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Inside cover

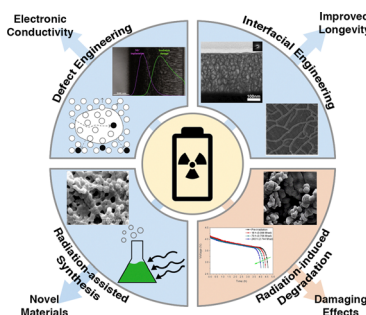
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REVIEWS

30761

Radiation effects on materials for electrochemical energy storage systems

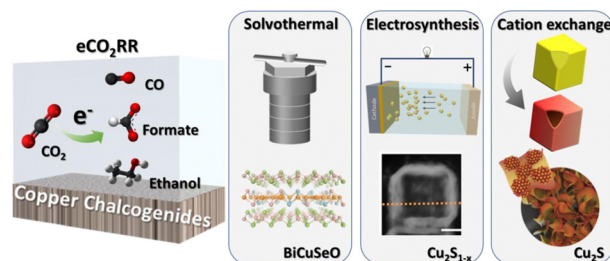
Tristan Olsen, Cyrus Koroni, Yuzi Liu, Joshua A. Russell, Janelle P. Wharry* and Hui Xiong*



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Recent advances in copper chalcogenides for CO₂ electroreduction

Wenjian Hu, Didier Grandjean, Jan Vaes, Deepak Pant* and Ewald Janssens*



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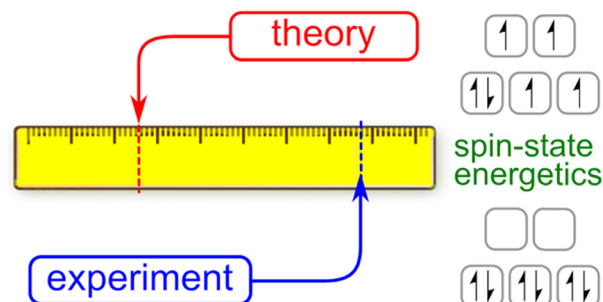


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Benchmarks for transition metal spin-state energetics: why and how to employ experimental reference data?

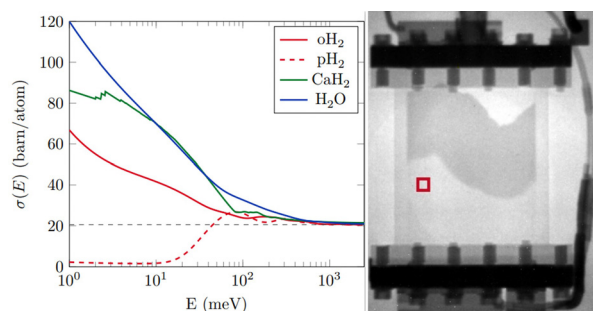
Mariusz Radoń



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Molecular specificity in neutron imaging: the case of hydrogen adsorption in metal organic frameworks

Margherita Simoni, Triestino Minniti, Roberto Senesi and Giovanni Romanelli*

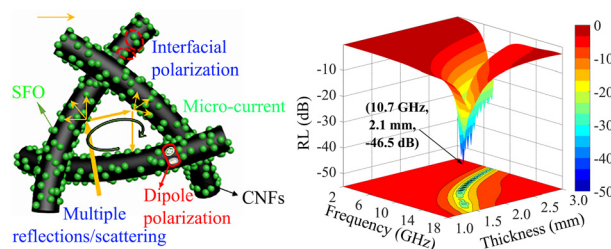


COMMUNICATION

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Ultrasmall SnFe₂O₄ nanoparticles anchored on N-doped carbon nanofibers for ultralight and high-performance microwave absorption

Guangguang Guan, Xiaoqiang Li, Yao Li, Siyi Tong, Jun Xiang* and Kaiyin Zhang*

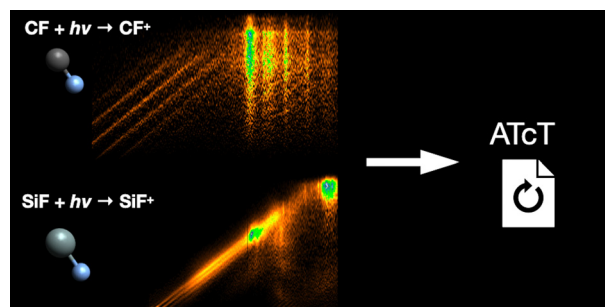


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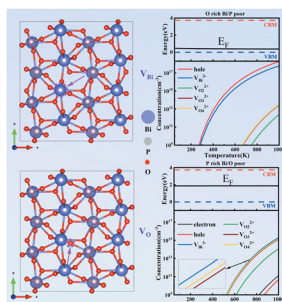
Refining the thermochemical properties of CF, SiF, and their cations by combining photoelectron spectroscopy, quantum chemical calculations, and the Active Thermochemical Tables approach

Ugo Jacovella,* Branko Ruscic,* Ning L. Chen, Hai-Linh Le, Séverine Boyé-Péronne, Sebastian Hartweg, Madhusree Roy Chowdhury, Gustavo A. Garcia, Jean-Christophe Loison and Bérenger Gans*



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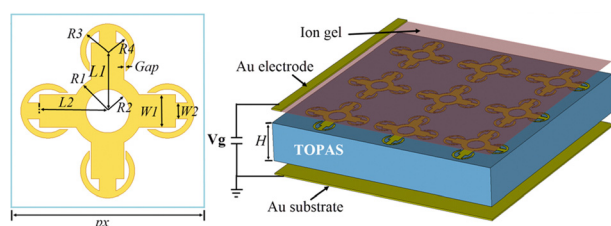
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Defect physics of intrinsic point defects in BiPO₄ photocatalysts: a hybrid functional study

Hongchun Zheng, Jincheng Wang, Bo Kong,* Xiang Xu, Min Zhang and Wentao Wang*

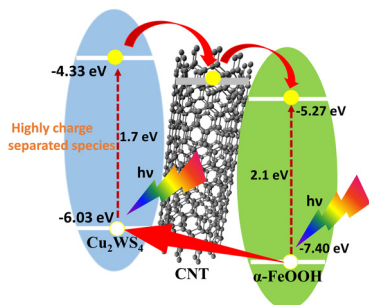
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A tunable broadband terahertz MoS₂ absorber using series-parallel hybrid network design

