

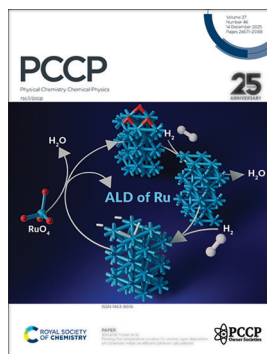
IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 27(46) 24671–25188 (2025)



Cover

See Shirin Faraji et al., pp. 24686–24688. Image reproduced by permission of Shirin Faraji from *Phys. Chem. Chem. Phys.*, 2025, 27, 24686.



Inside cover

See Alexandr Fonari et al., pp. 24704–24712. Image reproduced by permission of Alexandr Fonari from *Phys. Chem. Chem. Phys.*, 2025, 27, 24704.

EDITORIAL

24686

The role of electron spin in molecular photochemical and photophysical processes: theory and experiment

Shirin Faraji,* Martin Kleinschmidt, Bernd Engels and Andreas Dreuw

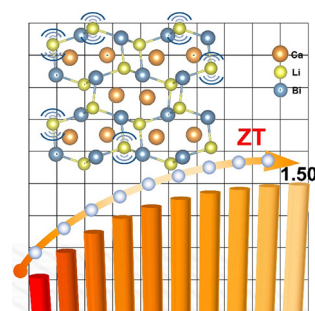


REVIEW

24689

Rattling vibration-induced low lattice thermal conductivity in Zintl-phase CaLiBi thermoelectrics

Zhiwei Zhang, Hao Wang, Shulin Bai, Da Wan, Peng Ai, Pengfei Zhang, Yunzhuo Zhang, Yujie Bao, Zhanpeng Xu and Shuwei Tang*



RSC Applied Interfaces

GOLD
OPEN
ACCESS

Interfacial and surface research with an applied focus

Interdisciplinary and open access



rsc.li/RSCApplInter

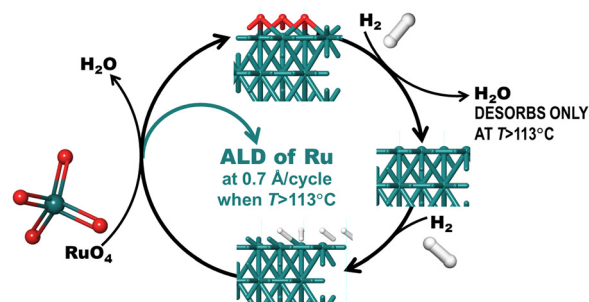
Fundamental questions
Elemental answers

RESEARCH PAPERS

24704

Finding the temperature window for atomic layer deposition of ruthenium metal *via* efficient phonon calculations

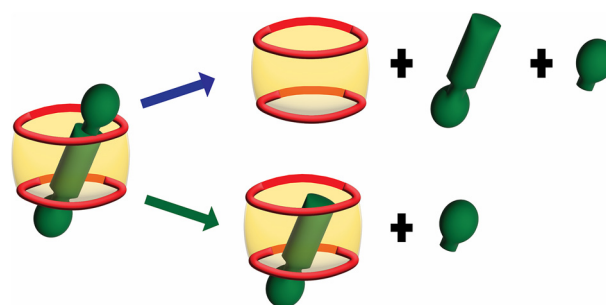
Alexandr Fonari,* Simon D. Elliott, Casey N. Brock, Yan Li, Jacob Gavartin and Mathew D. Halls



24713

Role of viologen substituents and host size in the gas-phase fragmentation of cucurbituril–viologen host–guest complexes

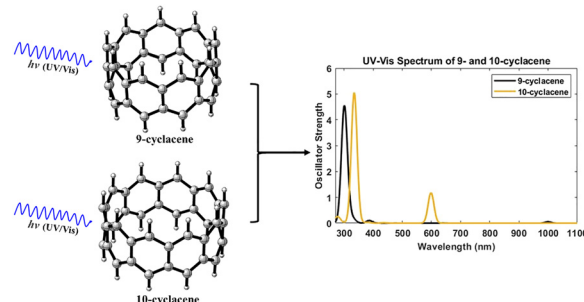
Hugo Y. Samayoa-Oviedo, Daniel M. Hristov, Bethany A. Phillips and Julia Laskin*



