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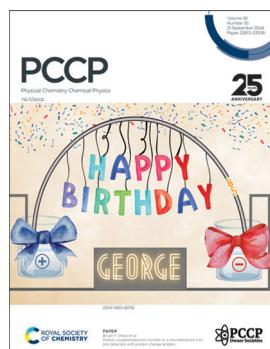
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ISSN 1463-9076 CODEN PPCFQ 26(35) 22813–23508 (2024)



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#### Inside cover

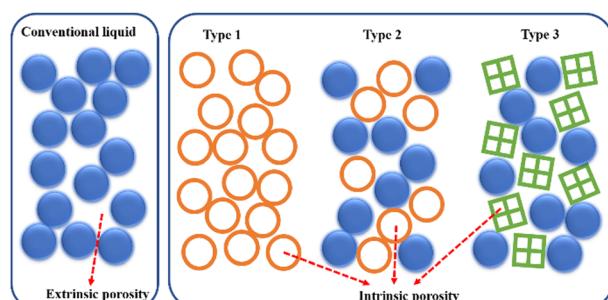
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### PERSPECTIVE

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\*

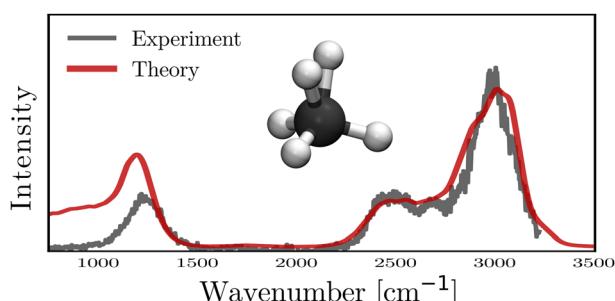


### COMMUNICATIONS

22846

#### Theoretical infrared spectroscopy of protonated methane isotopologues

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



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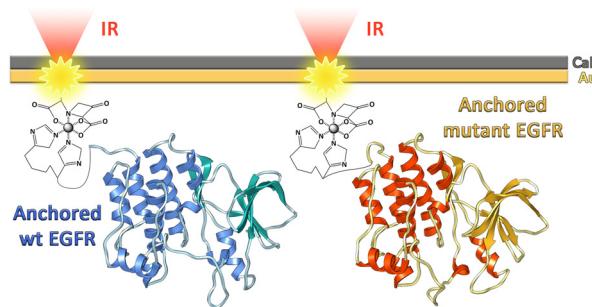


## COMMUNICATIONS

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**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\*

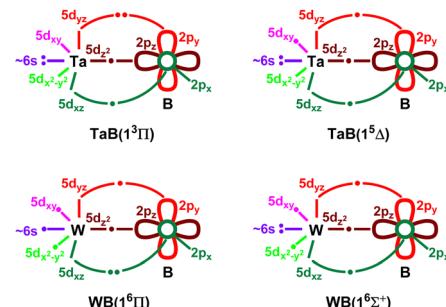


## RESEARCH PAPERS

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

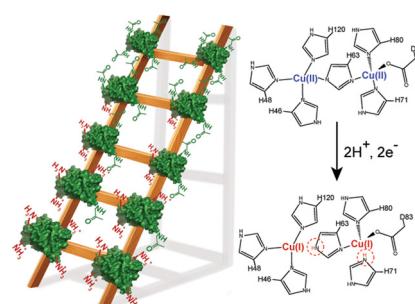
Isuru R. Ariyaratna



22870

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

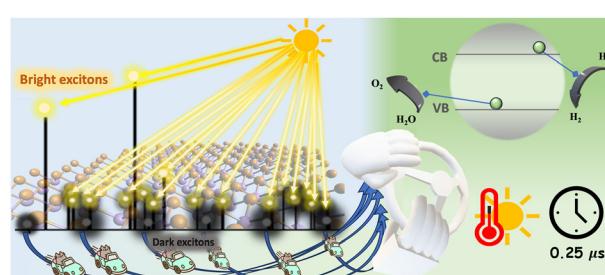
Mayte Gonzalez, Matthew J. Guberman-Pfeffer, Jordan C. Koone, Chad M. Dashnaw, Travis J. Lato and Bryan F. Shaw\*



22882

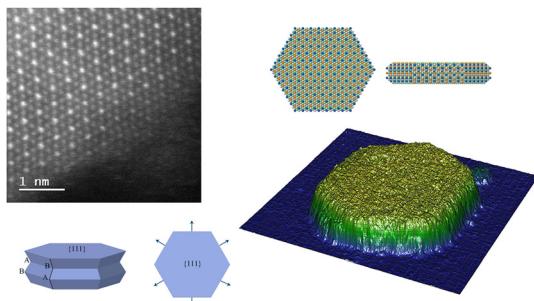
**Temperature-driven journey of dark excitons to efficient photocatalytic water splitting in  $\beta$ -AsP**