Fei Cai, Zhifei Kou and Guangsheng Deng*

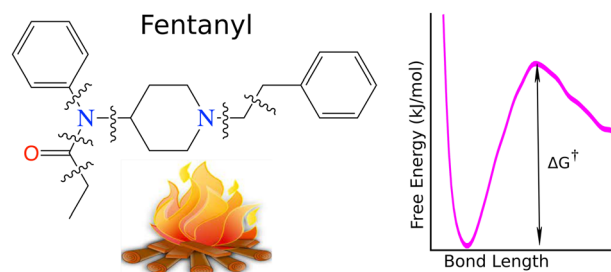
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Understanding the charge transfer dynamics of the Cu₂WS₄-CNT-FeOOH ternary composite for photo-electrochemical studies

Preeti Dagar, Nandan Ghorai, Manisha Bungla, Hirendra N. Ghosh* and Ashok K. Ganguli*

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Energetics of high temperature degradation of fentanyl into primary and secondary products

Bharat Poudel, Haley L. Monteith, Jason P. Sammon, Joshua J. Whiting, Matthew W. Moorman, Juan M. Vanegas* and Susan B. Rempe*

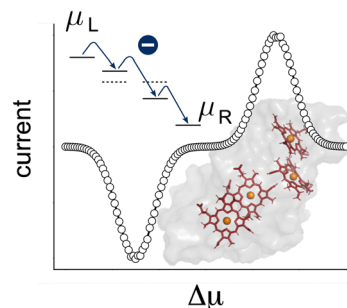


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Protein charge transfer far from equilibrium: a theoretical perspective

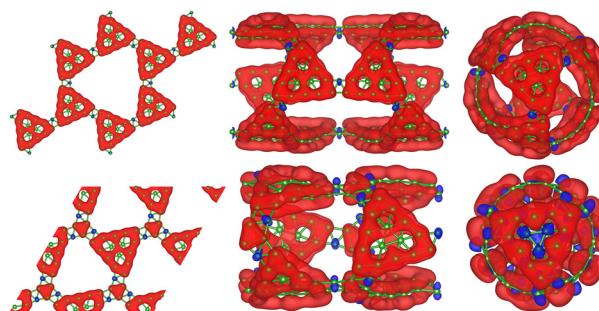
Mike Castellano, Christoph Kaspar, Michael Thoss and Thorsten Koslowski*



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Magnetic semiconducting borophenes and their derivatives

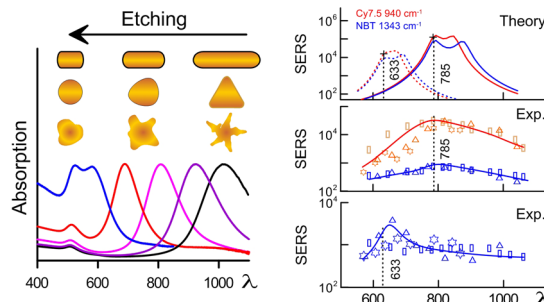
Bo Chen,* Lin Xue, Yan Han, Zhi Yang and Yong-Jia Zhang



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Surface-enhanced Raman scattering from Au nanorods, nanotriangles, and nanostars with tuned plasmon resonances

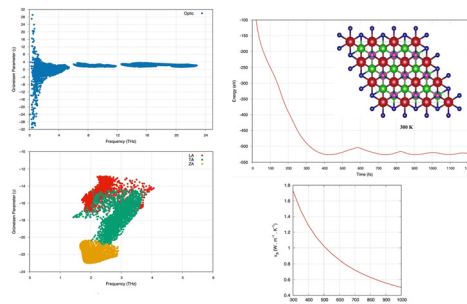
Boris N. Khlebtsov, Andrey M. Burov, Sergey V. Zarkov and Nikolai G. Khlebtsov*



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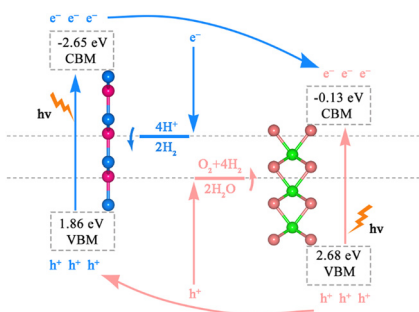
Unusual thermo-mechanical properties of the Janus Mo₂ScC₂OH MXene monolayer

Emre Bölen* and Engin Deligöz



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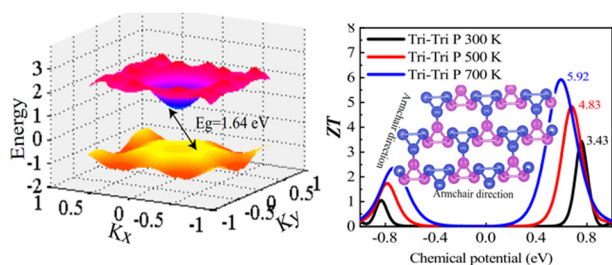
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Two-dimensional AlN/TMO van der Waals heterojunction as a promising photocatalyst for water splitting driven by visible light

Ji Tao, Liang Xu,* Can Li, Shixian Xiong,* Zhiqiang Xu, Jingyao Shao, Lei Cao, Ying Zhang, Kejun Dong* and Ling-Ling Wang

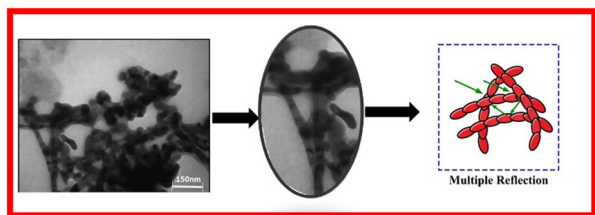
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Super-high carrier mobilities and excellent thermoelectric performances of Tri-Tri group-VA monolayers

Jia-He Lin, Tie Zhang and Tian Zhang*

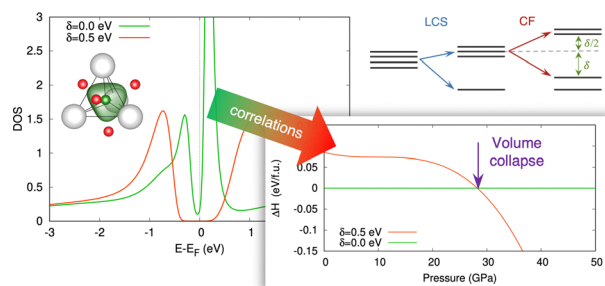
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GO-decorated chain-like Fe₂O₃/FeMn₂O₄ NPs (GO-Fe₂O₃/FeMn₂O₄ nanocomposites) with ultrabroad band microwave absorption

Mozhgan Arabi, Hoda Hekmatara* and Seyyed Mahdy Baizaei*

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Exploring correlation effects and volume collapse during electride dimensionality change in Ca₂N

Dmitry Y. Novoselov,* Mary A. Mazannikova, Dmitry M. Korotin, Alexey O. Shorikov, Vladimir I. Anisimov and Artem R. Oganov