24726

Impact of cyclacene size on their electronically excited singlet states

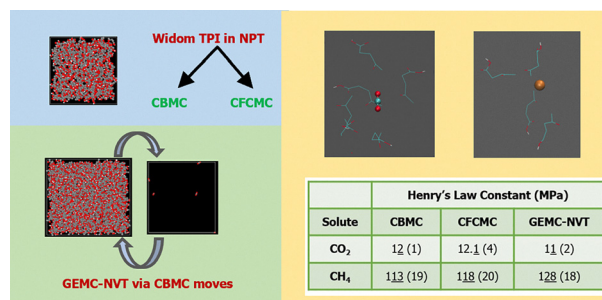
Abdollah Omran, Divanshu Gupta and Holger F. Bettinger*



24734

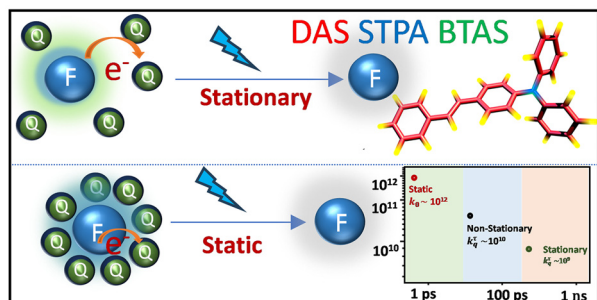
Prediction of Henry's law constants for CO₂ and CH₄ in levulinic acid *via* different Monte Carlo approaches

Prasil Kapadiya and Jhumpa Adhikari*



RESEARCH PAPERS

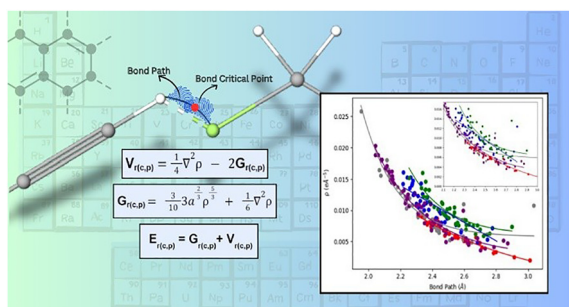
24747



Elucidation of the intrinsic and diffusion-driven electron transfer dynamics in *N,N*-diarylamino stilbenes: an ultrafast spectroscopic perspective

Preetika Verma, Megha Dinesh, Prajoy Kumar Mitra, Aarcha Santhosh and Yapamanu Adithya Lakshmana*

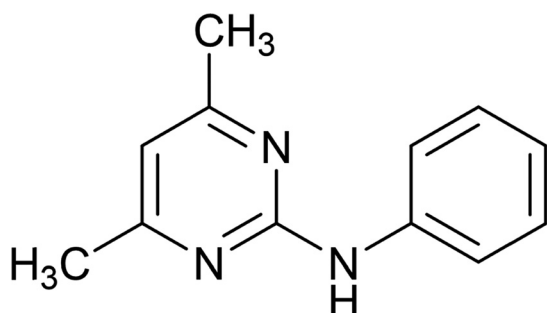
24759



Importance of intermolecular $-C\equiv C-H\cdots X-C$ ($X = F, O, N$) and $-Y-H\cdots F-C$ ($Y = O, N$) hydrogen bonds in crystal structures

Agantuk Saha, Sakshi and Angshuman Roy Choudhury*

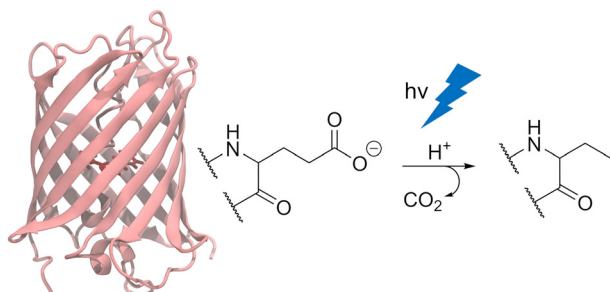
24766



Spectroscopic investigations of a pharmaceutical solid form analogue: pyrimethanil L-tartaric acid hemi-cocrystal

