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### IN THIS ISSUE

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#### Cover

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Michael J. Servis  
*et al.*, pp. 2877–2886.  
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2024, **26**, 2877.



#### Inside cover

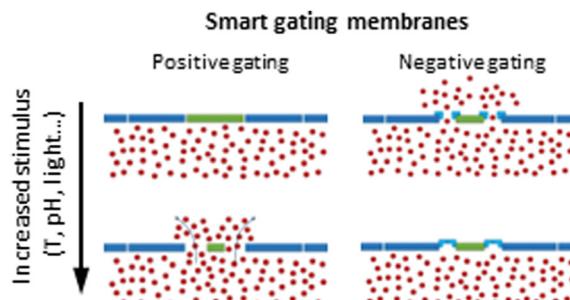
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### REVIEWS

2732

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

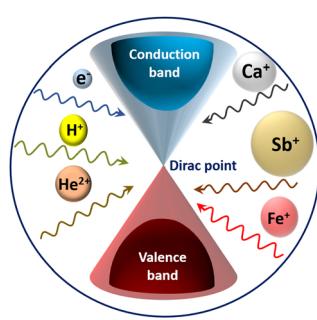
Stefanie Uredat, Aditi Gujare, Jonas Runge,  
Domenico Truzzolillo, Julian Oberdisse\* and  
Thomas Hellweg\*



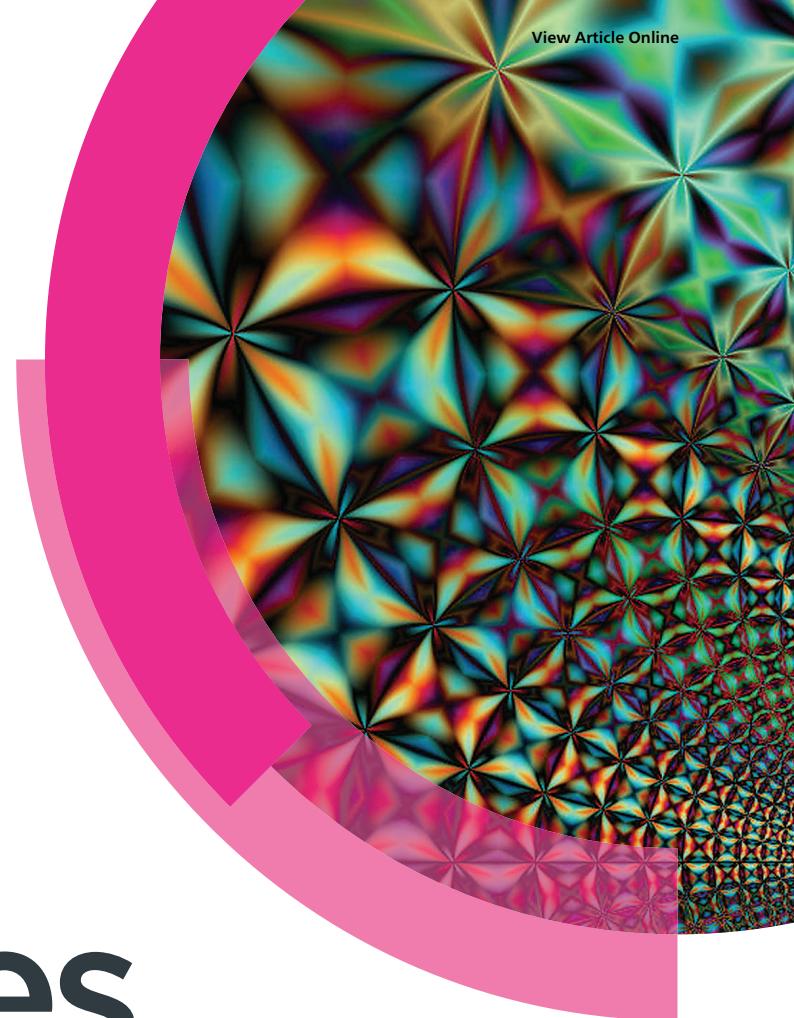
2745

#### 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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## PERSPECTIVES

2768

**Energy level measurement for organic semiconductors**Xuehua Zhou,\* Shixing Yang, Qingxia Li,  
Guoliang Bai, Chunhua Wang and Chao Han\*

## Organic Semiconductor

Vacuum Level

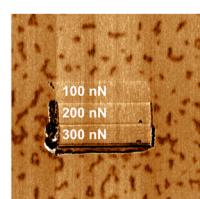
LUMO

HOMO

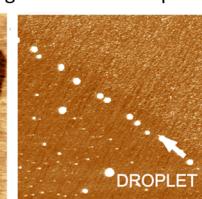
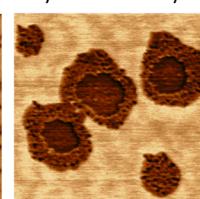
2780

**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

Calcite wear



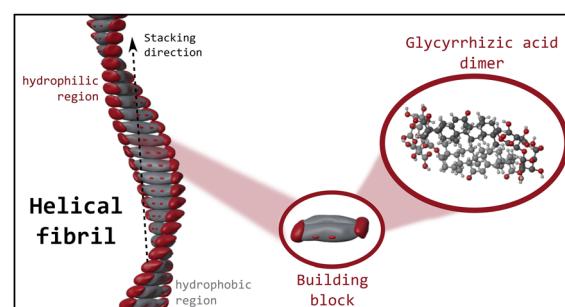
Fatty acid monolayer growth and disruption



2806

**Glycyrrhetic 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**

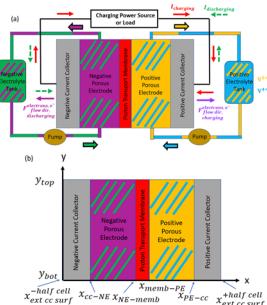
Frank Weinhold\* and Eric D. Glendening

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



## PERSPECTIVES

2823

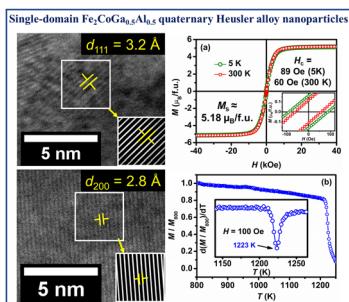


## Physics, electrochemistry, chemistry, and electronics of the vanadium redox flow battery by analyzing all the governing equations