Harshita Seksaria, Amal Kishore and Abir De Sarkar\*



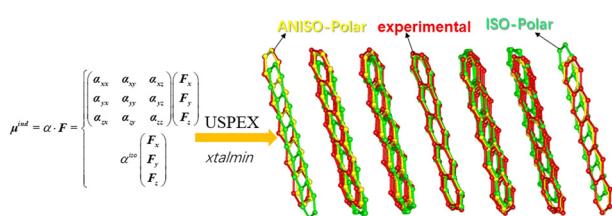
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**CoNiCuCrS alloy nanoparticles: synthesis and atomically resolved T/STEM studies**

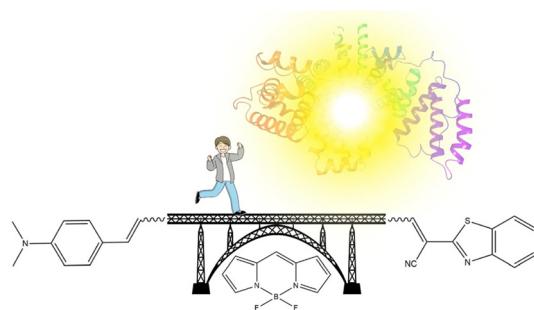
Carlos E. Rufino da Silva, Daniel Bahena Uribe, J. Jesús Velázquez Salazar, Dilip Karna, Joelin Agyei-Mensah and Miguel José Yacamán\*

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

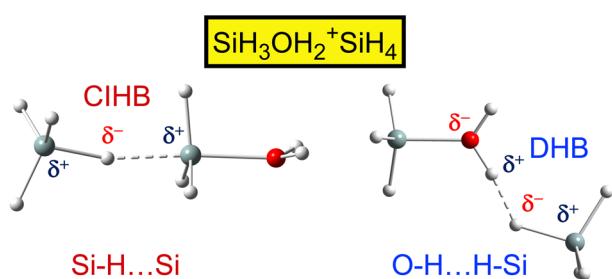
Yanyan Yang, Qianqian Jin and Shiwei Yin\*

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

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

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Martin Andreas Robert George and Otto Dopfer\*

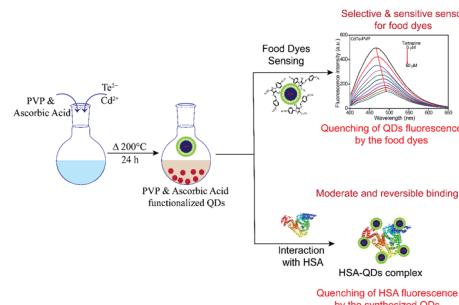


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**Formation of CdTe core and CdTe@ZnTe core–shell quantum dots via hydrothermal approach using dual capping agents: deciphering the food dye sensing and protein binding applications**

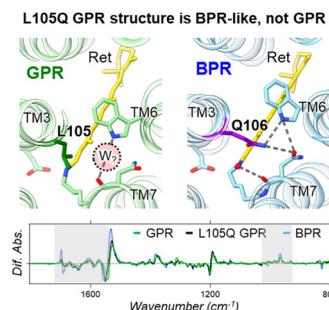
Mahabul Haque, Jintu Chutia, Amarjyoti Mondal, Sana Quraishi, Kalpana Kumari, Erica W. M. Marboh, Kripamoy Aguan and Atanu Singha Roy\*



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

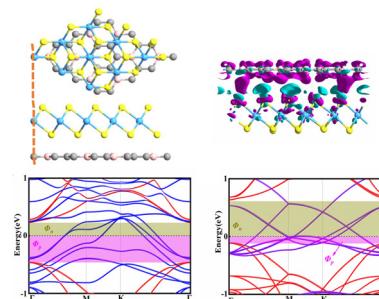
Tatsuro Nishikino, Teppei Sugimoto and Hideki Kandori\*



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**Electrical contact property and control effects for stable T(H)-TaS<sub>2</sub>/C<sub>3</sub>B metal–semiconductor heterojunctions**

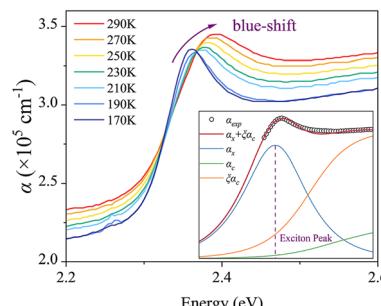
Shengguo Cao, Zhanhai Li, Jianing Han and Zhenhua Zhang\*



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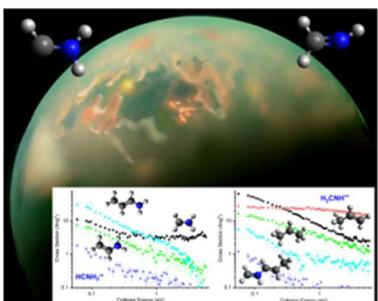
**Unravelling the mechanism of temperature modulated exciton binding energy for MAPbBr<sub>3</sub> perovskites**