Ramandeep S. Dosanjh, Adam Patterson, Joe Harris, Claire Wilson, Matthias J. Gutmann, Paul Collier, Timothy Johnson, Timothy Hyde, Andrew P. E. York, Stewart F. Parker and David Lennon*

24777



Photoinduced decarboxylation in fluorescent proteins: charge-transfer states and structure–function relationship

Janko Čivič,* Hideaki Mizuno and Jeremy N. Harvey*

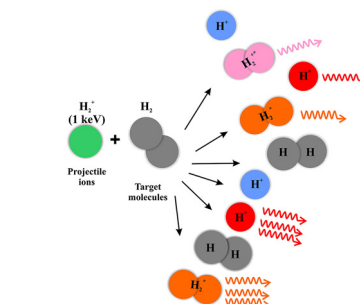


RESEARCH PAPERS

24789

The absolute total cross-sections of the charge transfer and the total luminescence in 1 keV $H_2^+-H_2$ collisions

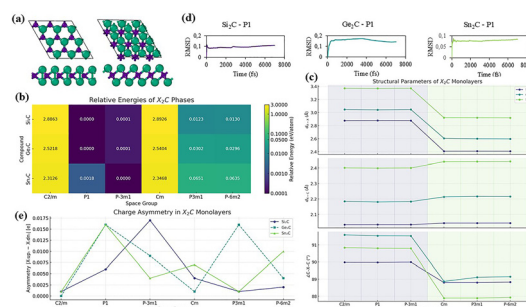
Ryszard Drozdowski* and Patryk Kamiński*



24797

Phase engineering of 2D X_2C monolayers: insights into metal–semiconductor transitions and multifunctional applications

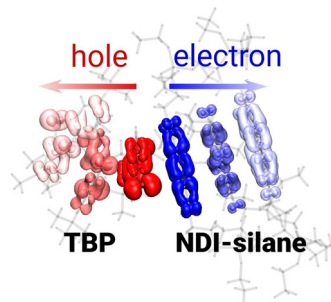
C. Pereyra Huelmo,* Ricardo Faccio,* Federico Iribarne, A. C. Garcia-Castro, Mauricio Vega-Tejido and Marc E. Segovia



24806

Optically induced charge separation at the naphthalenediimide–phenothiazine interface

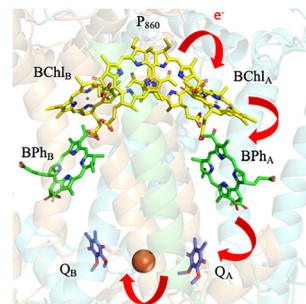
Thomas Trepl, Renan G. de Assis, Christine M. Isborn, Thiago B. de Queiroz and Stephan Kümmel*



24816

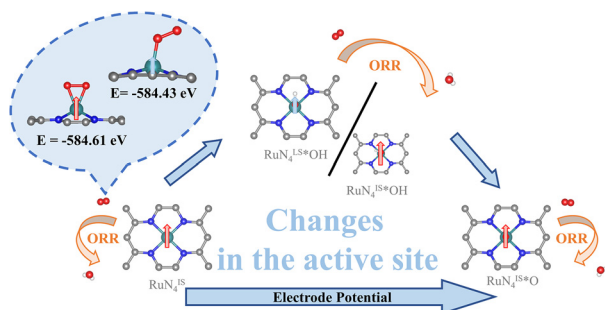
Why the electron chooses one of two symmetry-related paths in the type II bacterial photosynthetic reaction centers

Rongmei Judy Wei, Christine Kirmaier, Dewey Holten, Jan Kern, Philip D. Laible, Deborah K. Hanson, Gehan Ranepura, Md. Raihan Uddin, Jose Ortiz-Soto and M. R. Gunner*