Clifford M. Krown

## COMMUNICATIONS

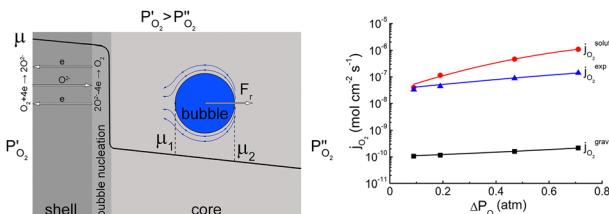
2863



## 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

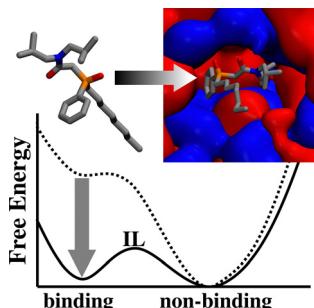


## Solutocapillary transport of oxygen bubbles in a diffusion-bubbling membrane core

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\*

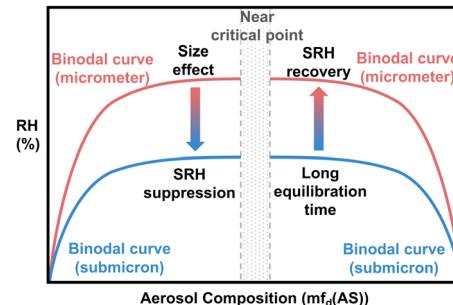


## RESEARCH PAPERS

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

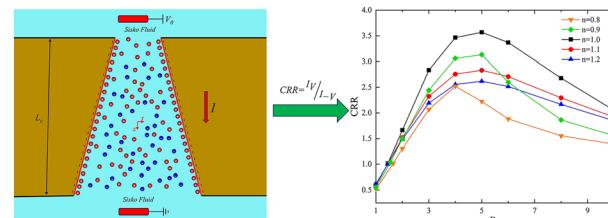
Qishen Huang, Kiran R. Pitta, Kayla Constantini, Emily-Jean E. Ott, Andreas Zuernd and Miriam Arak Freedman\*



2895

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

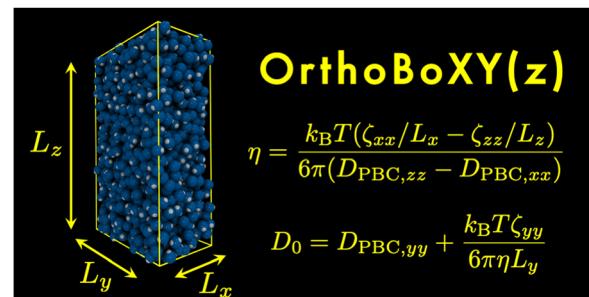
Lei Tang, Yu Hao, Li Peng, Runxin Liu, Yi Zhou and Jie Li\*



2907

## An OrthoBoXY-method for various alternative box geometries

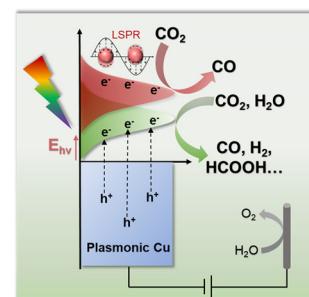
Johanna Busch and Dietmar Paschek\*



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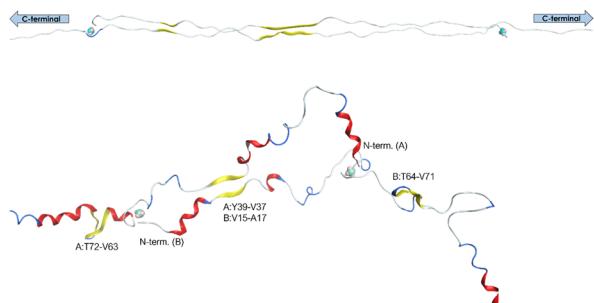
## The plasmonic effect of Cu on tuning CO<sub>2</sub> reduction activity and selectivity

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



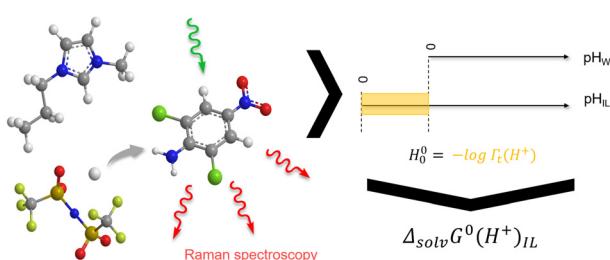
## RESEARCH PAPERS

2926

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

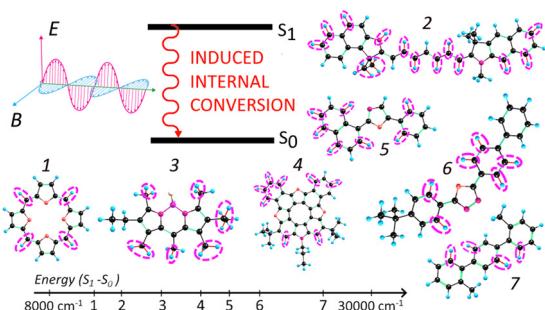
Loizos Savva and James A. Platts\*

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

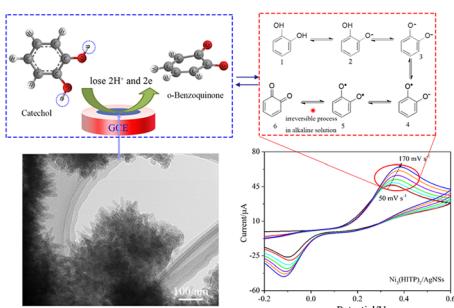
Aurelie Rensonnet and Cedric Malherbe\*

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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 Ni<sub>3</sub>(HITP)<sub>2</sub> 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\*

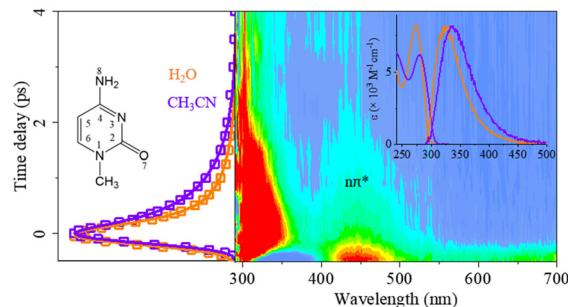


## RESEARCH PAPERS

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

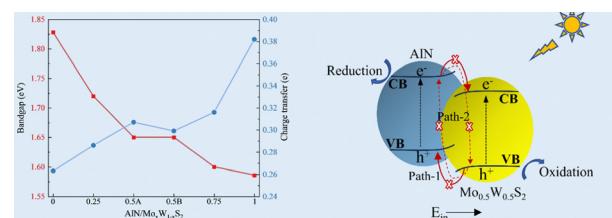
Chensheng Ma,\* Qingwu Xiong, Jingdong Lin, Xiaoyan Zeng, Mingliang Wang and Wai-Ming Kwok\*