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



## RESEARCH PAPERS

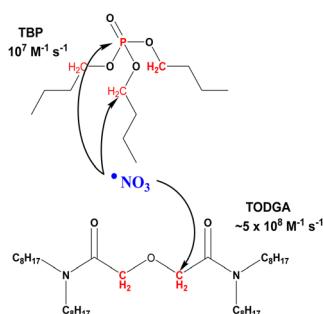
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**Combined experimental and computational study of the reactivity of the methanimine radical cation ( $\text{H}_2\text{CNH}^+$ ) and its isomer aminomethylene ( $\text{HCNH}_2^+$ ) with propene ( $\text{CH}_3\text{CHCH}_2$ )**

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

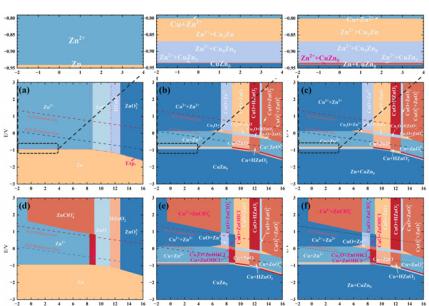
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**Reactions of the  $\cdot\text{NO}_3$  radical with nuclear extraction ligands in alkane solution**

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

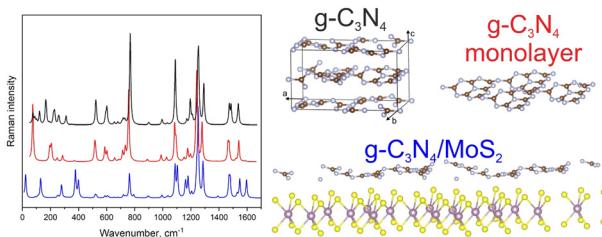
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**Electrochemical stability of biodegradable Zn–Cu alloys through machine-learning accelerated high-throughput discovery**

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

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**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

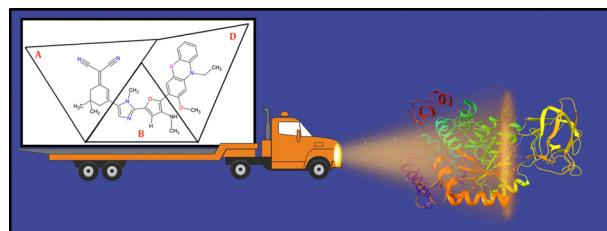


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**Optimizing 2-furylated imidazole  $\pi$ -bridges for NIR lipid droplet imaging**

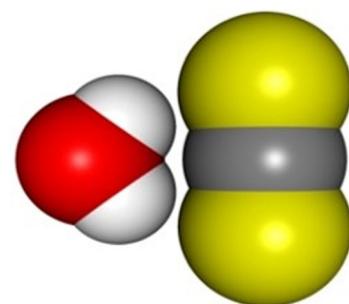
Anamika Suresh, Rohith Ramasamy, Deepa Kallumpurath and Rajadurai Vijay Solomon\*



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

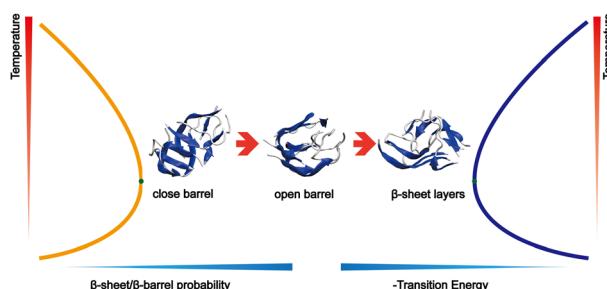
A. J. Barclay, A. R. W. McKellar, A. Pietropolli Charmet and N. Moazzen-Ahmadi\*



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**Energy gap of conformational transition related with temperature for the NACore of  $\alpha$ -synuclein**

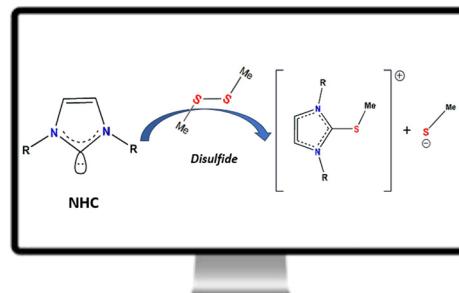
Pengxuan Xia, Yuanming Cao, Qingjie Zhao\* and Huiyu Li\*



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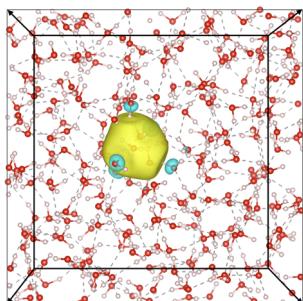
***In silico* investigation on the separation of disulfide bonds by N-heterocyclic carbene**