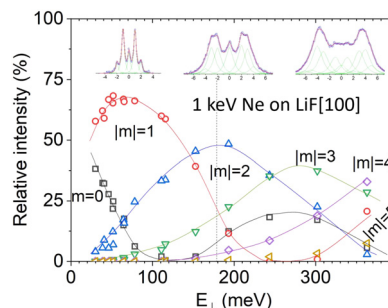


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Elastic and inelastic diffraction of fast neon atoms on a LiF surface

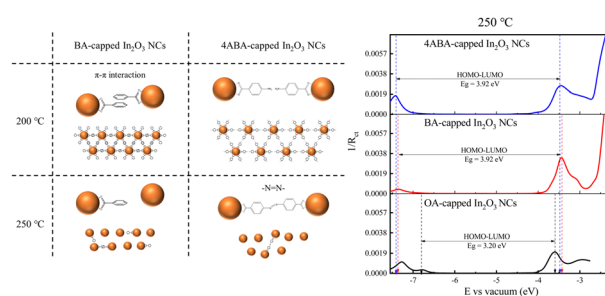
Maxime Debiossac, Peng Pan and Philippe Roncin*



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Effect of annealing temperature and capping ligands on the electron mobility and electronic structure of indium oxide nanocrystal thin films: a comparative study with oleic acid, benzoic acid, and 4-aminobenzoic acid

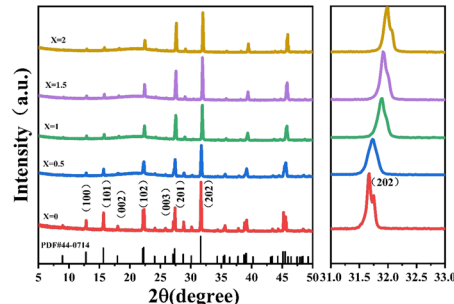
Quang Trung Le, Hyeok Yun, Hyeonbeom Park and Hyun-Dam Jeong*



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Bandgap lowering in mixed alloys of Cs₃Bi_{2-*x*}Sb_{*x*}Br₉ perovskite powders

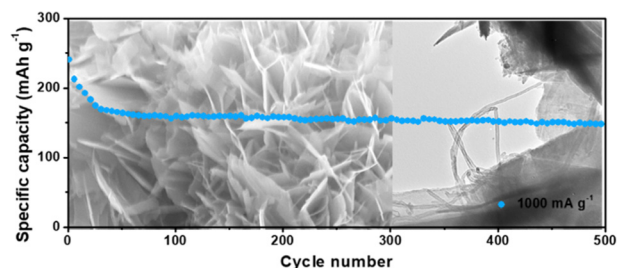
Siqi Dai, Xiaoyan Gan,* Kegui Li, Qiang Huang, Liling Guo and Hanxing Liu



31003

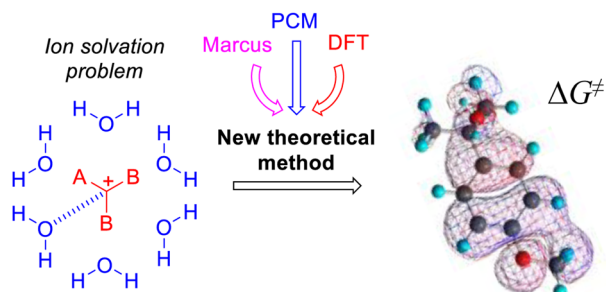
Enhancing the performance of aqueous zinc ion battery cathodes with a floral spherical V₅O₁₂·6H₂O/V₆O₁₃/CNT nanocomposite

Lingjiang Kou, Yong Wang, Jiajia Song,* Taotao Ai,* Panya Wattanapaphawong and Koji Kajiyoshi*



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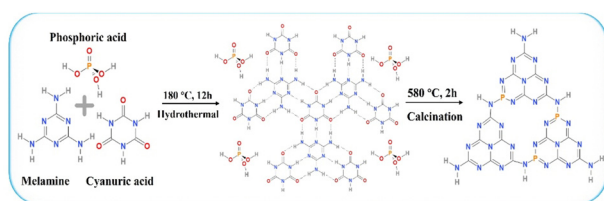
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Easy and accurate computation of energy barriers for carbocation solvation: an expeditious tool to face carbocation chemistry

Antonio G. Martínez,* Hans-Ulrich Siehl, Santiago de la Moya and Pedro C. Gómez*

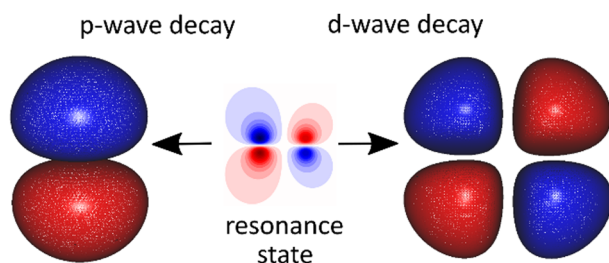
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Self-assembly synthesis of hollow phosphorus-doped graphitic carbon nitride microboxes for the photodegradation of organic pollutants

Si Cheng, Lifeng Miao,* Kunze Xue, Zhenhong Bao, Jian Liang, Xiaohong Li, Wenjun Zhu, Yunxia Chen* and Yongzhi Yu*

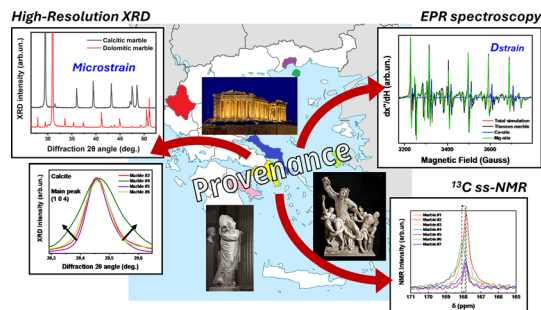
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Use of bound state methods to calculate partial and total widths of shape resonances

Michael F. Falcetta,* Mark C. Fair, Stephen R. Slimak, Kenneth D. Jordan* and Thomas Sommerfeld*

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Correlation of magnetic resonance (EPR, ssNMR) parameters and crystal-microstrain in marbles as a tool to probe their provenance

Loukas Belles, Christos Dimitriou, Constantinos Moularas, Maria Solakidou, Marinos Theodorakopoulos, Maria Louloudi and Yiannis Deligiannakis*

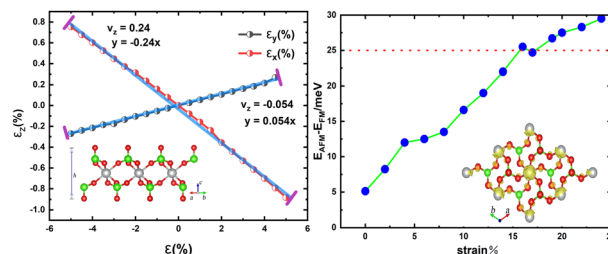


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A novel two-dimensional NiCl_2O_8 lattice with negative Poisson's ratio and magnetic modulation