2973

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

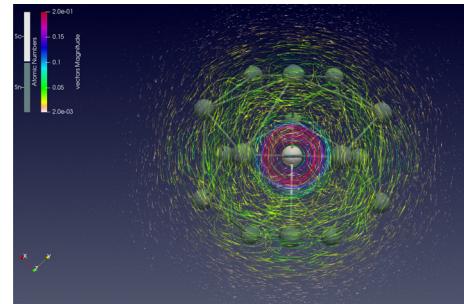
Liang Xu,\* Can Li, S. X. Xiong,\* Shuaihao Tang, Zhiqiang Xu, Lei Cao, Ji Tao, Ying Zhang, Kejun Dong\* and Ling-Ling Wang



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

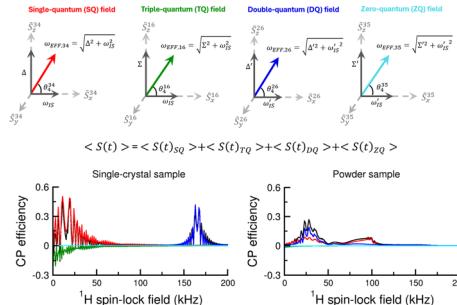
Jin-Kun Zeng, Huai-Qian Wang,\* Hui-Fang Li, Hao Zheng, Jia-Ming Zhang, Xun-Jie Mei, Yong-Hang Zhang and Xun-Lei Ding



2995

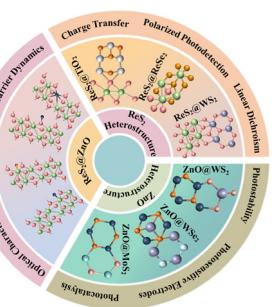
**Unravelling the mechanism of polarization transfer from spin-1/2 to spin-1 system in solids**

Ekta Nehra and Manoj Kumar Pandey\*



## RESEARCH PAPERS

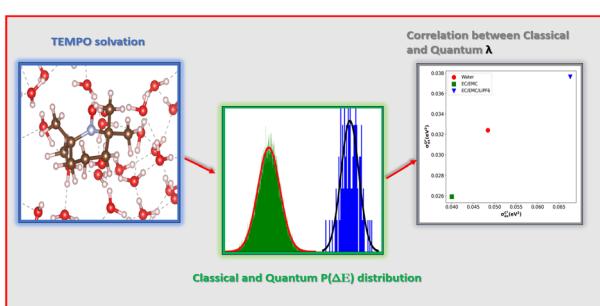
3008



**Study on interface engineering and chemical bonding of the  $\text{ReS}_2@\text{ZnO}$  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\*

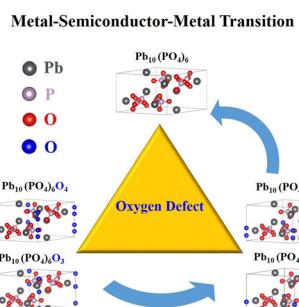
3020



**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\*

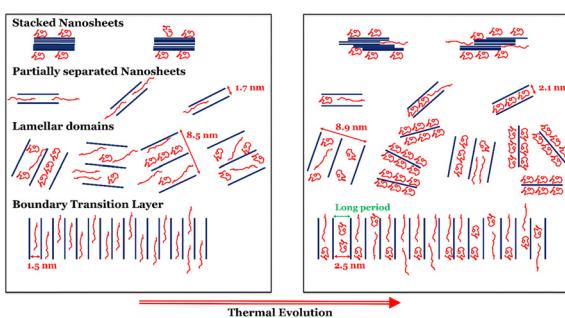
3029



**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\*

3036



**Thermal evolution of a polymer–nanoparticle binary mixture**

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

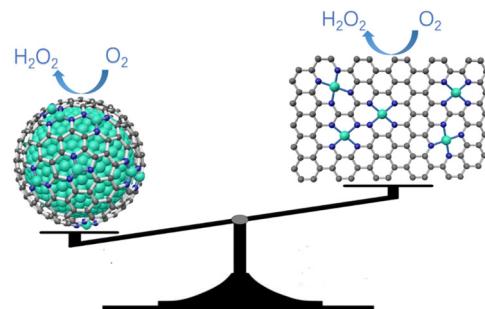


## RESEARCH PAPERS

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

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

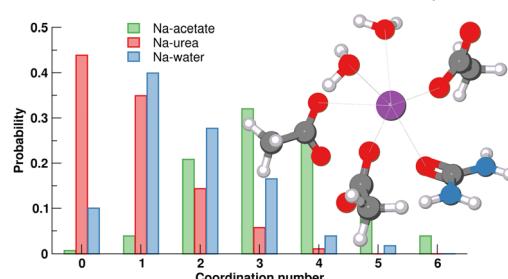


3051

**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\*

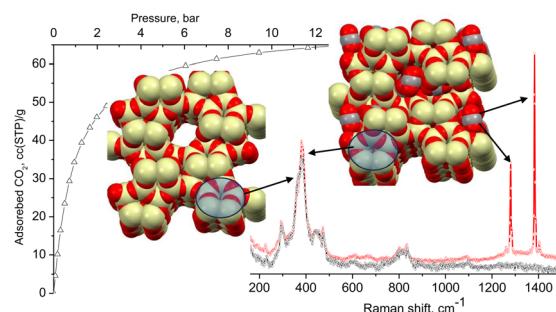
Sodium environment in SAT-urea eutectic liquid



3060

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

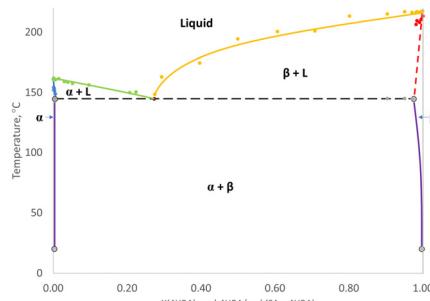
Dimitar V. Tzankov and Peter A. Georgiev\*



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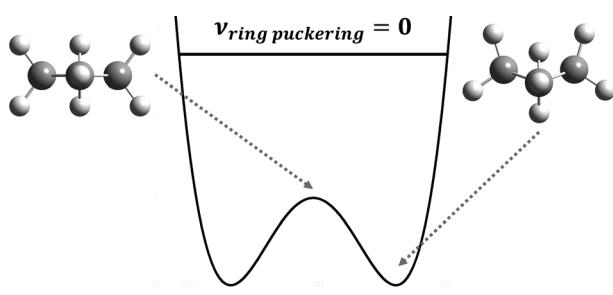
**Terminal crystalline solid solutions, solubility enhancements and T-X phase diagram of salicylic acid – 4-hydroxybenzoic acid**