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



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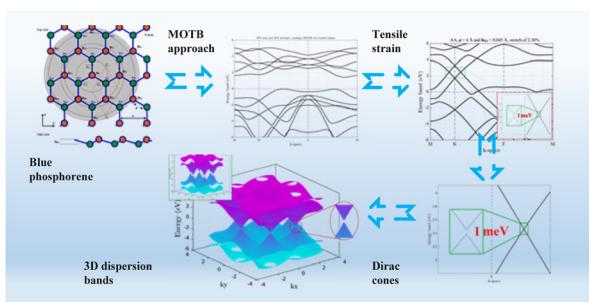
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## Enhanced deep potential model for fast and accurate molecular dynamics: application to the hydrated electron

Ruiqi Gao, Yifan Li and Roberto Car\*

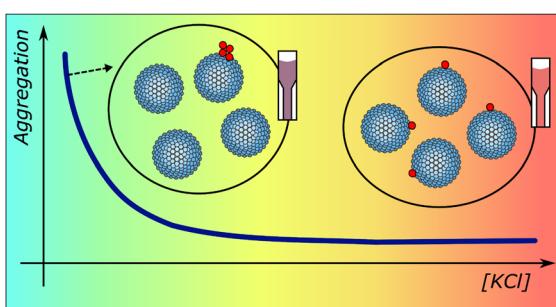
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## Two-dimensional bilayer blue phosphorus Dirac-like material: a multi-orbital tight-binding investigation

Amine Benhaij\* and Omar Mounkachi\*

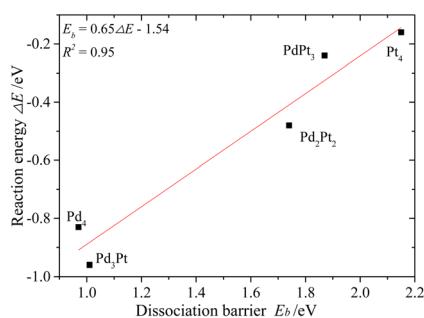
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## Cooperative aggregation of gold nanoparticles on phospholipid vesicles is electrostatically driven

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## H-assisted $CO_2$ dissociation on $Pd_nPt_{(4-n)}/In_2O_3$ catalysts: a density functional theory study

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

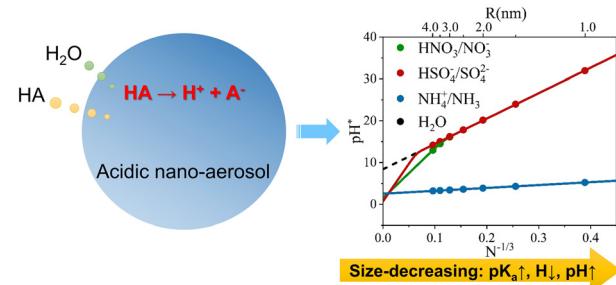


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**Size-dependent acidity of aqueous nano-aerosols**

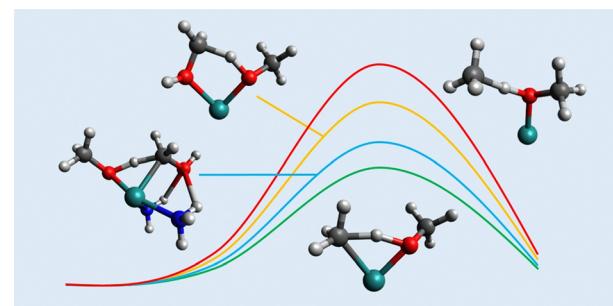
Wanrong Song, Shaoxun Guo and Hui Li\*



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

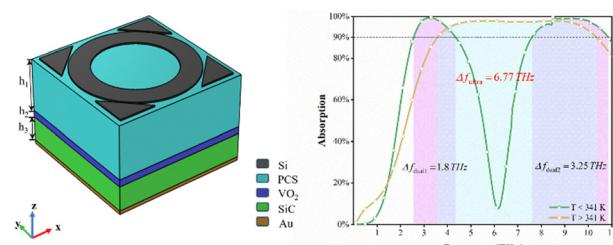
Shahriar N. Khan, Brody Quebedeaux and Evangelos Miliordos\*



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**Photocontrolled ultra-broadband metamaterial absorber around the terahertz regime**

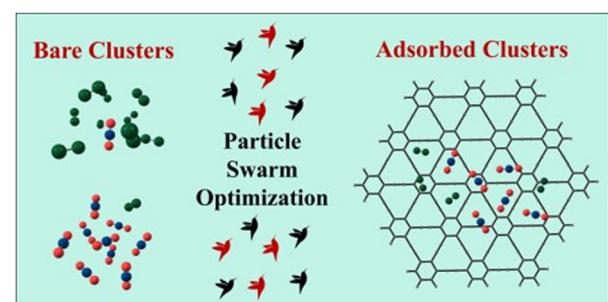
Guozheng Wu, Chao Li,\* Dong Wang, Song Gao, Haijun Guo, Wenyu Chen, Shijing Guo, Jiaran Xiong and Yue Che