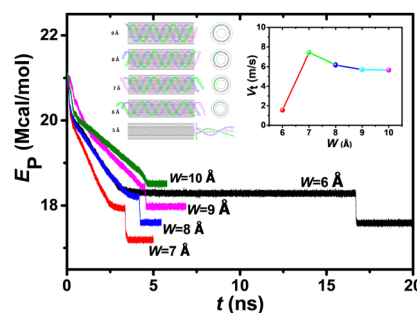
Hongbo Zhao, Hongguang Wang, Wei Tan, Na Ren, Longhua Ding, Xin Yu* and Aizhu Wang*



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Helical insertion of polyphenylene chains into confined cylindrical slits composed of two carbon nanotubes

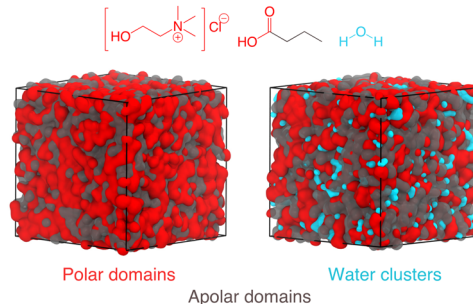
Xueyin Yang, Xuemei Sun, Shuqiong Xu, Hongjin Fu and Yunfang Li*



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Bulk nanostructure of a deep eutectic solvent with an amphiphilic hydrogen bond donor

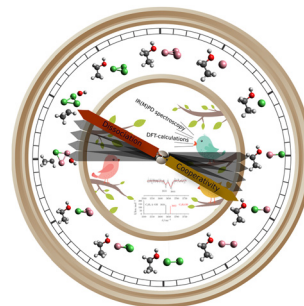
Lucas N. Wong, Silvia. Imberti, Gregory G. Warr and Rob. Atkin*



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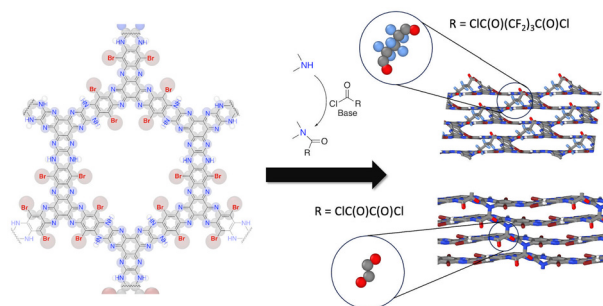
Investigating cooperative effects in small cobalt and cobalt–nickel alloy clusters with attached ethanol

Fabian Dietrich,* Markus Becherer, Daniel Bellaire, Paulina Martínez-Rodríguez and Markus Gerhards



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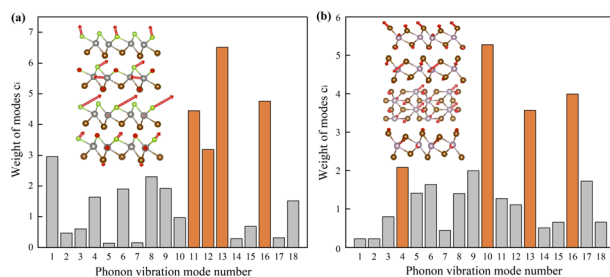
31090



Computationally directed manipulation of cross-linked covalent organic frameworks for membrane applications

Alathea E. Davies, Michael J. Wenzel, Cailin L. Brugger, Jordan Johnson, Bruce A. Parkinson, John O. Hoberg and Laura de Sousa Oliveira*

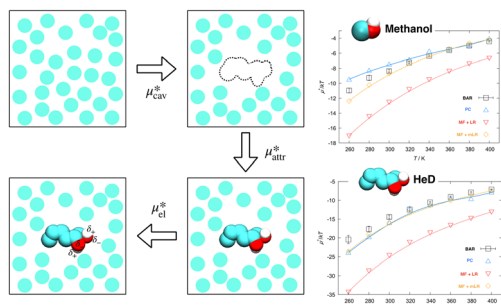
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Key phonon modes to determine the phase transition of two dimensional Janus transition metal dichalcogenides: a DFT and tight-binding study

Chengyue Sun, Jiming Zheng,* Sujuan Zhang, Pujun Zhao, Ping Guo and Zhenyi Jiang*

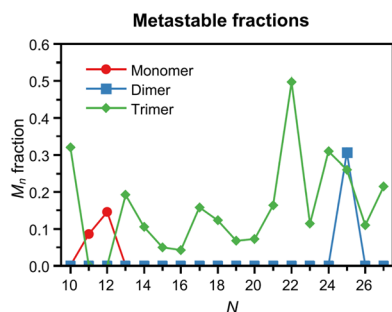
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Solvation free energies of alcohols in water: temperature and pressure dependences

Aoi Taira, Ryuichi Okamoto, Tomonari Sumi and Kenichiro Koga*

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Fragmentation channels of non-fullerene cationic carbon clusters

Piero Ferrari, Klavs Hansen,* Ozan Lacinbala, Ewald Janssens and Peter Lievens

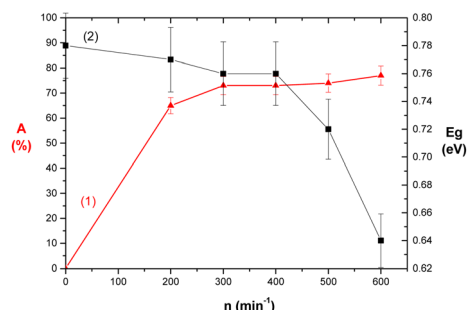


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The manipulation of natural mineral chalcopyrite CuFeS_2 via mechanochemistry: properties and thermoelectric potential

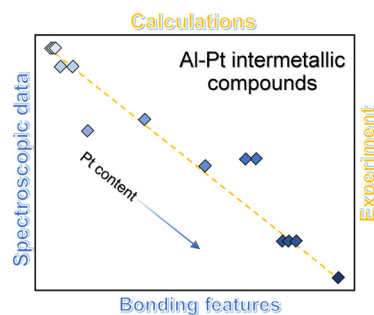
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31137