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



## RESEARCH PAPERS

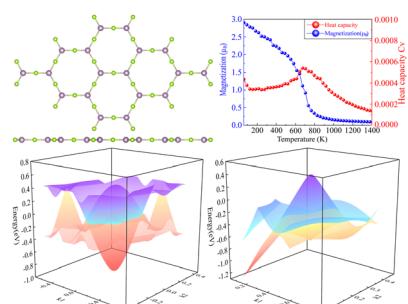
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### High-resolution infrared spectroscopy of jet cooled cyclobutyl in the $\alpha$ -CH stretch region: large-amplitude puckering dynamics in a 4-membered ring radical

Ya-Chu Chan and David J. Nesbitt\*

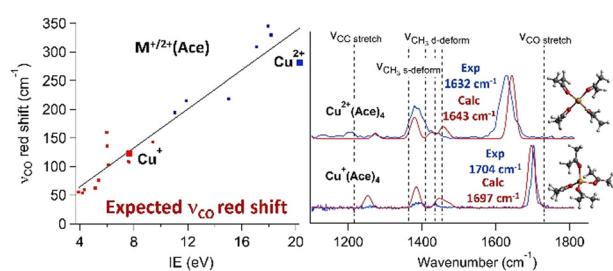
3092



### 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\*

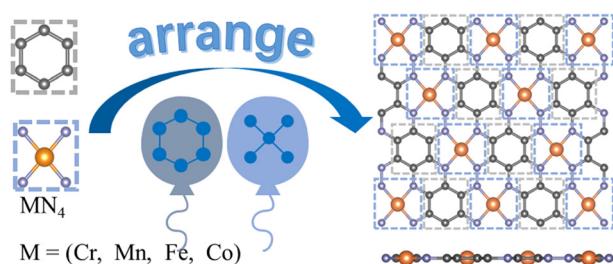
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### How the nature and charge of metal cations affect vibrations in acetone solvent molecules

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

3110



### Prediction of transition metal carbonitride monolayers $MN_4C_6$ ( $M = Cr, Mn, Fe$ , 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\*



## RESEARCH PAPERS

3117

**Structural and electronic changes in the  $\text{Ni}_{13}@\text{Ag}_{42}$  nanoparticle under surface oxidation: the role of silver coating**

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

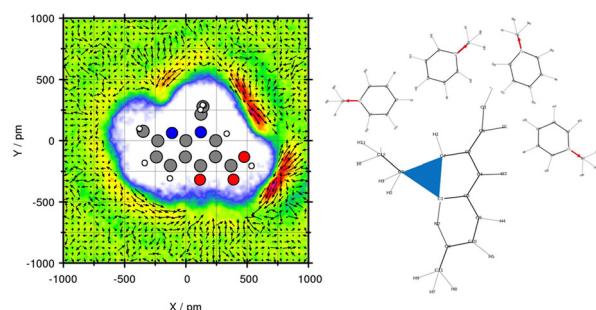


$\text{Ag}_{42}\text{Ni}_{13}$  nanoparticle oxidation.

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**

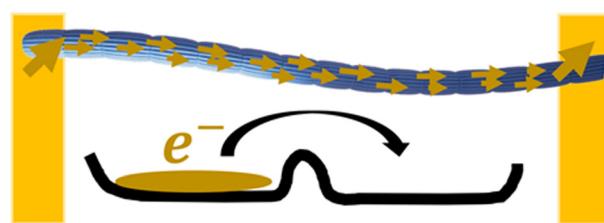
Miriam Sprick and Gabriele Raabe\*



3139

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

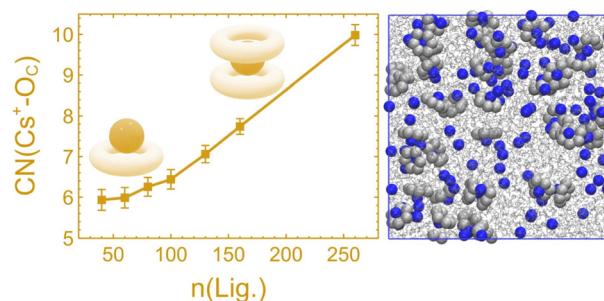
Jasper R. van der Veen,\* Stephanie Valianti, Herre S. J. van der Zant, Yaroslav M. Blanter and Filip J. R. Meysman\*



3152

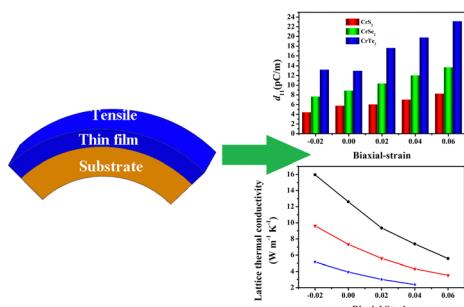
**Exclusive ion recognition using host–guest sandwich complexes**