RESEARCH PAPERS

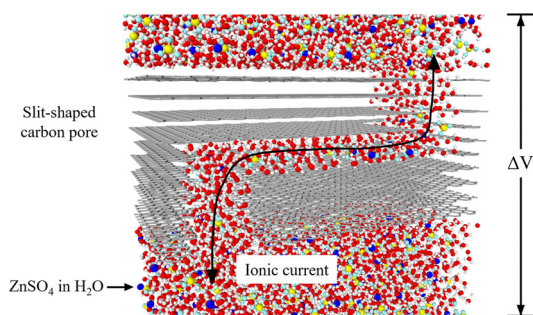
24827



Spin-dominated oxygen activation and reduction mechanism on a Ru–N–C single-atom-catalyst

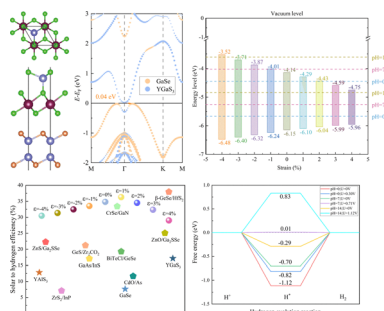
Zixian Zhao, Mingyuan Yu, Erjun Kan and Cheng Zhan*

24835

Pore size and counterion effects on ionic transport of a ZnSO_4 electrolyte in carbon slit pores via molecular dynamics

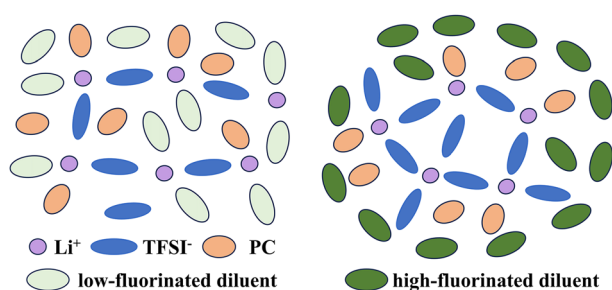
Matteo Alberghini,* Fabrizio Silveri and Alessio Tommasi

24846

Prediction of 2D heterostructure GaSe/YGaS₃ for highly efficient photocatalytic water splitting

Chao He,* Hui-Tang Liu, Qinghua Lv, Bao-Hua Tan, Bei Peng,* Hao Wang, JunHui Yuan and Jiafu Wang

24856

Fluorinated-diluent-driven modulation of Li^+ solvation structure and ion transport in localized high concentration electrolytes by molecular dynamics simulation

Yan Zhang, Zexin Zhang, Yilong Fan, Weizhong Zheng,* Weizhen Sun* and Ling Zhao

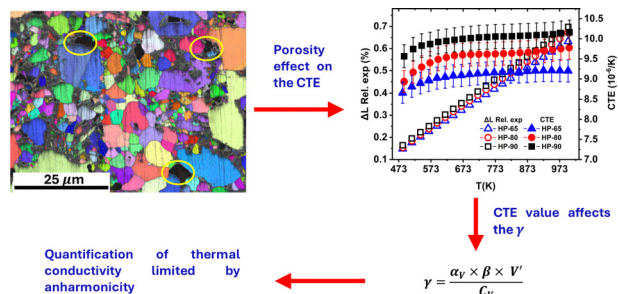


RESEARCH PAPERS

24872

Experimental and theoretical determination of the Grüneisen parameter to analyze the density effect on anharmonicity and thermal conductivity in the NbCoSb system

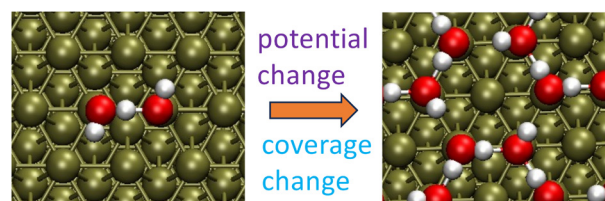
Inder Kumar, Jipin Peter, Anjali Gawande, Gowtham Venkatesan, Praveen Kumar, Satyam Suwas, Raju K. Biswas and Ramesh Chandra Mallik*



24888

Computational analysis of water coverage formation on Pt(111) surface under humid conditions with the effect of applied voltage

