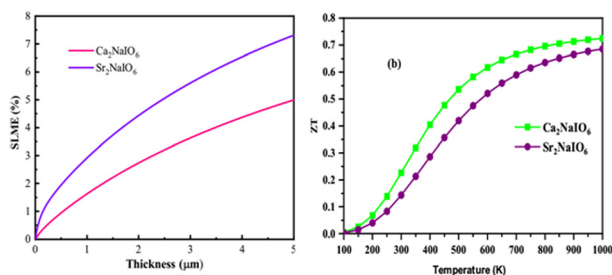
3605



### Lanthanium nitride $\text{LaN}_9$ 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

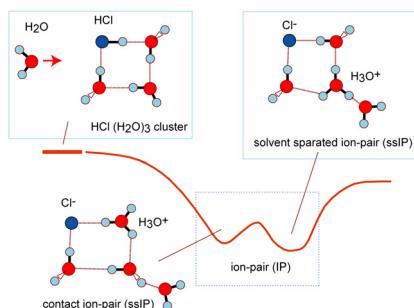
3614



### Optoelectronic and thermoelectric properties of novel stable lead-free cubic double perovskites $\text{A}_2\text{NaIO}_6$ ( $\text{A} = \text{Ca}, \text{Sr}$ ) 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

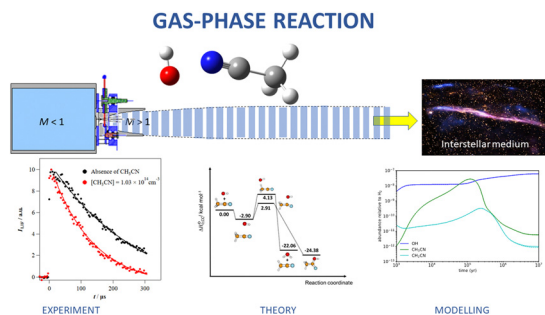
Hiroto Tachikawa



3632

**Effect of temperature on the gas-phase reaction of CH<sub>3</sub>CN 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

