

IN THIS ISSUE

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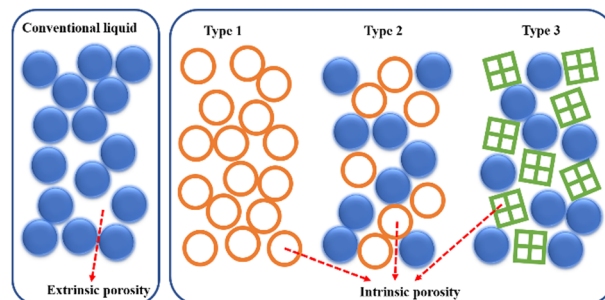
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PERSPECTIVE

22832

Porous liquids: a novel porous medium for efficient carbon dioxide capture

Xiao Zhang, Jiayi Li, Fei Lu, Fengjin Xie, Xinming Xu, Long Su, Xinpei Gao* and Liqiang Zheng*

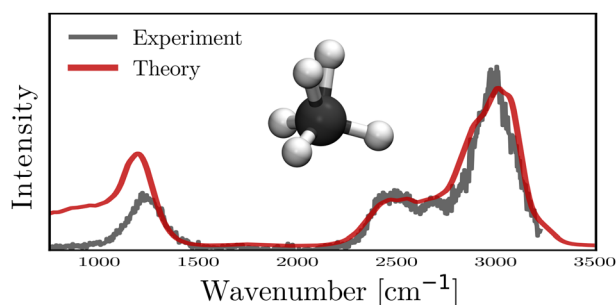


COMMUNICATIONS

22846

Theoretical infrared spectroscopy of protonated methane isotopologues

Richard Beckmann, Christoph Schran,* Fabien Brieuc and Dominik Marx



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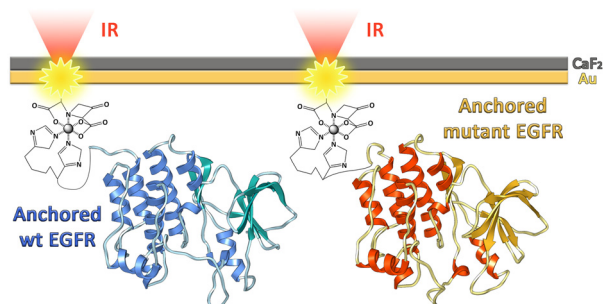
Fundamental questions
Elemental answers

COMMUNICATIONS

22853

Probing conformational dynamics of EGFR mutants via SEIRA spectroscopy: potential implications for tyrosine kinase inhibitor design

Emiliano Laudadio, Federica Piccirilli, Henrick Vondracek, Giovanna Mobbili, Marta S. Semrau, Paola Storici, Roberta Galeazzi, Elena Romagnoli, Leonardo Sorci, Andrea Toma, Vincenzo Aglieri, Giovanni Birarda* and Cristina Minnelli*

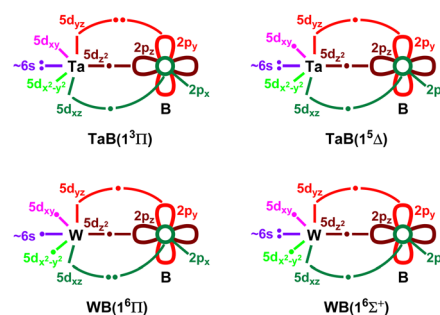


RESEARCH PAPERS

22858

Wavefunction theory and density functional theory analysis of ground and excited electronic states of TaB and WB

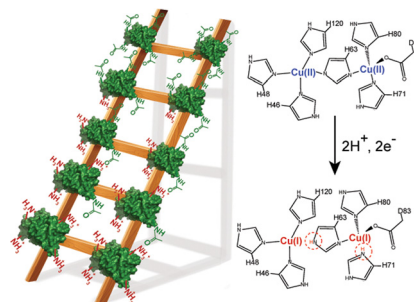
Isuru R. Ariyaratna



22870

Proton-coupled electron transfer at a mis-metalated zinc site detected with protein charge ladders

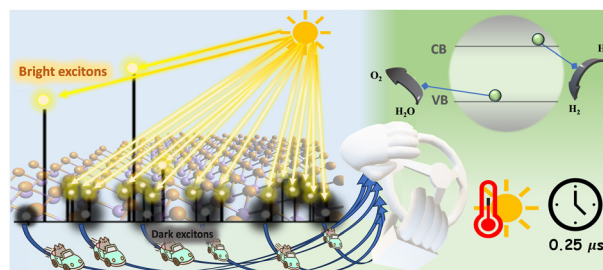
Mayte Gonzalez, Matthew J. Guberman-Pfeffer, Jordan C. Koone, Chad M. Dashnaw, Travis J. Lato and Bryan F. Shaw*



22882

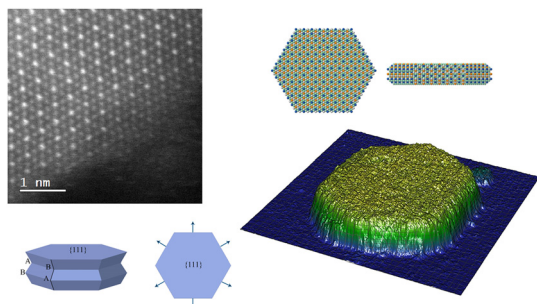
Temperature-driven journey of dark excitons to efficient photocatalytic water splitting in β -AsP