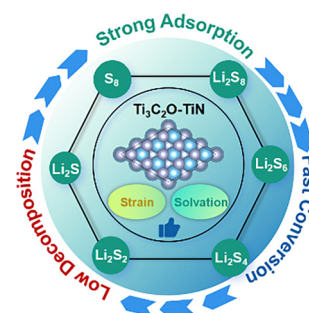
Maxim Shishkin* and Takeo Yamaguchi*



24899

Strain and solvation effects on Ti₃C₂O–TiN heterostructures as bifunctional electrocatalysts for Li–S batteries: a first-principles study

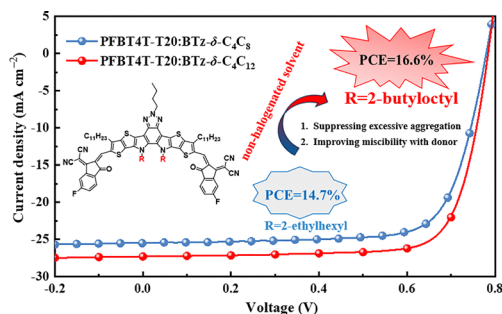
Mei Yang, Minhui Song, Lu Xie, Ping Qian* and Yanjing Su*



24911

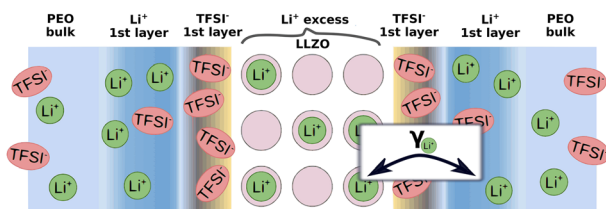
Side chain engineering of mono-fluorinated acceptors for efficient non-halogenated solvent-processed organic solar cells

Mei Luo,* Siyu Zhao, Lingchen Kong, Zesheng Zhang, Jialong Xie, Xuanchen Liu and Junwu Chen*



RESEARCH PAPERS

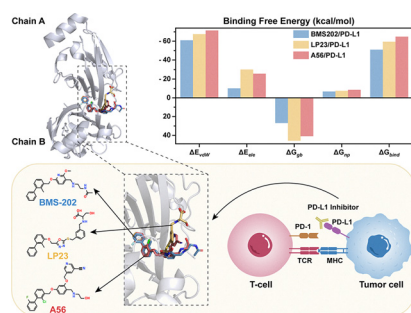
24918



Equilibration of ion distribution at polymer/ceramic interfaces

Melania Kozdra, Laura Hölzer, Daniel Brandell and Andreas Heuer*

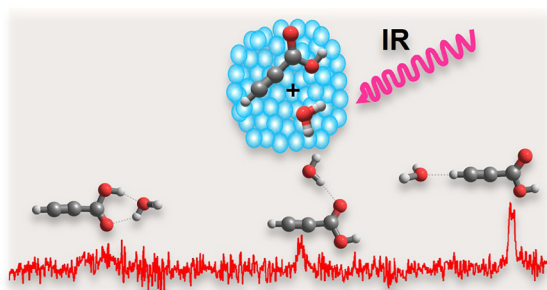
24932



Molecular dynamics reveals novel small-molecule inhibitors block PD-1/PD-L1 by promoting PD-L1 dimer stability

Shuhan Li, Danyang Xiong, Vladimir V. Klochkov, Ilya A. Khodov and Xiao He*

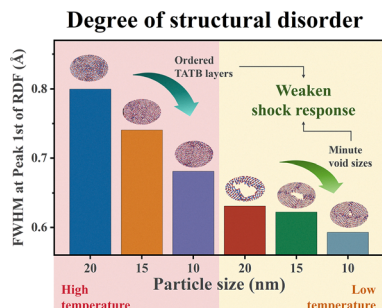
24948



Probing binding-site preferences in a propionic acid complex with water at 0.4 K

Arghya Chakraborty, Stefan Henkel, Gerhard Schwaab and Martina Havenith*

24958



Size-dependent shock response mechanisms in stacked nanoparticles of 1,3,5-triamino-2,4,6-trinitrobenzene