Nitesh Kumar



## RESEARCH PAPERS

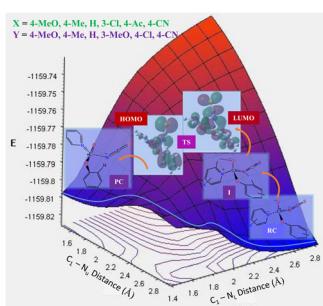
3159



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

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

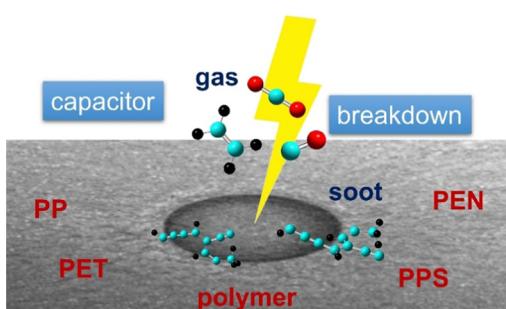
3168



## 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\*

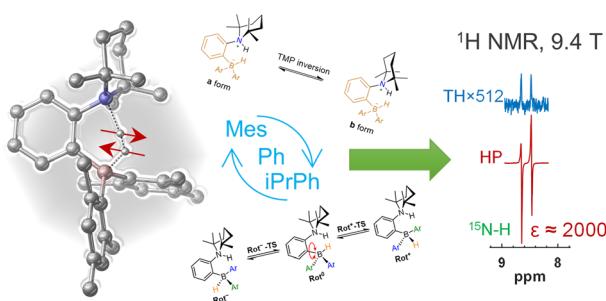
3184



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

Vitaly V. Chaban\* and Nadezhda A. Andreeva

3197



## Activation of H<sub>2</sub> using ansa-aminoboranes: solvent effects, dynamics, and spin hyperpolarization

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

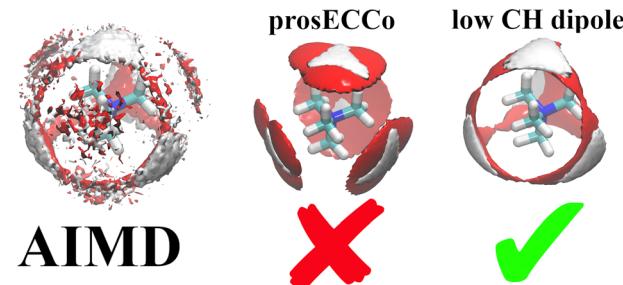


## RESEARCH PAPERS

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

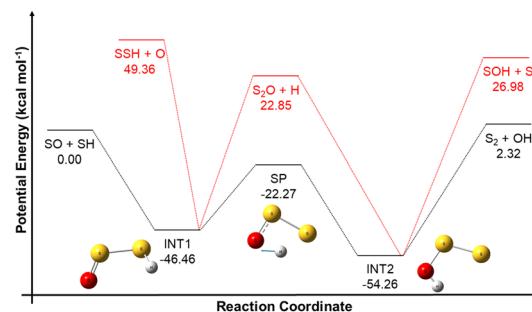
Philip E. Mason,\* Tomas Martinek, Balázs Fábián, Mario Vazdar, Pavel Jungwirth, Ondrej Tichacek, Elise Duboué-Dijon and Hector Martinez-Seara\*



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**Quantum chemistry and kinetics of hydrogen sulphide oxidation**

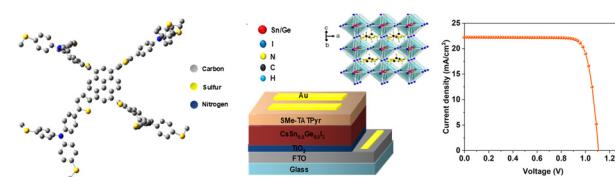
M. Monge-Palacios,\* Q. Wang,\* A. Alshaarawi, A. C. Cavazos Sepulveda and S. M. Sarathy



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**Improved eco-friendly CsSn<sub>0.5</sub>Ge<sub>0.5</sub>I<sub>3</sub> perovskite photovoltaic efficiency beyond 20% with SMe-TATPyr hole-transporting layer**

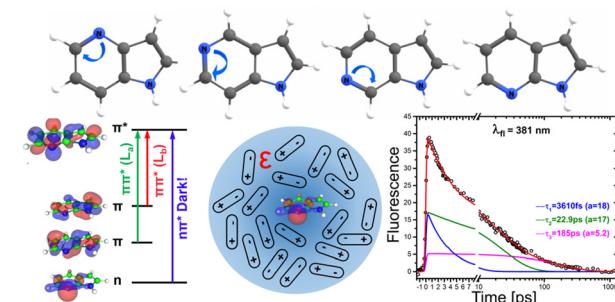
Mustafa K. A. Mohammed,\* Moaed E. Al-Gazally, Omar A. Khaleel, Ali K. Al-Mousoi, Zuhair Mohammed Ali Jeddoa, Hasan Sh. Majdi, Majid S. Jabir, M. Khalid Hossain, Mohammad Rafe Hatshan, Md. Ferdous Rahman and Davoud Dastan



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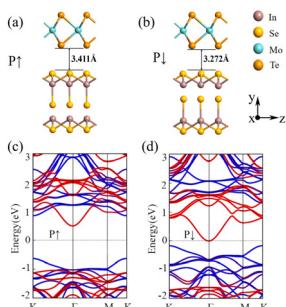
**Photodynamics of azaindoles in polar media: the influence of the environment**

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



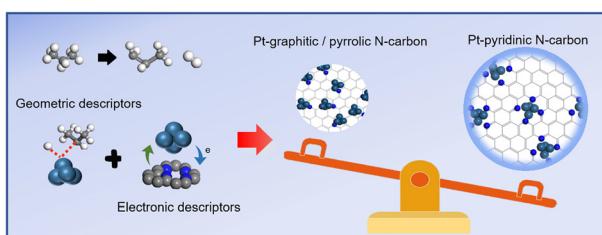
## RESEARCH PAPERS

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**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**

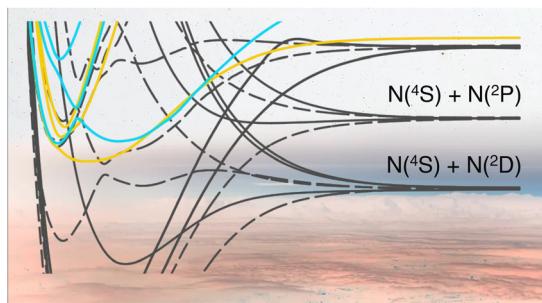
Leitao Lei, Yan-Hong Zhou,\* Xiaohong Zheng,\* Wenqiang Wan and Weiyang Wang

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

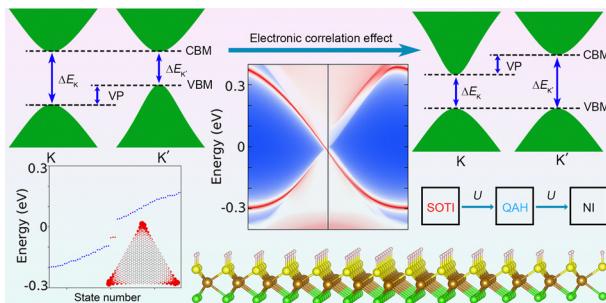
Ziwei Zhai, Bofeng Zhang,\* Yutong Wang and Guozhu Liu\*

3274

**Nonadiabatic quantum dynamics explores non-monotonic photodissociation branching of  $\text{N}_2$  into the  $\text{N}^{(4)\text{S}} + \text{N}^{(2)\text{P}}$  and  $\text{N}^{(4)\text{S}} + \text{N}^{(2)\text{D}}$  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\*

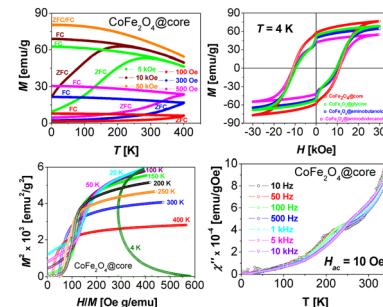


## RESEARCH PAPERS

3296

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

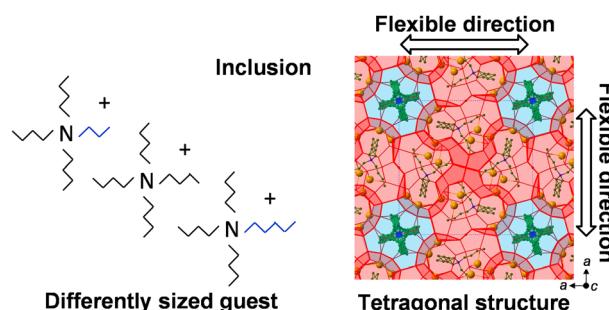
Ewa Mosiniewicz-Szablewska,\* Leandro Carlos Figueiredo, Atailson Oliveira da Silva, Marcelo Henrique Sousa and Paulo César de Morais