Harshita Seksaria, Amal Kishore and Abir De Sarkar*



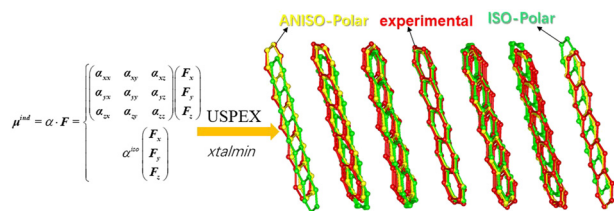
RESEARCH PAPERS

22894

**CoNiCuCrS alloy nanoparticles: synthesis and atomically resolved T/STEM studies**

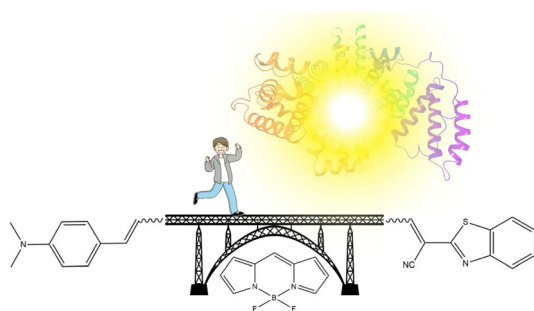
Carlos E. Rufino da Silva, Daniel Bahena Uribe, J. Jesús Velázquez Salazar, Dilip Karna, Joelin Agyei-Mensah and Miguel José Yacamán*

22900

**Development of an anisotropic polarizable model for the all-atom AMOEBA force field**

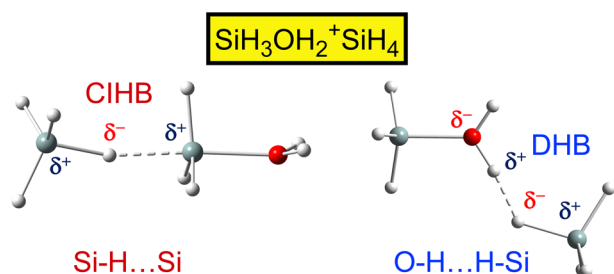
Yanyan Yang, Qianqian Jin and Shiwei Yin*

22912

**Molecular engineering of BODIPY-bridged fluorescent probes for lysosome imaging – a computational study**

Prince Joby, Rohith Ramasamy, Rajadurai Vijay Solomon* and Paul Wilson*

22931

**IR spectrum of $\text{SiH}_3\text{OH}_2^+\text{SiH}_4$: cationic $\text{OH}\cdots\text{HSi}$ dihydrogen bond versus charge-inverted $\text{SiH}\cdots\text{Si}$ hydrogen bond**

Martin Andreas Robert George and Otto Dopfer*

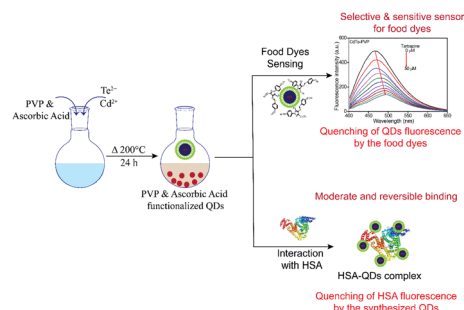


RESEARCH PAPERS

22941

Formation of CdTe core and CdTe@ZnTe core–shell quantum dots *via* hydrothermal approach using dual capping agents: deciphering the food dye sensing and protein binding applications

Mahabul Haque, Jintu Chutia, Amarjyoti Mondal, Sana Quraishi, Kalpana Kumari, Erica W. M. Marboh, Kripamoy Aguan and Atanu Singha Roy*

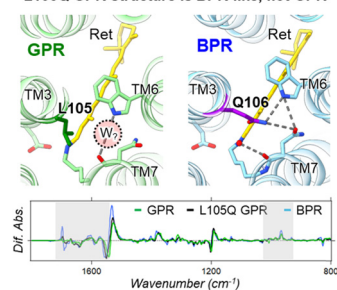


22959

Low-temperature FTIR spectroscopy of the L/Q switch of proteorhodopsin

Tatsuro Nishikino, Teppei Sugimoto and Hideki Kandori*

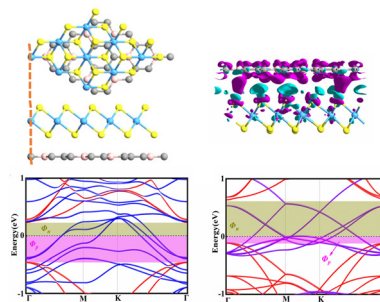
L105Q GPR structure is BPR-like, not GPR



22968

Electrical contact property and control effects for stable T(H)-TaS₂/C₃B metal–semiconductor heterojunctions

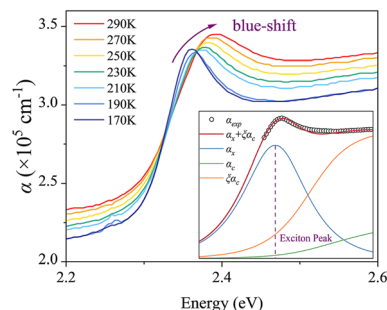
Shengguo Cao, Zhanhai Li, Jianing Han and Zhenhua Zhang*



22982

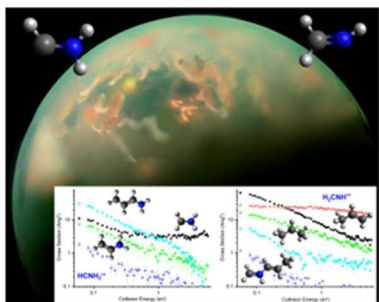
Unravelling the mechanism of temperature modulated exciton binding energy for MAPbBr₃ perovskites

Yanzhuo Hu, Dong Liu,* Ying-Bo Lu,* Hao Wang, Zhongchen Wu, Hexin Bao, Ruijie Zou, Xianyuan Jiang, Wei-Yan Cong and Chengbo Guan