Al–Pt intermetallic compounds: HAXPES study

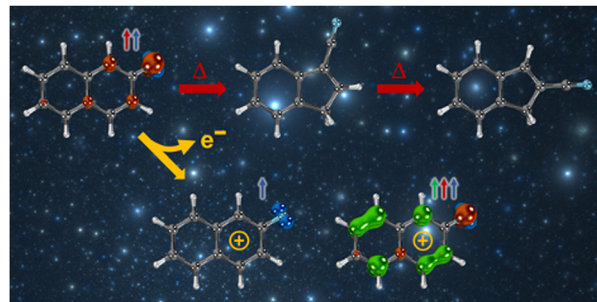
Iryna Antonyshyn,* Olga Sichevych, Ulrich Burkhardt, Ana María Barrios Jiménez, Anna Melendez-Sans, Yen-Fa Liao, Ku-Ding Tsuei, Deepa Kasinathan, Daisuke Takegami and Alim Ormeci



31146

Photoelectron spectroscopic study of 2-naphthyl nitrene and its thermal rearrangement to cyanoindenes

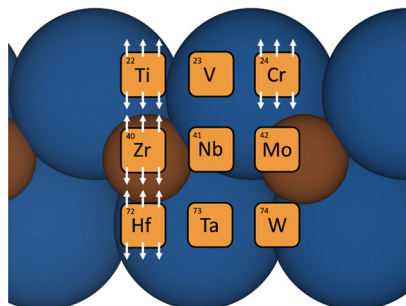
Mayank Saraswat, Adrian Portela-Gonzalez, Enrique Mendez-Vega, Ginny Karir, Wolfram Sander* and Patrick Hemberger*



31153

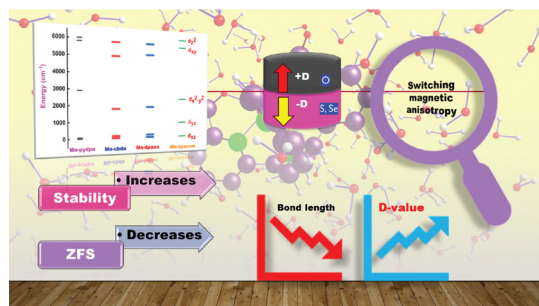
The nature of the electronic ground state of M_2C ($\text{M} = \text{Ti, V, Cr, Zr, Nb, Mo, Hf, Ta, and W}$) MXenes

Néstor García-Romeral, Ángel Morales-García,* Francesc Viñes, Ibério de P. R. Moreira and Francesc Illas*



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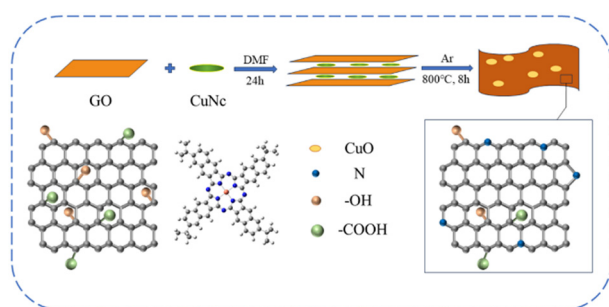
31165



Probing the dynamic behaviour and magnetic identification of seven coordinated Mn(II) complexes: a combined AIMD and multi-reference approach

Niharika Keot and Manabendra Sarma*

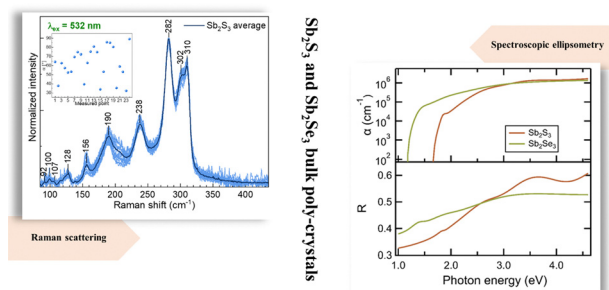
31178



Synthesis of copper naphthalocyanine/graphene oxide composites as anode materials for lithium-ion batteries

Qiuya Li, Bin Li,* Dongjun Lv,* Ping Wu, Qiwei Tang, Tianyong Zhang, Shuang Jiang and Ning Zhang

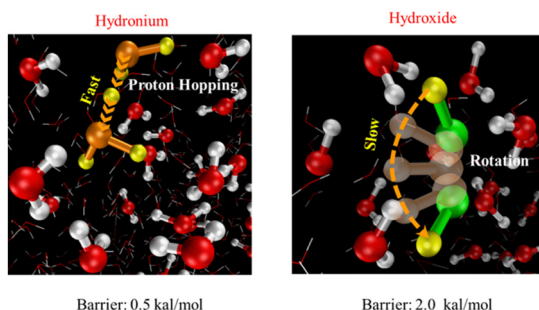
31188



Raman scattering and spectroscopic ellipsometry studies of Sb₂S₃ and Sb₂Se₃ bulk polycrystals

Elena Hajdeu-Chicarosh,* Victoria Rotaru, Sergiu Levcenko, Rosalia Serna, Ivan A. Victorov, Maxim Guc, Raquel Caballero, José Manuel Merino, Ernest Arushanov and Máximo León

31194



Identifying the acidic or basic behavior of surface water: a QM/MM-MD study

Md Al Mamunur Rashid, Mofizur Rahman, Tamina Acter and Nizam Uddin*

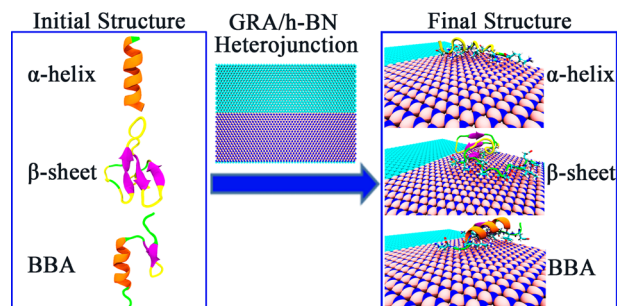


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31206

Theoretical study of protein adsorption on graphene/h-BN heterostructures

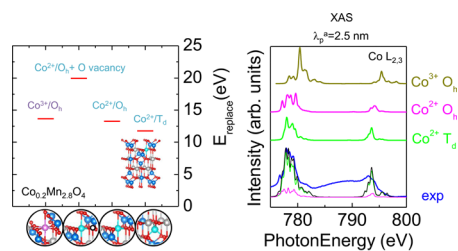
Jun Lan, Yiran Peng, Lijun Liang,* Xing Duan, Zhe Kong, Li Zhang and Jia-Wei Shen*



31222

Growth and electronic properties of Co-doped Mn_3O_4 thin films: a combined experimental and theoretical investigation