3315

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

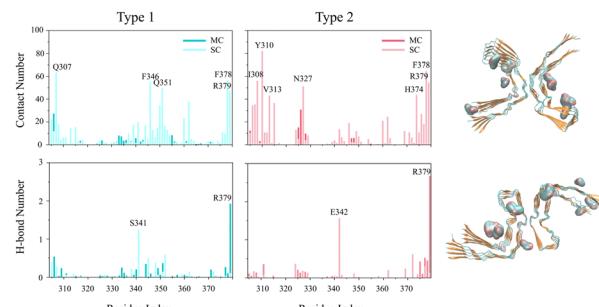
Sanehiro Muromachi\* and Satoshi Takeya



3322

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

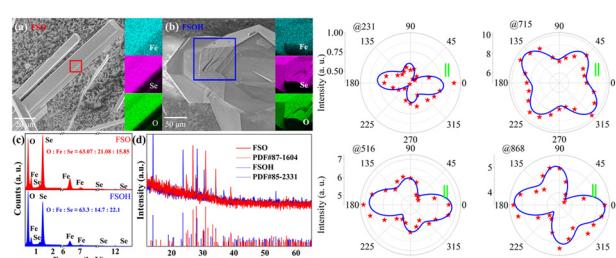
Jiaxing Tang, Ruiqing Sun, Jiaqian Wan, Yu Zou\* and Qingwen Zhang\*



3335

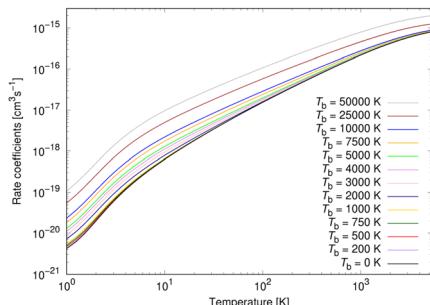
**Optical properties of ferroic  $\text{Fe}_2\text{O}(\text{SeO}_3)_2$  and  $\text{Fe}_2(\text{SeO}_3)_3 \cdot 3\text{H}_2\text{O}$** 

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



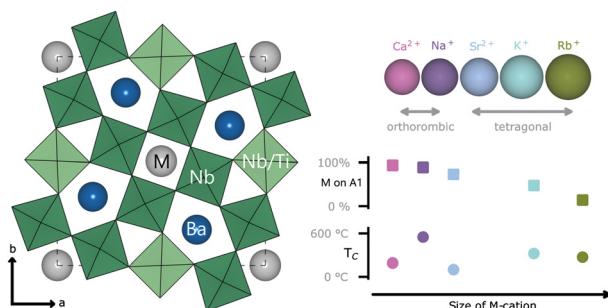
## RESEARCH PAPERS

3342

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

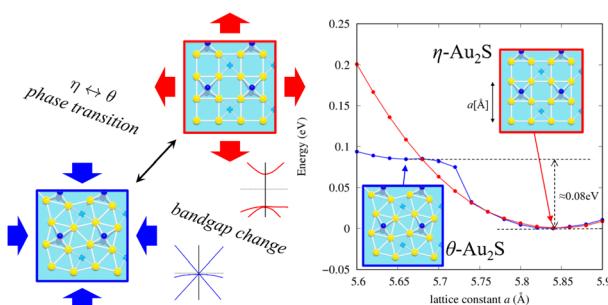
Martina Šimsová née Zámečníková,\* Magnus Gustafsson, Gunnar Nyman and Pavel Soldán

3350

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

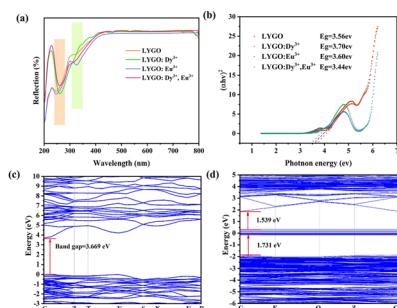
Nora Statle Løndal, Benjamin Albert Dobson Williamson, Julian Walker, Mari-Ann Einarsrud and Tor Grande\*

3367

**Electronic band structure change with structural transition of buckled  $\text{Au}_2\text{X}$  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

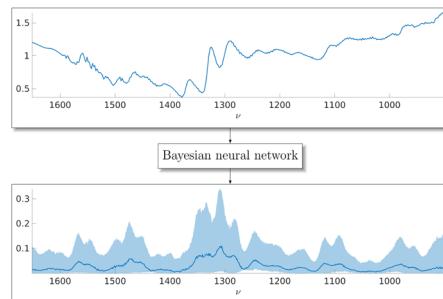


## RESEARCH PAPERS

3389

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

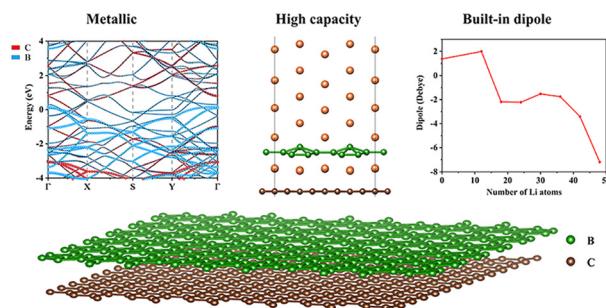
Teemu Häkkinen,\* Erik M. Vartiainen, Lasse Lensu, Matthew T. Moores and Lassi Roininen



3400

**Enhancement of multilayer lithium storage in a  $\beta_{12}$ -borophene/graphene heterostructure with built-in dipoles**

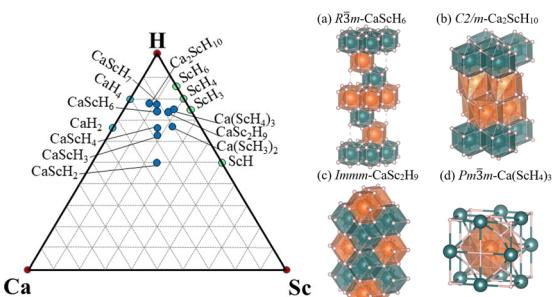
Xiaowei Jiang, Wenjun Tang, Xiaobin Niu and Haiyuan Chen\*