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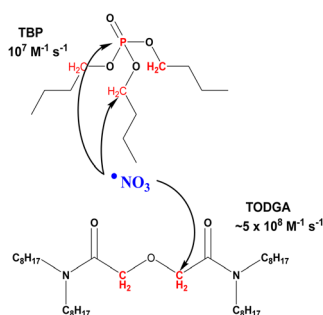
22990



Combined experimental and computational study of the reactivity of the methanimine radical cation ($\text{H}_2\text{CNH}^{\bullet+}$) and its isomer aminomethylene ($\text{HCNH}_2^{\bullet+}$) with propene (CH_3CHCH_2)

Vincent Richardson,* David Sundelin, Claire Romanzin, Roland Thissen, Christian Alcaraz, Miroslav Polášek, Jean-Claude Guillemin, Jan Žabka, Wolf D Geppert and Daniela Ascenzi*

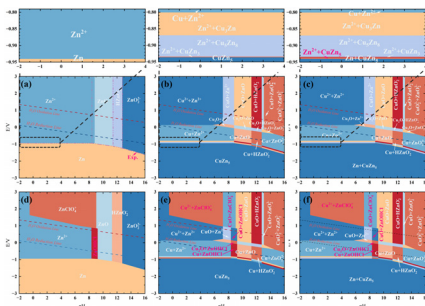
23003



Reactions of the $\bullet\text{NO}_3$ radical with nuclear extraction ligands in alkane solution

Anh N. Dang, Maya H. Rogalski, Dean R. Peterman, Bruce J. Mincher and Stephen P. Mezyk*

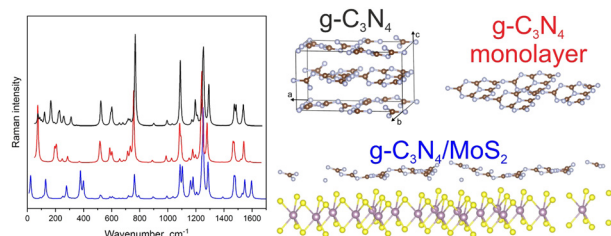
23010



Electrochemical stability of biodegradable Zn–Cu alloys through machine-learning accelerated high-throughput discovery

Kun Luo, Zhaorui Liu, Rui Yu, Tengfei Xu, Dominik Legut, Xing Yin* and Ruifeng Zhang*

23023



Electronic transitions and vibrational properties of bulk and monolayer $\text{g-C}_3\text{N}_4$, and a $\text{g-C}_3\text{N}_4/\text{MoS}_2$ heterostructure from a DFT study

A. S. Oreshonkov,* E. V. Sukhanova, D. V. Pankin and Z. I. Popov

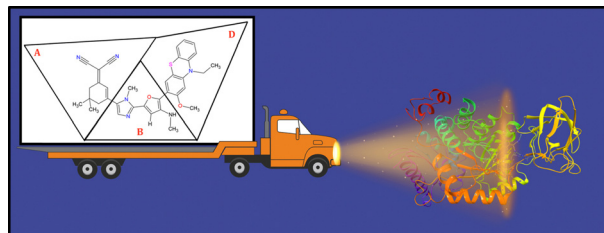


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23032

Optimizing 2-furylated imidazole π -bridges for NIR lipid droplet imaging

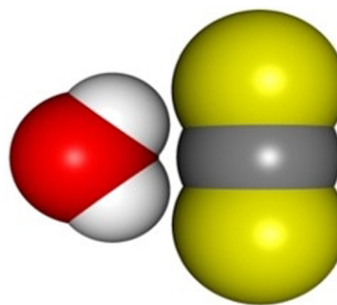
Anamika Suresh, Rohith Ramasamy, Deepa Kallumpurath and Rajadurai Vijay Solomon*



23053

Water–carbon disulfide dimers: observation of a new isomer and *ab initio* structure theory

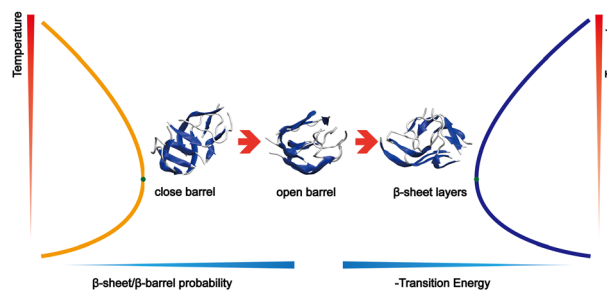
A. J. Barclay, A. R. W. McKellar, A. Pietropolli Charmet and N. Moazzen-Ahmadi*



23062

Energy gap of conformational transition related with temperature for the NACore of α -synuclein

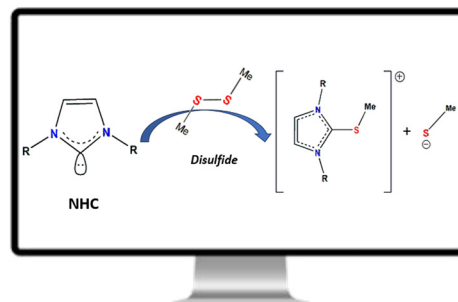
Pengxuan Xia, Yuanming Cao, Qingjie Zhao* and Huiyu Li*



23073

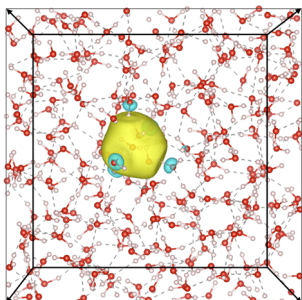
***In silico* investigation on the separation of disulfide bonds by N-heterocyclic carbene**