Astrid Alí, Eduardo Cisternas, Fernando Stavale and Emilia Annese*

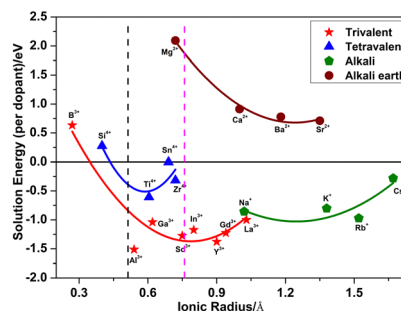


- Co (8%) doping of Mn_3O_4 thin film
- Co adopts $2+$ oxidation state and occupies mainly T_d sites
- Co 3d states appear in Co- Mn_3O_4 valence band

31230

Defect properties and solution energies of dopants in NASICON-type $\text{LiGe}_2(\text{PO}_4)_3$ solid electrolyte: a first-principles study

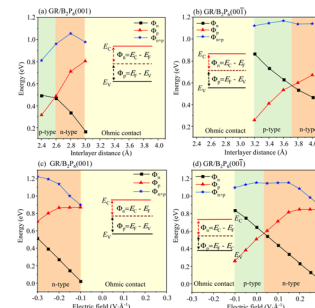
Anurup Das, Madhumita Goswami and P. S. Ghosh*



31238

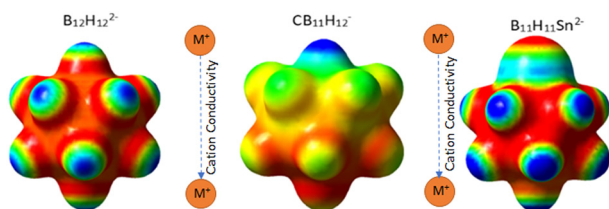
A graphene/Janus B_2P_6 heterostructure with a controllable Schottky barrier via interlayer distance and electric field

Tian Xie, Xinguo Ma,* Youyou Guo, Gang Yuan, JiaJun Liao, Nan Ma and Chuyun Huang*



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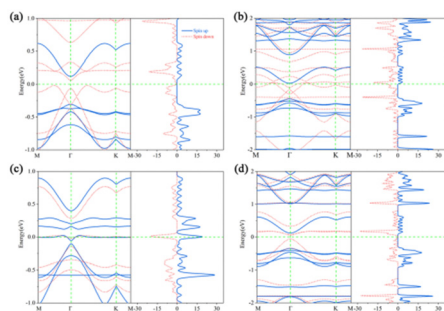
31249



Stannaborates: tuning the ion conductivity of dodecaborate salts with tin substitution

Thomas A. Hales, Kasper T. Møller, Terry D. Humphries, Anita M. D'Angelo, Craig E. Buckley and Mark Paskevicius*

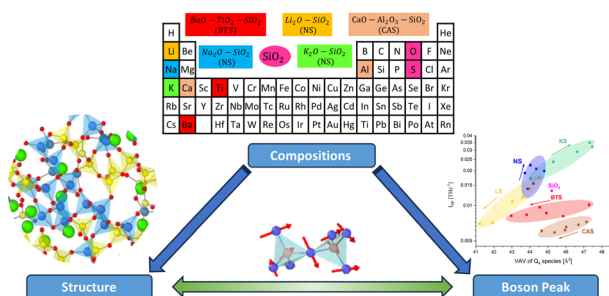
31257



The metal atomic substitution induced half-metallic properties, metallic properties and semiconducting properties in X-N₄ nanoribbons

Dong Fan, Zhihao Wang, Maoye Yin, Hengshuai Li,* Haiquan Hu, Feng Guo, Zhenbao Feng, Jun Li, Dong Zhang, Zhi Li and Minghui Zhu

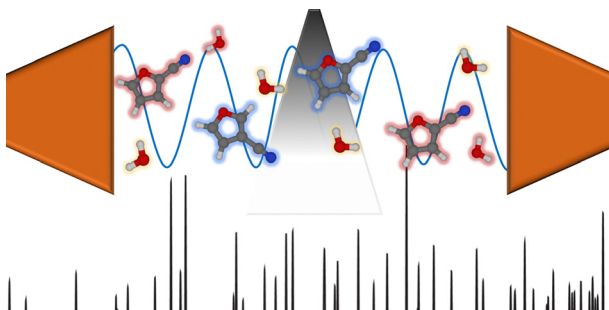
31270



The boson peak in silicate glasses: insight from molecular dynamics

Ahmed El Hamdaoui,* El Mehdi Ghardi,* Achraf Atila, Hicham Jabraoui, Michael Badawi, Abdellatif Hasnaoui and Said Ouaskit*

31281



Rotational spectra and semi-experimental structures of furonitrile and its water cluster

Mattia Melosso,* Silvia Alessandrini, Lorenzo Spada,* Alessio Melli, Xiujuan Wang, Yang Zheng, Chunguo Duan, Jiayi Li, Weiping Du, Qian Gou,* Luca Bizzocchi, Luca Dore, Vincenzo Barone and Cristina Puzzarini

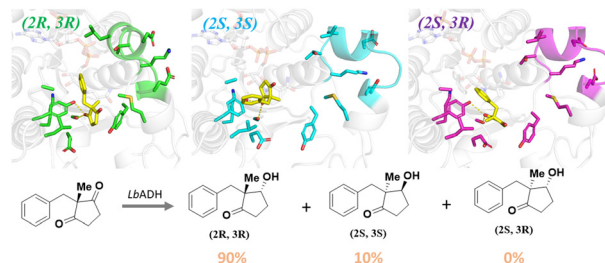


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31292

Origin of the enantioselectivity of alcohol dehydrogenase

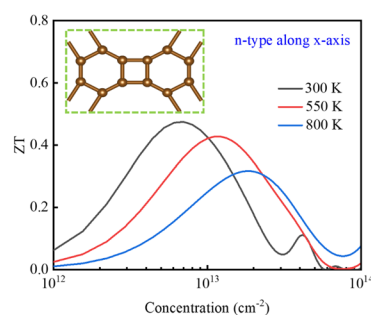
Jiahui Zhou, Tao Han, Shahbaz Ahmad, Derek Quinn, Thomas S. Moody, Qi Wu* and Meilan Huang*



31301

Thermal and electrical transport properties of two-dimensional Dirac grapheneylene: a first-principles study

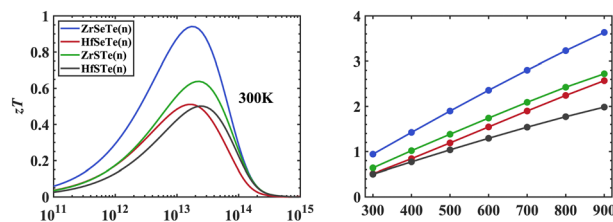
Changhong Zhang, Chengyi Hou, Yi Lu, Le Zhao, Haorong Wu, Hongyuan Song, Ju Rong,* Lan Yu* and Xiaohua Yu