3408

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

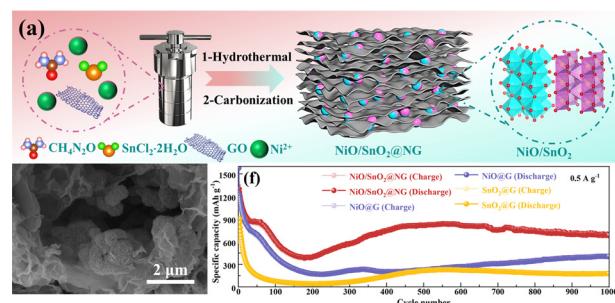
Wenjie Yuan, Xu Yang, Shichang Li,\* Chunbao Feng, Bole Chen, Ying Chang and Dengfeng Li\*



3415

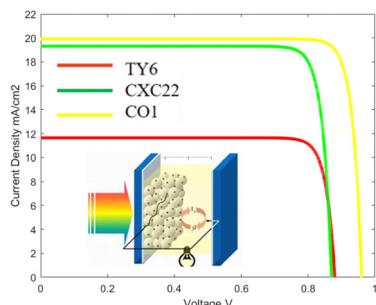
**Synthesis of heterointerfaces in NiO/SnO<sub>2</sub> coated nitrogen-doped graphene for efficient lithium storage**

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



## RESEARCH PAPERS

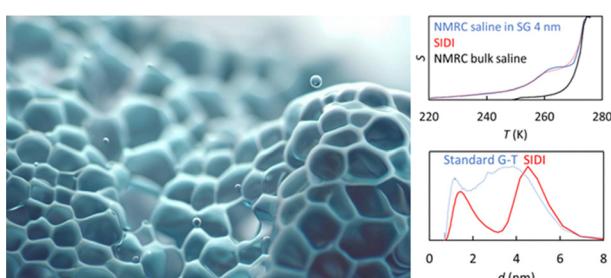
3424



### 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\*

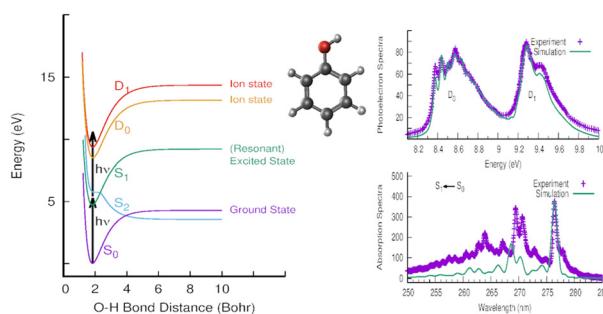
3441



### 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\*

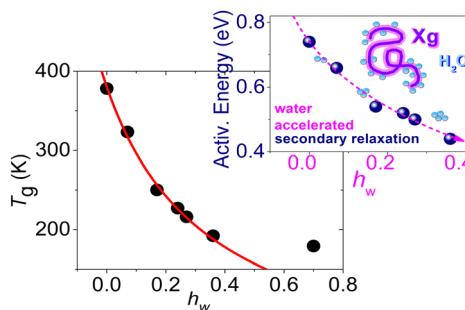
3451



### 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\*

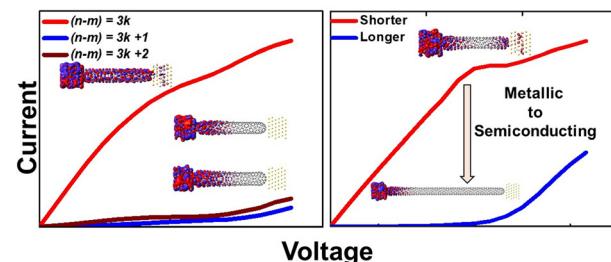


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3474

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

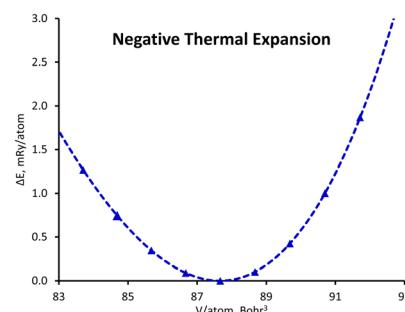
Ameet Kumar, Sudip Sarkar\* and Daeheum Cho\*



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**

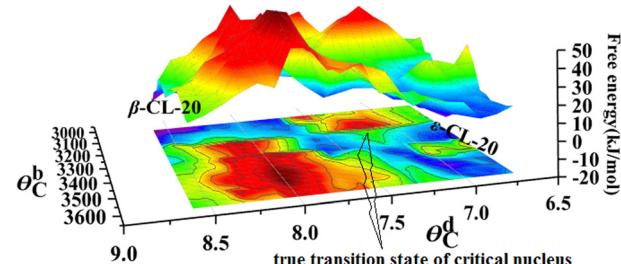
Dmitry Vasilyev



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  $\varepsilon$ -CL-20**

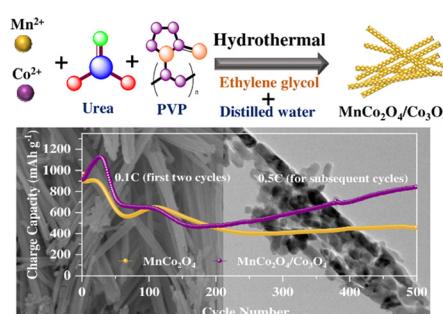
Fu-de Ren,\* Ying-Zhe Liu, Ke-wei Ding, Ling-ling Chang, Duan-lin Cao and Shubin Liu\*



3516

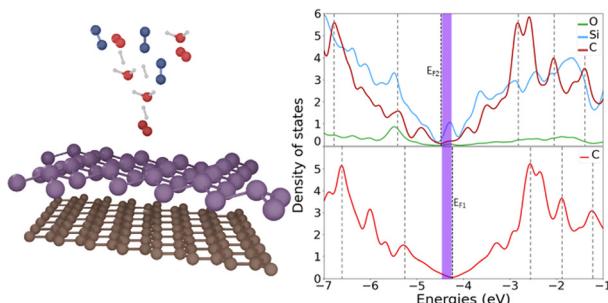
**Boosting the high-rate performance of lithium-ion battery anodes using  $\text{MnCo}_2\text{O}_4/\text{Co}_3\text{O}_4$  nanocomposite interfaces**

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



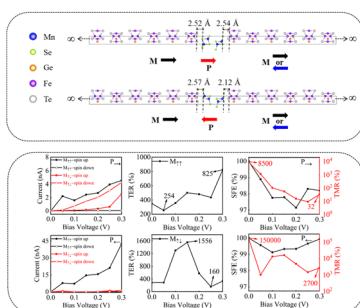
## RESEARCH PAPERS

3525

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

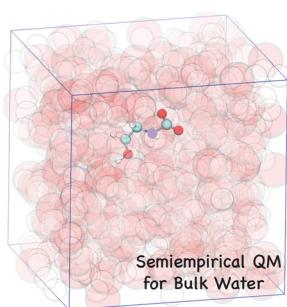
Xuhong Zhao, Haiyuan Chen, Jianwei Wang\* and Xiaobin Niu\*