Swapan Sinha, Subhra Das, Kritish Kumar Ray, Sibaprasad Maity, Gourisankar Roymahapatra and Santanab Giri*



RESEARCH PAPERS

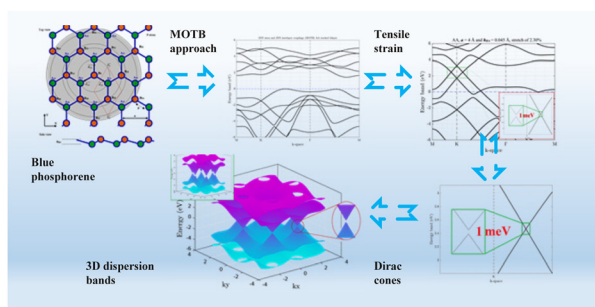
23080



Enhanced deep potential model for fast and accurate molecular dynamics: application to the hydrated electron

Ruiqi Gao, Yifan Li and Roberto Car*

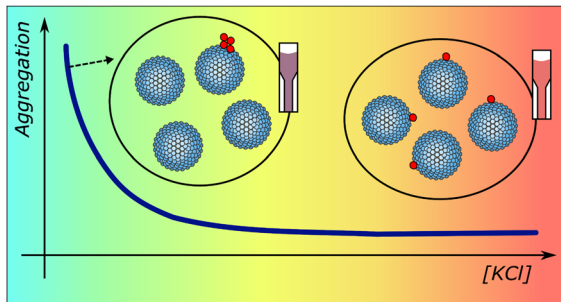
23089



Two-dimensional bilayer blue phosphorus Dirac-like material: a multi-orbital tight-binding investigation

Amine Benhajj* and Omar Mounkachi*

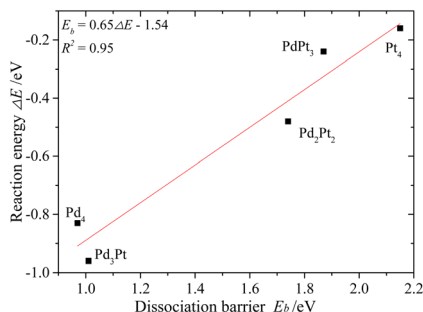
23103



Cooperative aggregation of gold nanoparticles on phospholipid vesicles is electrostatically driven

Helena Mateos*, Antonia Mallardi, Miquel Oliver, Marcella Dell'Aglio, Pamela Giannone and Gerardo Palazzo

23116



H-assisted CO₂ dissociation on Pd_nPt_(4-n)/In₂O₃ catalysts: a density functional theory study

Xiaowen Wang, Jiaying Pan*, Haiqiao Wei*, Wenjia Li, Jun Zhao and Zhen Hu

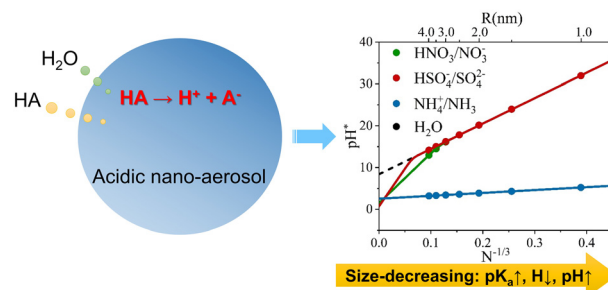


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23125

Size-dependent acidity of aqueous nano-aerosols

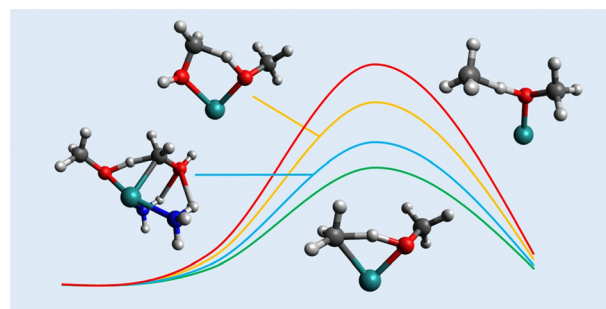
Wanrong Song, Shaoxun Guo and Hui Li*



23136

Selective conversion of methane to methanol facilitated by molecular metal–methoxy complexes via a self-correcting chemical cycle

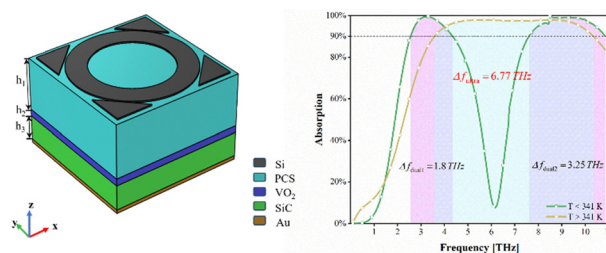
Shahriar N. Khan, Brody Quebedeaux and Evangelos Miliordos*



23144

Photocontrolled ultra-broadband metamaterial absorber around the terahertz regime

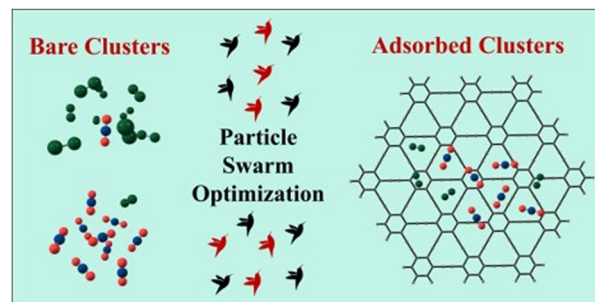
Guozheng Wu, Chao Li,* Dong Wang, Song Gao, Haijun Guo, Wenya Chen, Shijing Guo, Jiaran Xiong and Yue Che