31312

Janus 2H-MXTe (M = Zr, Hf; X = S, Se) monolayers with outstanding thermoelectric properties and low lattice thermal conductivities

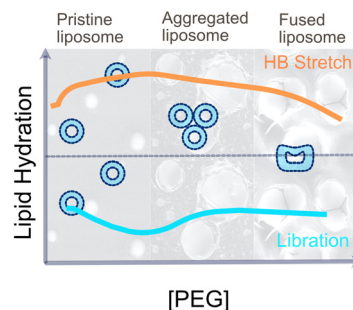
Ying-Qin Lin, Qiu Yang, Zhao-Qi Wang,* Hua-Yun Geng and Yan Cheng*



31326

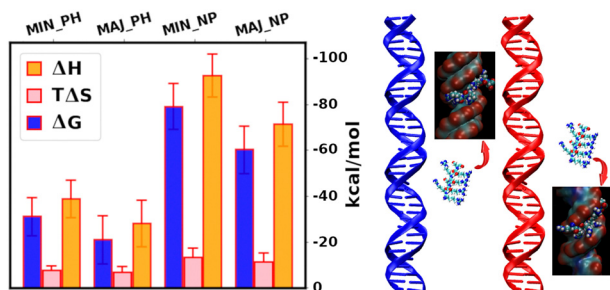
The explicit role of interfacial hydration during polyethylene glycol induced lipid fusion: a THz spectroscopic investigation

Sumana Pyne, Partha Pyne and Rajib Kumar Mitra*



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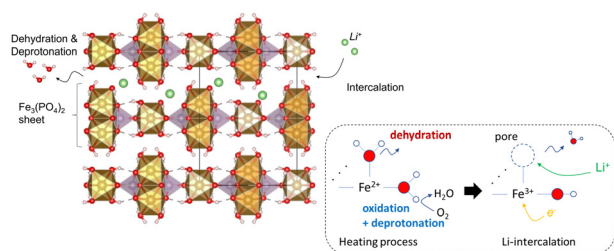
31335



DNA groove preference shift upon phosphorylation of a protamine-like cationic peptide

Khadka B. Chhetri, Yun Hee Jang, Yves Lansac and Prabal K. Maiti*

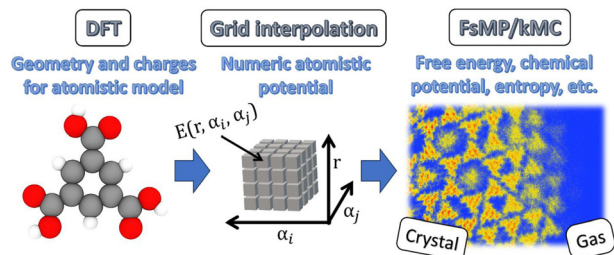
31346



Li intercalation in 2D iron phosphate synthesized from the partial dehydration and deprotonation of vivianite

Ryo Yamane,* Hongyi Li, Tetsu Ichitsubo and Kazumasa Sugiyama

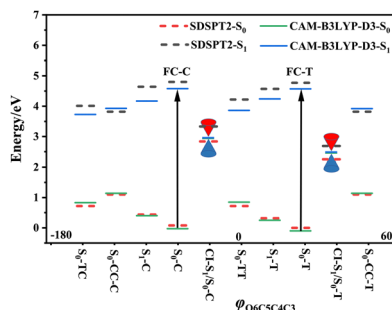
31352



Equilibrium structure of a dense trimesic acid monolayer on a homogeneous solid surface: from atomistic simulation to thermodynamics

Sergey S. Akimenko, Vitaly A. Gorbunov* and Eugene A. Ustinov

31363



Nonadiabatic molecular dynamics simulations for ultrafast photo-induced ring-opening and isomerization reactions of 2,2-diphenyl-2H-chromene

He Wang, Tianhe Yang, Yuechun Li, Le Yu,* Yibo Lei* and Chaoyuan Zhu*

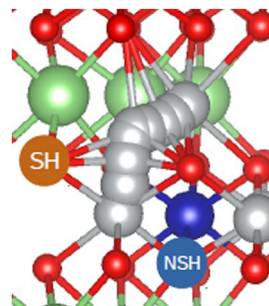


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31374

Effect of the oxygen vacancy electronic state on Ni migration in $\text{Li}_{0.5}(\text{Ni}_{0.8}\text{Mn}_{0.1}\text{Co}_{0.1})\text{O}_2$ cathode material

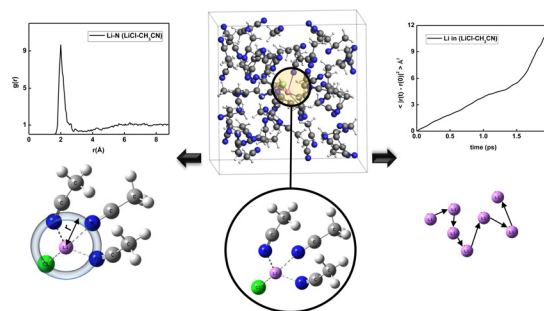
Ravanny W. M. Komalig, Ganes Shukri,*
 Mohammad Kemal Agusta,* Muhammad Haris Mahyuddin,
 Afriyanti Sumboja, Adhitya Gandaryus Saputro,
 Ryo Maezono, Ahmad Nuruddin* and
 Hermawan Kresno Dipojono



31382

Structure and dynamics of the Li^+ ion in water, methanol and acetonitrile solvents: *ab initio* molecular dynamics simulations

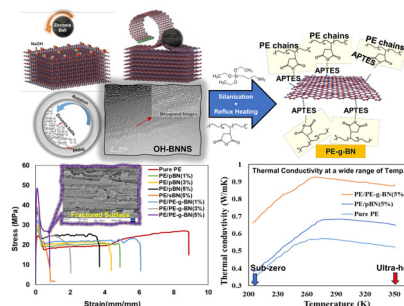
Reman Rana, Sk. Musharaf Ali* and Dilip K. Maity*



31396

Covalently bonded interface in polymer/boron nitride nanosheet composite toward enhanced mechanical and thermal behaviour

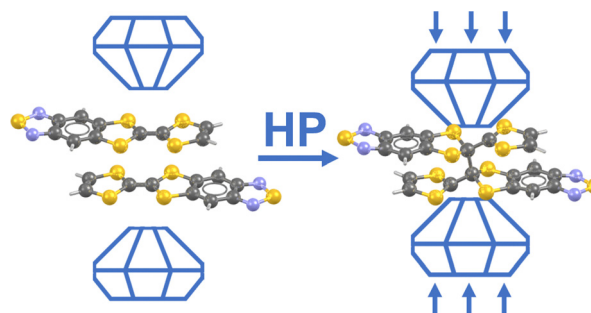
Ankur Chaurasia, Kaushlendra Kumar, S. P. Harsha and
 Avinash Parashar*