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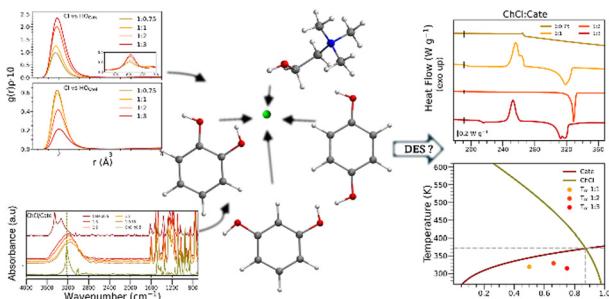
**On assessing the carbon capture performance of graphynes with particle swarm optimization**

Megha Rajeevan, Chris John and Rotti Srinivasamurthy Swathi\*



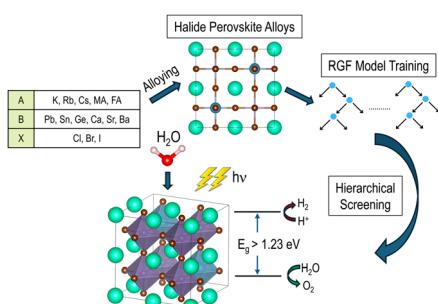
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**On the composition and isomerism effect in the thermal and structural properties of choline chloride/hydroxyphenol deep eutectic solvents**

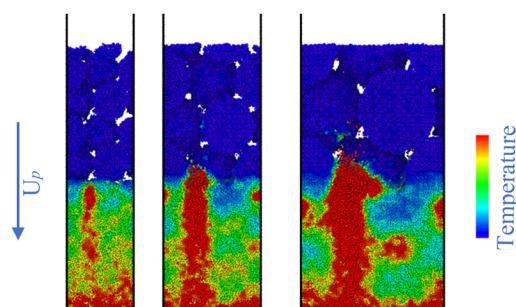
Paolo Casu, Matteo Busato,\* Matteo Palluzzi, Riccardo Spezia and Paola D'Angelo\*

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

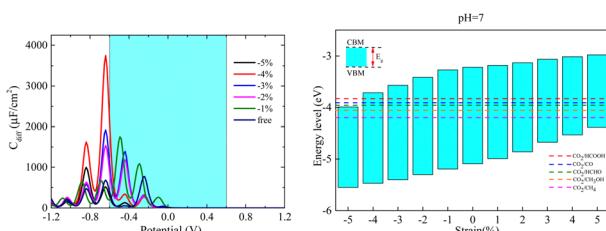
Maitreyo Biswas, Rushik Desai and Arun Mannodi-Kanakkithodi\*

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**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\*

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**Regulating the electronic properties, quantum capacitance and photocatalytic activity of Sc₂CO₃ based on Y doping and strain**

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

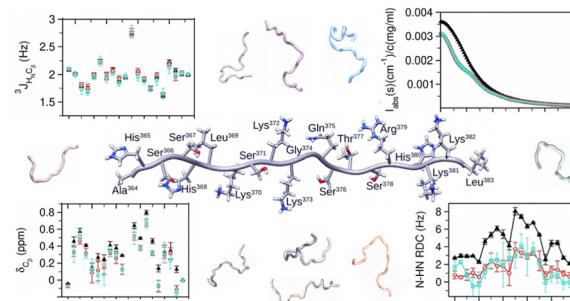


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**Statistical accuracy of molecular dynamics-based methods for sampling conformational ensembles of disordered proteins**

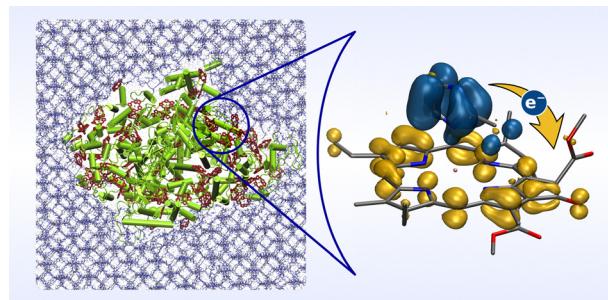
Adolfo Bastida,\* José Zúñiga, Federico Fogolari and Miguel A. Soler\*



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

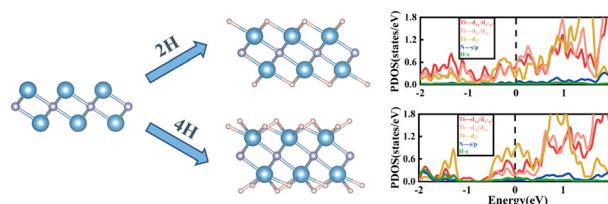
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**Realization of hydrogenation-induced superconductivity in two-dimensional Ti<sub>2</sub>N MXene**