23152

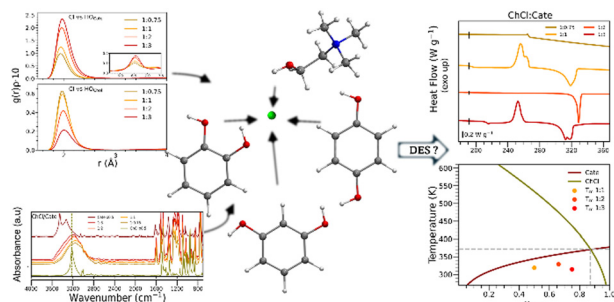
On assessing the carbon capture performance of graphynes with particle swarm optimization

Megha Rajeevan, Chris John and Rotti Srinivasamurthy Swathi*



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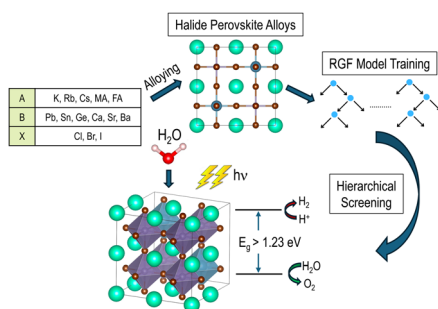
23168



On the composition and isomerism effect in the thermal and structural properties of choline chloride/hydroxyphenol deep eutectic solvents

Paolo Casu, Matteo Busato,* Matteo Palluzzi, Riccardo Spezia and Paola D'Angelo*

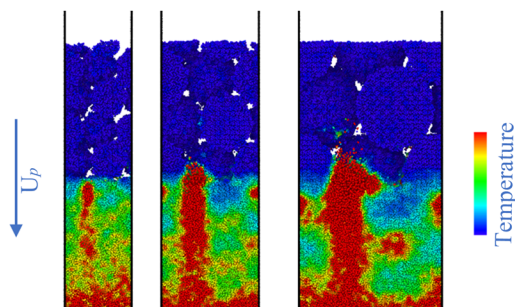
23177



Screening of novel halide perovskites for photocatalytic water splitting using multi-fidelity machine learning

Maitreyo Biswas, Rushik Desai and Arun Mannodi-Kanakkithodi*

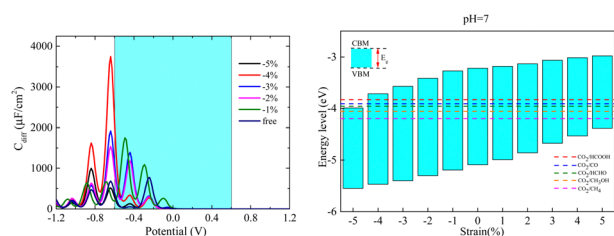
23189



Size-dependent shock response mechanisms in nanogranular RDX: a reactive molecular dynamics study

Xiaona Huang, Chunliang Ji, Xiaoxia Ma, Lixiao Hao, Feng Guo, Guangcheng Yang, Jichun Huang, Yushi Wen* and Zhiqiang Qiao*

23201



Regulating the electronic properties, quantum capacitance and photocatalytic activity of Sc₂CO₂ based on Y doping and strain

Qing-Feng Ren, Rui-Zhou Zhang,* Xiao-Hong Li* and Hong-Ling Cui

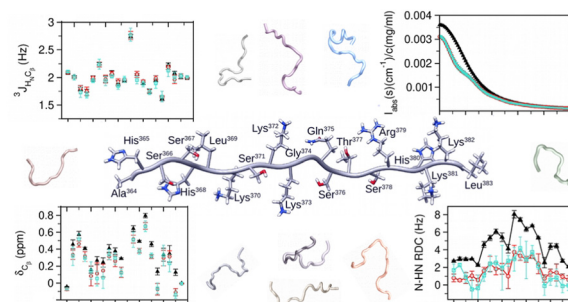


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23213

Statistical accuracy of molecular dynamics-based methods for sampling conformational ensembles of disordered proteins

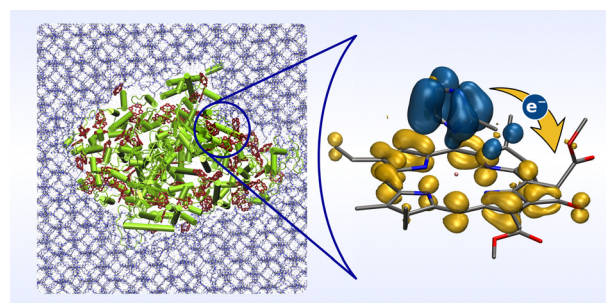
Adolfo Bastida,* José Zúñiga, Federico Fogolari and Miguel A. Soler*



23228

Molecular interactions of photosystem I and ZIF-8 in bio-nanohybrid materials

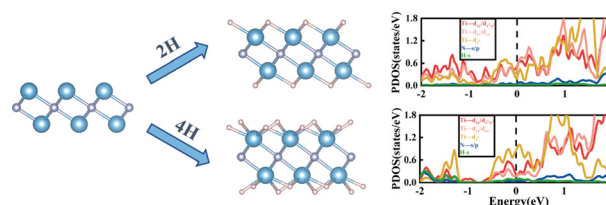
Sebastian Reiter,* Igor Gordiy, Kathrin L. Kollmannsberger, Feng Liu, Erling Thyraug, Dario Leister, Julien Warnan, Jürgen Hauer* and Regina de Vivie-Riedle



23240

Realization of hydrogenation-induced superconductivity in two-dimensional Ti₂N MXene