31410

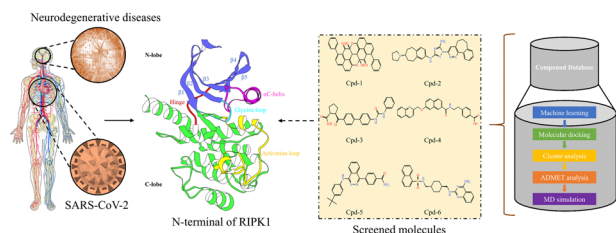
High pressure behaviour of the organic semiconductor salt $(\text{TTF-BTD})_2\text{I}_3$

Fabio Montisci, Arianna Lanza, Martin Fisch,
 Camille Sonnevile, Yan Geng, Silvio Decurtins,
 Christian Reber, Shi-Xia Liu* and Piero Macchi*



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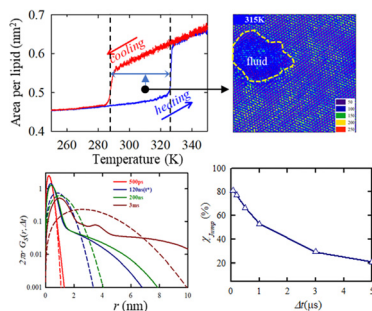
31418



Discovery of potential RIPK1 inhibitors by machine learning and molecular dynamics simulations

Ji-xiang Liu, Ri-song Na, Lian-juan Yang, Xu-ri Huang and Xi Zhao*

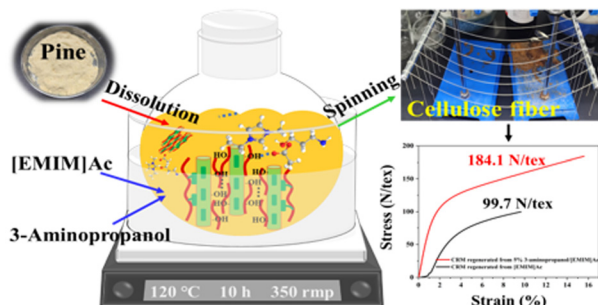
31431



Anomalous lateral diffusion of lipids during the fluid/gel phase transition of a lipid membrane

Abhay Kumar and Snehasis Daschakraborty*

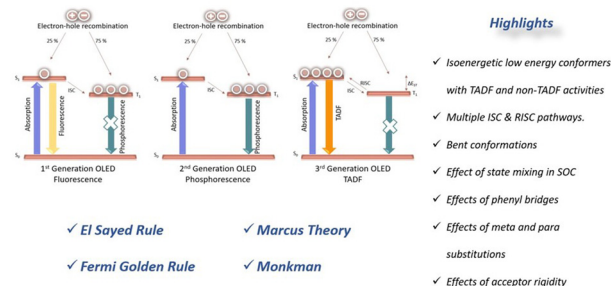
31444



Alcoholamine enhanced fractionation of cellulose from lignocellulosic biomass in ionic liquids

Yiwei Zhu, Jian Kang, Die Gao, Bingtong Chen, Yi Nie, Hui Wang* and Xiaowen Wu*

31457



The photophysical properties of sulfone-based TADF emitters in relation to their structural properties

Aslihan Hepguler, Pelin Ulukan and Saron Catak*

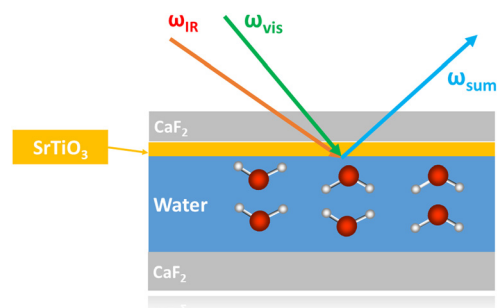


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31471

Unravelling the interfacial water structure at the photocatalyst strontium titanate by sum frequency generation spectroscopy

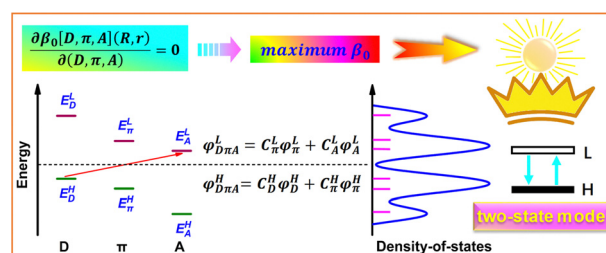
Martin Buessler, Shingo Maruyama, Moritz Zelenka, Hiroshi Onishi and Ellen H.G. Backus*



31481

The search for a maximum of the D- π -A paradigm for second order nonlinear optical molecular materials

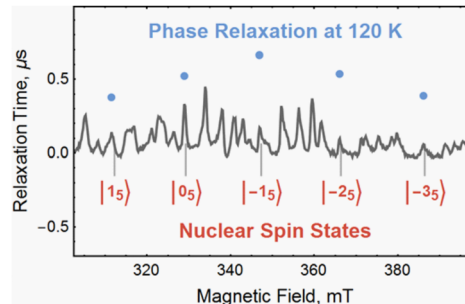
Cui-Cui Yang, Xiao Su, Qi-Zheng Zheng, Jiu Chen, Wei Quan Tian,* Wei-Qi Li* and Ling Yang*



31493

Low-temperature motion of the scandium bimetal in endofullerene $\text{Sc}_2\text{@C}_{80}(\text{CH}_2\text{Ph})$

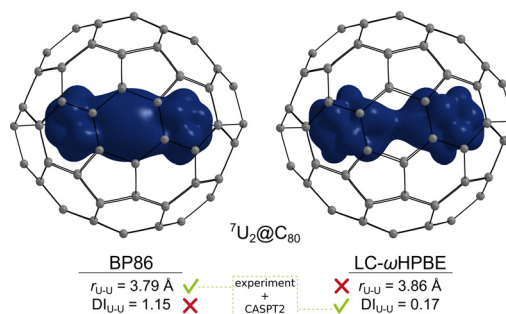
Yuri E. Kandrashkin* and Ruslan B. Zaripov



31500

Unraveling actinide–actinide bonding in fullerene cages: a DFT *versus* *ab initio* methodological study

Adam Jaroš and Michal Straka*



CORRECTION

31514

Correction: Optical absorption and shape transition in neutral Sn_N clusters with $N \leq 40$: a photodissociation spectroscopy and electric beam deflection study

Andreas Lehr,* Filip Rivic, Marc Jäger, Martin Gleditzsch and Rolf Schäfer