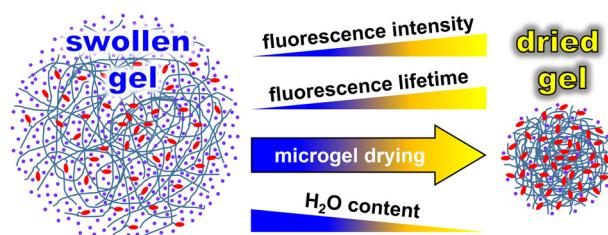
Yamin Xue, Zebang Cheng, Shunwei Yao, Ben Wang, Jiajun Jiang, Lin Peng,\* Tingting Shi, Jing Chen, Xiaolin Liu and Jia Lin\*



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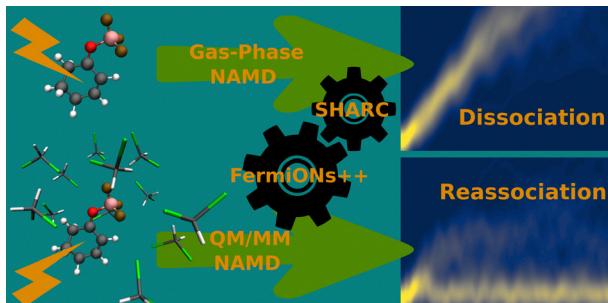
**Moisture changes inside hydrogel particles during their drying process investigated with fluorescence lifetime imaging**

Sankar Jana and Dominik Wöll\*



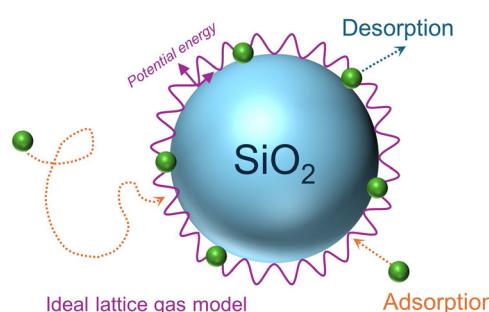
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**Simulation of the non-adiabatic dynamics of an enone-Lewis acid complex in an explicit solvent**

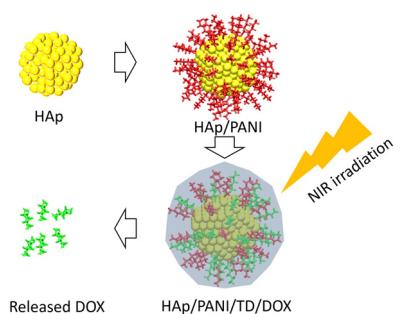
Martin T. Peschel, Jörg Kussmann,\* Christian Ochsenfeld\* and Regina de Vivie-Riedle

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

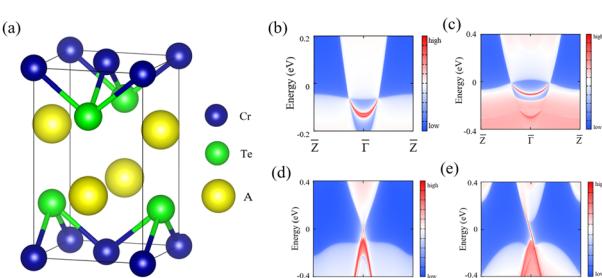
Kristen N. Johnson, Yixin Li, Michael J. Ezell, Pascale S. J. Lakey, Manabu Shiraiwa and Barbara J. Finlayson-Pitts\*

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**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\*

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**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\*

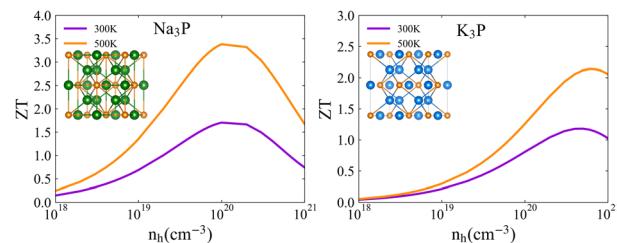


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**Excellent thermoelectric performance in alkali metal phosphides  $M_3P$  ( $M = \text{Na}$  and  $\text{K}$ ) with phonon-glass electron-crystal like behaviour**

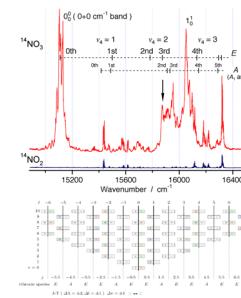
Xinji Xu, Weiyu Zhou, Wei Zhan, Ziyi Pan, Hao Huang,\* Geng Li,\* Shuming Zeng\* and Yusong Tu



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**Laser induced fluorescence spectroscopy of the  $\tilde{\text{B}}^2\text{E}' - \tilde{\text{X}}^2\text{A}'$  transition of jet cooled  $^{14}\text{NO}_3$  and  $^{15}\text{NO}_3$  II: the dispersed fluorescence spectrum from the 3rd E level of the  $\nu_4$  mode (approximately the  $2\nu_4$  ( $e'$ ),  $l = 0$ , level)**