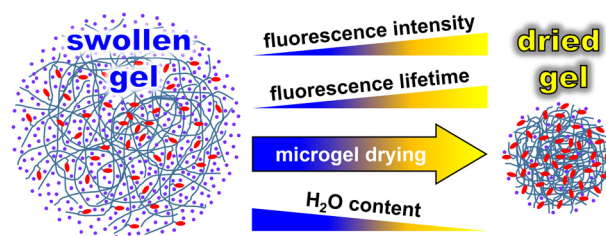
Yamin Xue, Zebang Cheng, Shunwei Yao, Ben Wang, Jiajun Jiang, Lin Peng,* Tingting Shi, Jing Chen, Xiaolin Liu and Jia Lin*



23250

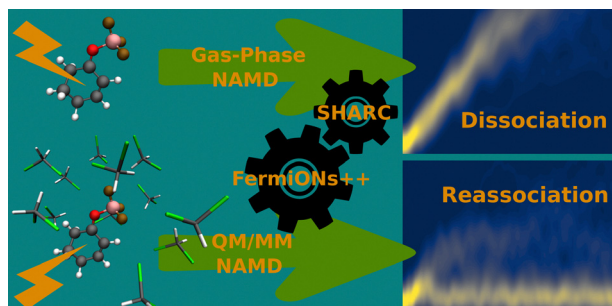
Moisture changes inside hydrogel particles during their drying process investigated with fluorescence lifetime imaging

Sankar Jana and Dominik Wöll*



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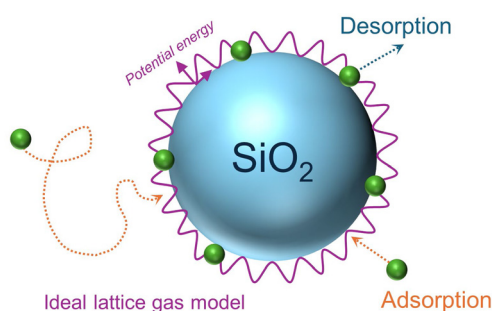
23256



Simulation of the non-adiabatic dynamics of an enone-Lewis acid complex in an explicit solvent

Martin T. Peschel, Jörg Kussmann,*
Christian Ochsenfeld* and Regina de Vivie-Riedle

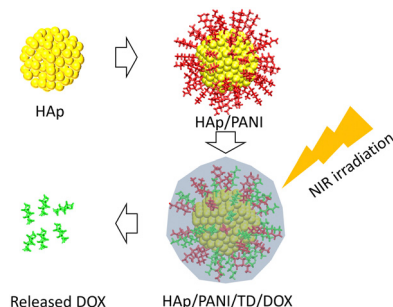
23264



Elucidating gas-surface interactions relevant to atmospheric particle growth using combined temperature programmed desorption and temperature-dependent uptake

Kristen N. Johnson, Yixin Li, Michael J. Ezell,
Pascale S. J. Lakey, Manabu Shiraiwa and
Barbara J. Finlayson-Pitts*

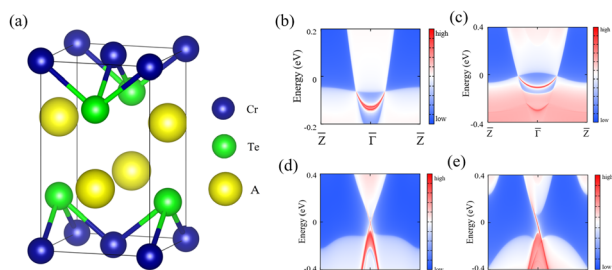
23277



Loading polyaniline (PANI) nanoparticles to mesoporous hydroxyapatite (HAp) spheres for near infrared (NIR) induced doxorubicin (DOX) drug delivery and colon cancer treatment

Jiamin Jin, Yujing Chen, Houzhong Li, Yongping Xu* and
Liyan Wang*

23288



The multiple topological phases in a new family of compounds ACrTe (A = Na, K, Rb, Cs) predicted by first-principles calculations

Shuaiqi Peng, Qing Wang,* Xinliang Huang and
Ning Hao*

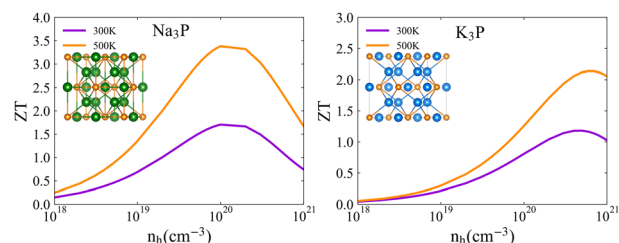


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23297

Excellent thermoelectric performance in alkali metal phosphides M_3P ($M = Na$ and K) with phonon-glass electron-crystal like behaviour

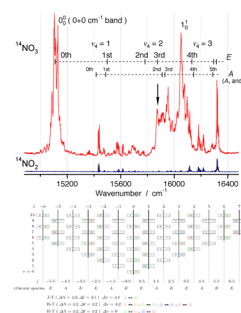
Xinji Xu, Weiyu Zhou, Wei Zhan, Ziyi Pan, Hao Huang,*
Geng Li,* Shuming Zeng* and Yusong Tu



23307

Laser induced fluorescence spectroscopy of the $\tilde{B}^2E' - \tilde{X}^2A'_2$ transition of jet cooled $^{14}NO_3$ and $^{15}NO_3$ II: the dispersed fluorescence spectrum from the 3rd E level of the ν_4 mode (approximately the $2\nu_4$ (e'), $l = 0$, level)