3531

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

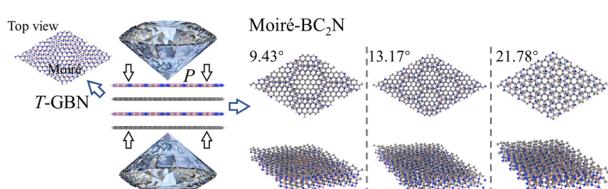
Xiao-Hui Guo, Lin Zhu,\* Zeng-Lin Cao and Kai-Lun Yao

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\*

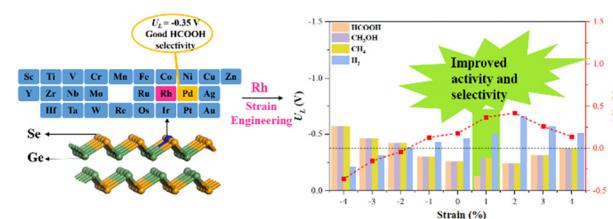


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3560

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

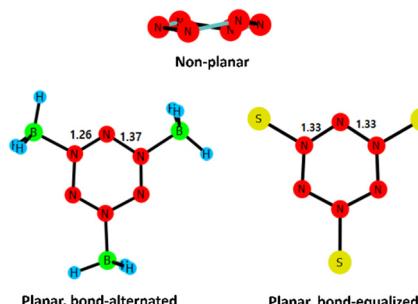
Yu-wang Sun, Lei Liu and Jing-yao Liu\*



3569

## Bond-alternated and bond-equalized hexazine derivatives

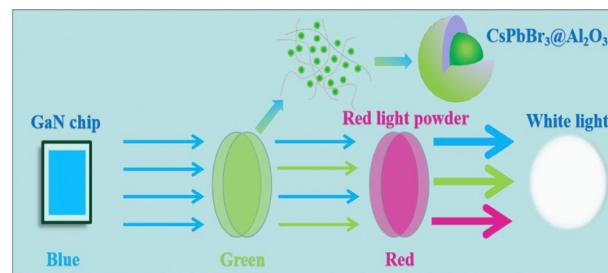
Kunnumma Chelladath Krishnapriya, Ashith Thayyil, Mithu Kumari and Priyakumari Chakkalingal Parambil\*



3578

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

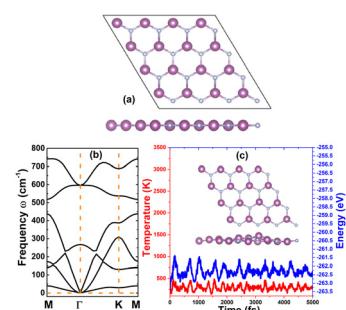
Sheng Huang,\* Ce Bian, Wenjie Xu, Hui Zhang, Shasha Gao, Yue Wang\* and Yuling Wang\*



3587

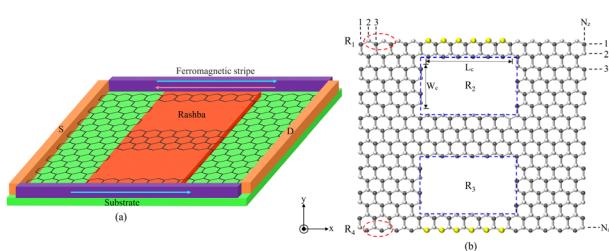
## Modifying the electronic and magnetic properties of the scandium nitride semiconductor monolayer via vacancies and doping

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



## RESEARCH PAPERS

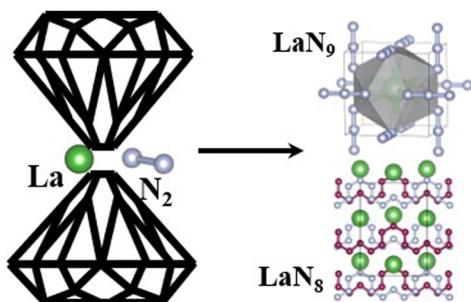
3597



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

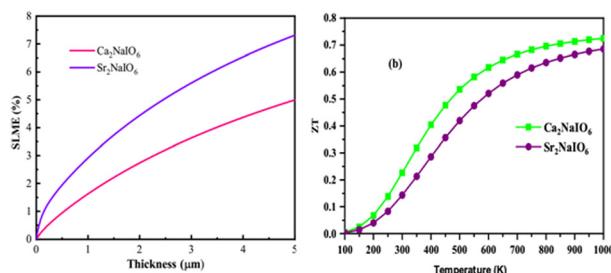
Xiang Gao, Cheng Ma, Lei Li,\* Xiaowei Zhang, Zhihong Deng, Xu Li and Zigang Zhou

3605

Lanthanum nitride  $\text{LaN}_9$  featuring azide units: the first metal nine-nitride as a high-energy-density material

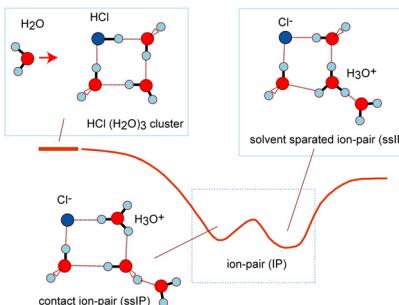
Shuyi Lin, Jingyan Chen, Bi Zhang, Jian Hao,\* Meiling Xu\* and Yinwei Li

3614

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

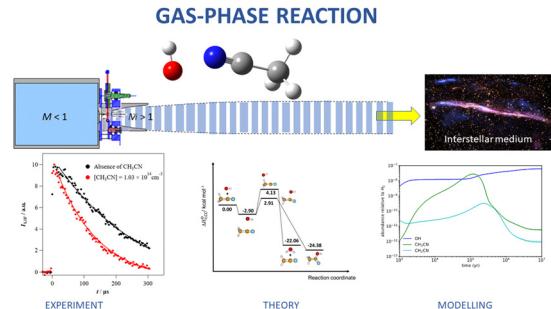


## RESEARCH PAPERS

3632

**Effect of temperature on the gas-phase reaction of CH<sub>3</sub>CN with OH radicals: experimental ( $T = 11.7\text{--}177.5\text{ K}$ ) and computational ( $T = 10\text{--}400\text{ K}$ ) 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<sub>2</sub> → FH + H reaction at  $E_{\text{trans}} = 62.09\text{ meV}$**

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