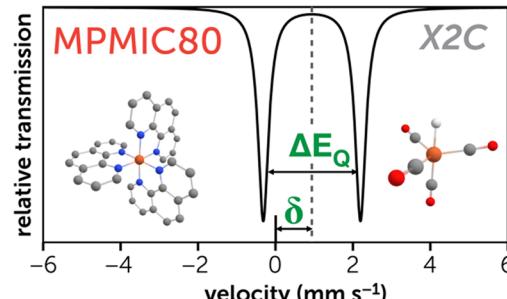
Masaru Fukushima



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

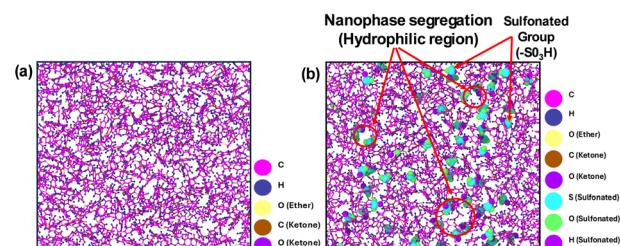
Golokesh Santra, Frank Neese\* and Dimitrios A. Pantazis\*



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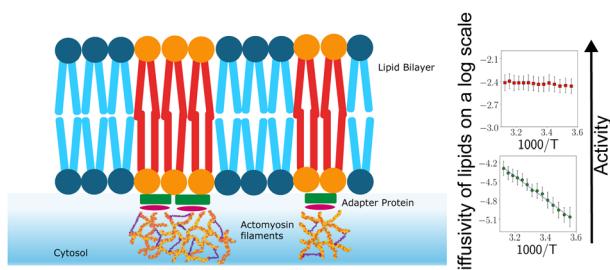
**Effect of the degree of polymerization, crystallinity and sulfonation on the thermal behaviour of PEEK: a molecular dynamics-based study**

Ashutosh Mittal and Avinash Parashar\*



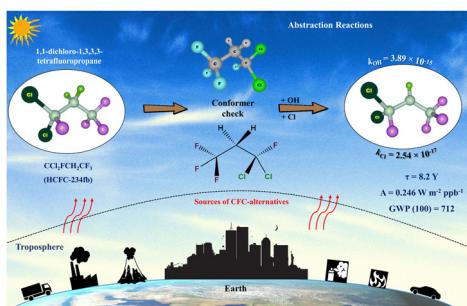
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**Self-diffusion is temperature independent on active membranes**

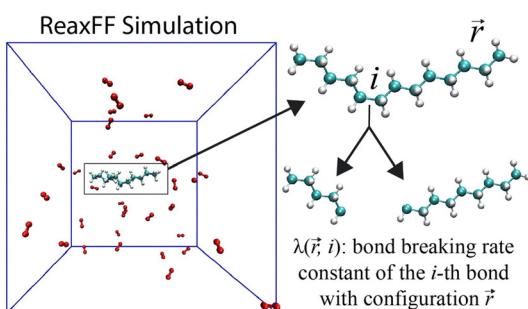
Saurav G. Varma, Argha Mitra and Sumantra Sarkar\*

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**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**

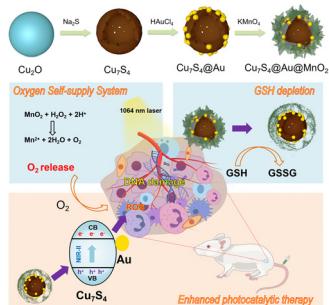
Rabu Ranjan Changmai, Samsung Raja Daimari, Anand Kumar Yadav and Manabendra Sarma\*

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

Jiang Wang,\* Zhiling Li and Wenli Zhang\*

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**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\*

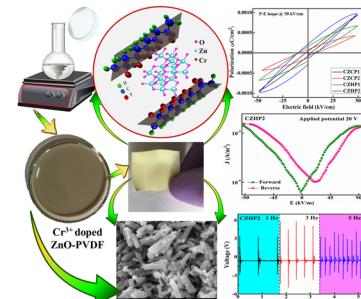


## RESEARCH PAPERS

23393

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

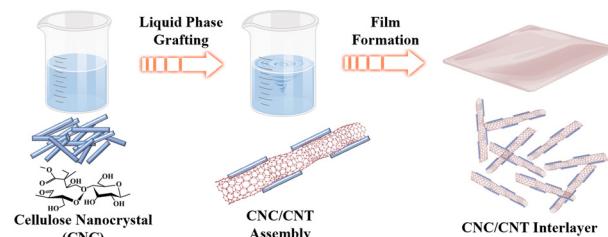
Tanmoy Chakraborty, Suman Saha, Dhananjay Mondal, Subhojit Dutta, Abhik Sinha Mahapatra, Kishan Gupta, Partha Sona Maji, Sukhen Das and Soumyaditya Sutradhar\*