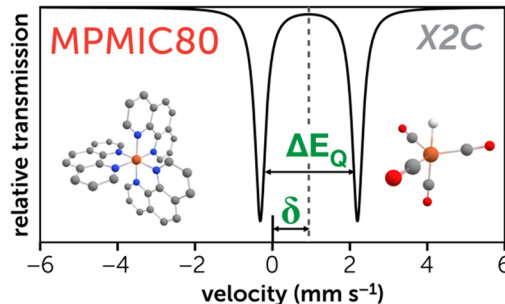
Masaru Fukushima



23322

Extensive reference set and refined computational protocol for calculations of ^{57}Fe Mössbauer parameters

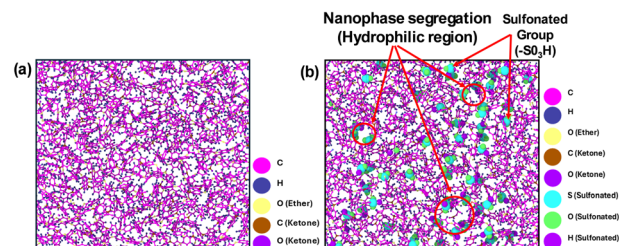
Golokesh Santra, Frank Neese* and
Dimitrios A. Pantazis*



23335

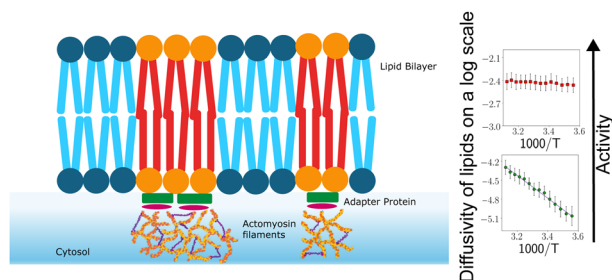
Effect of the degree of polymerization, crystallinity and sulfonation on the thermal behaviour of PEEK: a molecular dynamics-based study

Ashutosh Mittal and Avinash Parashar*



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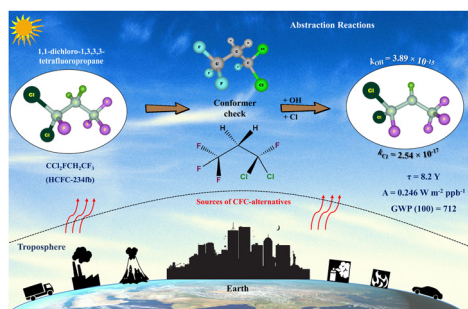
23348



Self-diffusion is temperature independent on active membranes

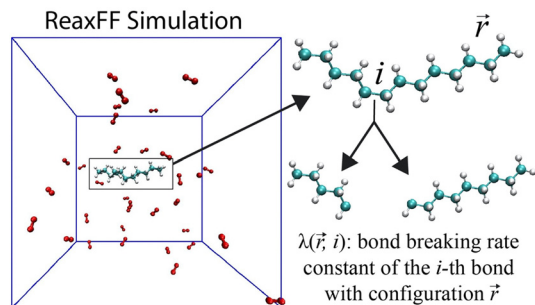
Saurav G. Varma, Argha Mitra and Sumantra Sarkar*

23363

Atmospheric oxidation pathways of $\text{CF}_3\text{CH}_2\text{CFCl}_2$ (HCFC-234fb) with OH-radicals and Cl-atoms: insights into the mechanism, thermodynamics, and kinetics

Rabu Ranjan Changmai, Samsung Raja Daimari, Anand Kumar Yadav and Manabendra Sarma*

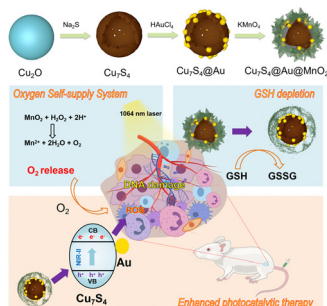
23372



The impact of molecular configuration on the bond breaking rates of hydrocarbons: a computational study

Jiang Wang,* Zhiling Li and Wenli Zhang*

23386



An endogenous oxygen self-supplied nanoplatform with GSH-depleted and NIR-II triggered electron–hole separation for enhanced photocatalytic anti-tumor therapy

Yao Huang, Hanlin Wei, Hui Feng, Fengyu Tian,* Qi Zheng* and Zhiming Deng*

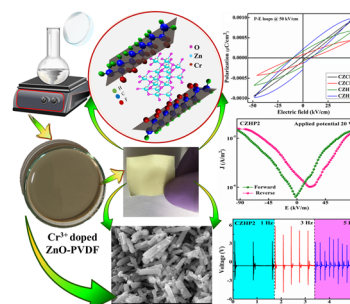


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23393

Promising ferroelectric and piezoelectric response of Cr-doped ZnO nanofiller-incorporated PVDF flexible and laminated nanocomposite system

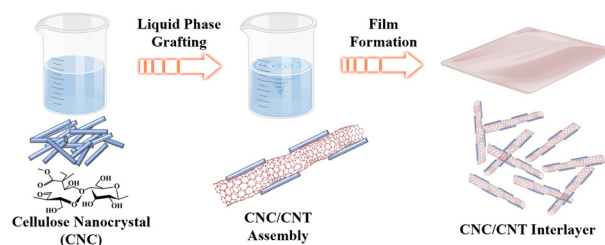
Tanmoy Chakraborty, Suman Saha, Dhananjoy Mondal, Subhojit Dutta, Abhik Sinha Mahapatra, Kishan Gupta, Partha Sona Maji, Sukhen Das and Soumyaditya Sutradhar*



23411

An anti-corrosive cellulose nanocrystal/carbon nanotube derived Zn anode interface for dendrite-free aqueous Zn-ion batteries

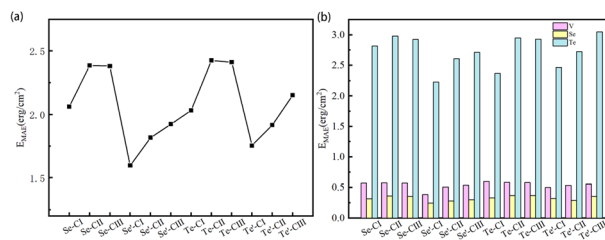
Hai Wang,* Qin Zhao, Yue Wang, Junliang Lin, Weimin Li, Shun Watanabe* and Xiaobo Wang*



23419

The electronic and magnetic properties modulated by ferroelectric polarization switching in two-dimensional VSeTe/Sc₂CO₂ van der Waals heterostructures

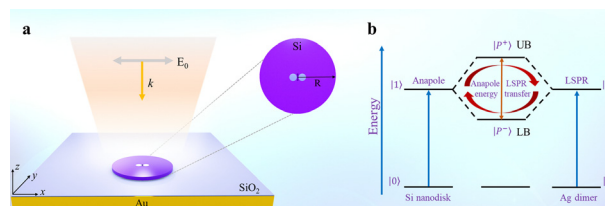
Weiyang Yu,* Xiaoli Zhang, Yuling Zhang, Yali Wu, Rui Li and Wei-Bing Zhang



23429

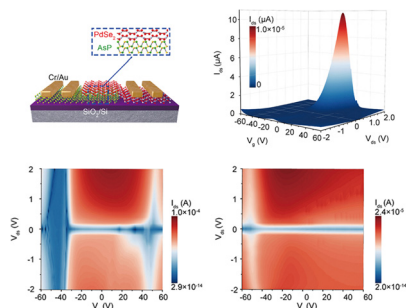
Strong anapole–plasmon coupling in dielectric–metallic hybrid nanostructures

Jingyu Wang,* Suze Wu, Weimin Yang and Xiaojun Tian



RESEARCH PAPERS

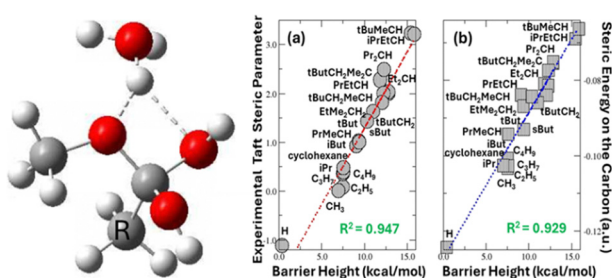
23438



Thermally tunable anti-ambipolar heterojunction devices

Shengyao Chen, Jiyou Jin, Wenxiang Wang, Shu Wang, Xiaoshan Du, Feng Wang, Lijun Ma, Junqi Wang, Cong Wang,* Xinzheng Zhang* and Qian Liu*

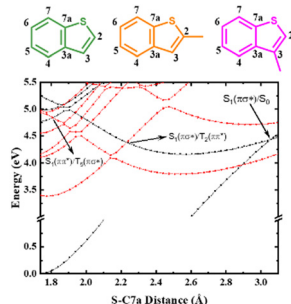
23447



Density-based quantification of steric effects: validation by Taft steric parameters from acid-catalyzed hydrolysis of esters

Jingwen Zhang, Xin He, Bin Wang, Chunying Rong,* Dongbo Zhao* and Shubin Liu*

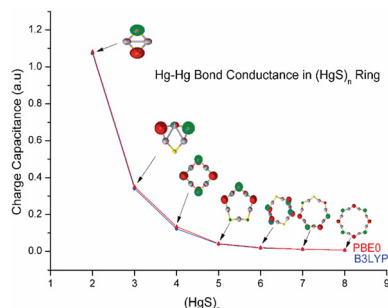
23457



Carbon–sulfur bond elongation as the promoting reaction coordinate in the efficient sub-nanosecond intersystem crossing in thianaphene derivatives

Cameron Griffith, Erqian Mao, Sean J. Hoehn, Sarah E. Krul and Carlos E. Crespo-Hernández*

23468

Hg–Hg bonding and its influence on the stability of $(\text{HgS})_n$ clusters

Thankan Jayasekharan

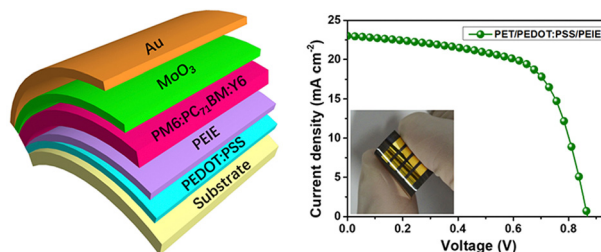


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23487

An organic cathode for low-temperature processed, flexible ternary organic solar cells with high-performance

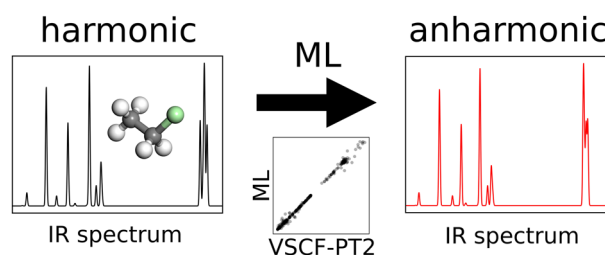
Xia Liu, Lei Wang, Xi Liu, Shuangcui Li, Zhihai Liu* and Ping Chen*



23495

Machine-learning to predict anharmonic frequencies: a study of models and transferability

Jamoliddin Khanifaev, Tim Schrader and Eva Perlt*



CORRECTIONS

23503

Correction: Visualizing and characterizing excited states from time-dependent density functional theory

John M. Herbert

23505

Correction: Polymer mechanochemistry: from single molecule to bulk material

Qifeng Mu* and Jian Hu*