23411

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

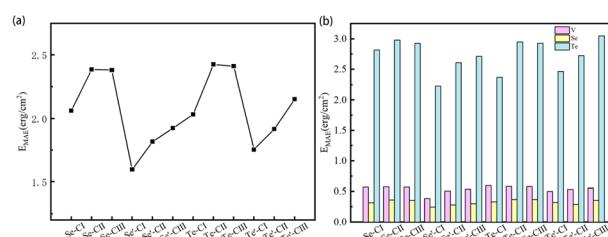
Hai Wang,\* Qin Zhao, Yue Wang, Junliang Lin, Weimin Li, Shun Watanabe\* and Xiaobo Wang\*



23419

**The electronic and magnetic properties modulated by ferroelectric polarization switching in two-dimensional VSeTe/Sc<sub>2</sub>CO<sub>2</sub> van der Waals heterostructures**

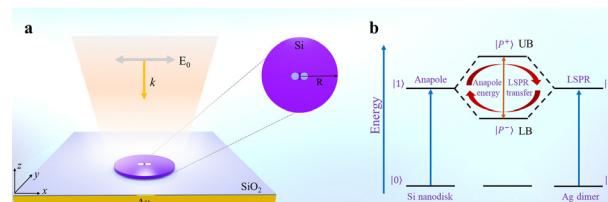
Weiyang Yu,\* Xiaoli Zhang, Yuling Zhang, Yali Wu, Rui Li and Wei-Bing Zhang



23429

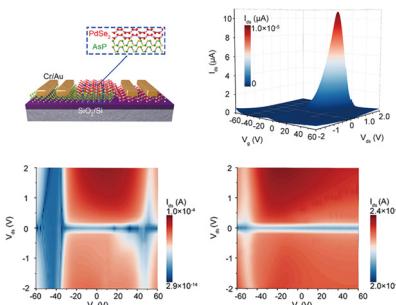
**Strong anapole–plasmon coupling in dielectric–metallic hybrid nanostructures**

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



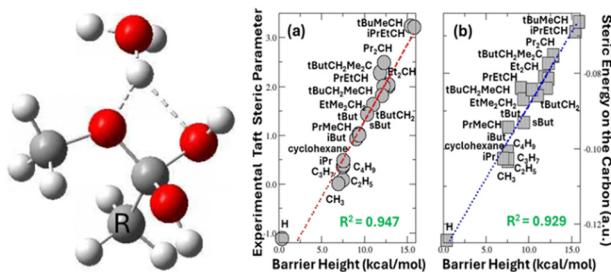
## RESEARCH PAPERS

23438

**Thermally tunable anti-ambipolar heterojunction devices**

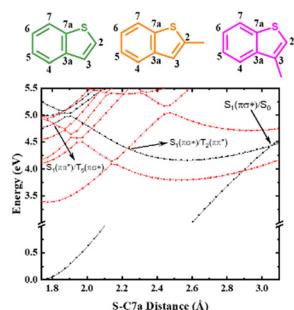
Shengyao Chen, Jiyou Jin, Wenxiang Wang, Shu Wang, Xiaoshan Du, Feng Wang, Lijun Ma, Junqi Wang, Cong Wang,\* Xinzheng Zhang\* and Qian Liu\*

23447

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

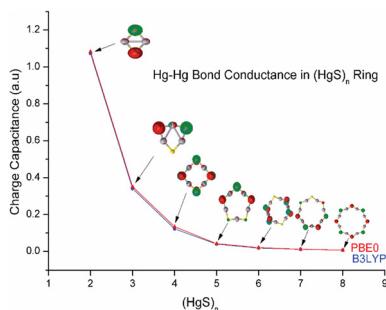
Jingwen Zhang, Xin He, Bin Wang, Chunying Rong,\* Dongbo Zhao\* and Shubin Liu\*

23457

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

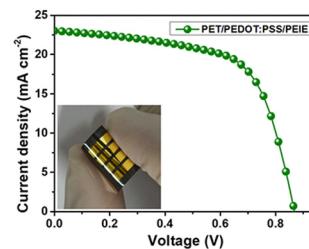
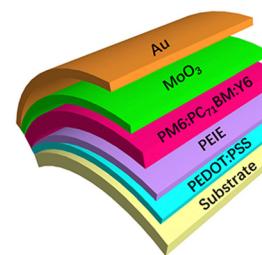


## RESEARCH PAPERS

23487

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

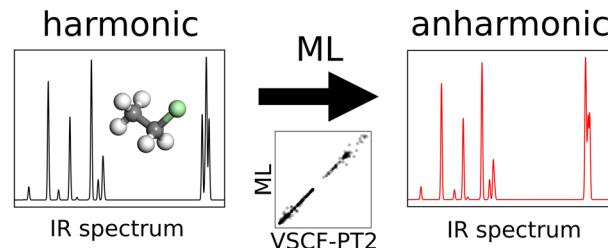
Xia Liu, Lei Wang, Xi Liu, Shuangcui Li, Zhihai Liu\* and Ping Chen\*



23495

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

Jamiliddin 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\*