Guanchen Dong, Jialu Guan, Jing Lv, Linghua Tan,* Xiaona Huang* and Guangcheng Yang*

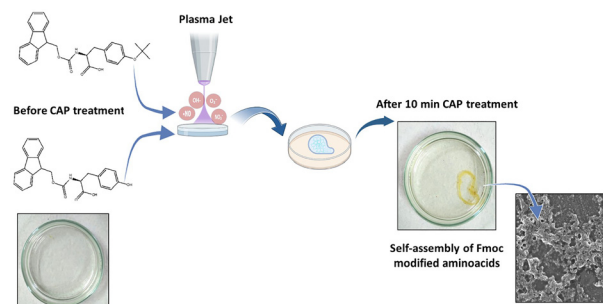


RESEARCH PAPERS

24969

Stimuli-responsive gelation of Fmoc-L-tyrosine derivatives to form supramolecular architectures via cold atmospheric plasma treatment

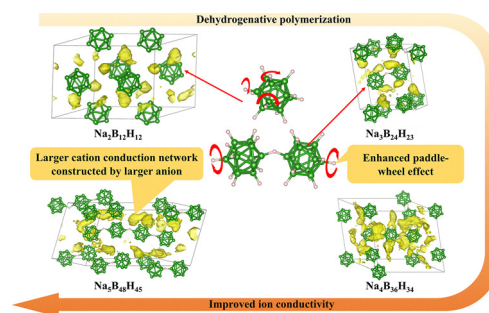
Priya Bhatt, Pranadhika Das and Kamatchi Sankaranarayanan*



24986

An anionic polymerization strategy for improving ionic conductivity in solid hydroborate electrolytes: the anion paddle-wheel effect

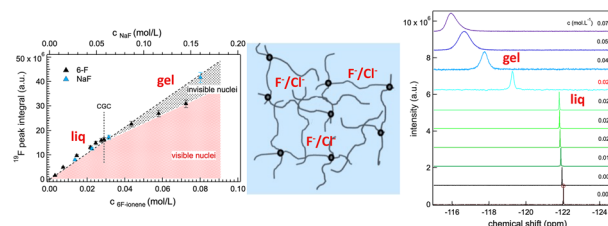
Jiahui Ji, Yujin Ji,* Yanhui Guo and Youyong Li*



24994

Ionene-based physical hydrogels: probing the liquid-gel transition, chain and counterion dynamics by means of NMR

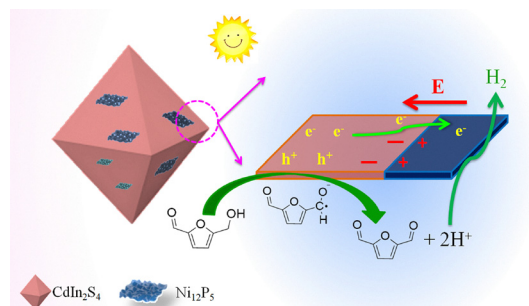
Sarrah Mezdari, Lingsam Tea, Juliette Sirieix-Plénet, François Ribot and Natalie Malikova*



25003

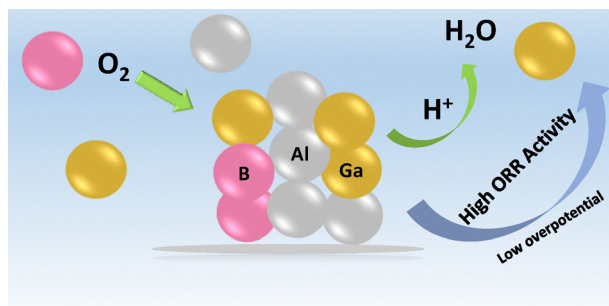
Constructing a 2D/3D Ni12P5/CdIn2S4 ohmic junction for enhanced photocatalytic selective oxidation of 5-hydroxymethylfurfural and H2 production

Zhenyu Liu,* Xiaoman Li,* Zhenyu Zhang, Yaming Zhao, Cheng Xue, Chenggong Gong and Weisheng Liu*



RESEARCH PAPERS

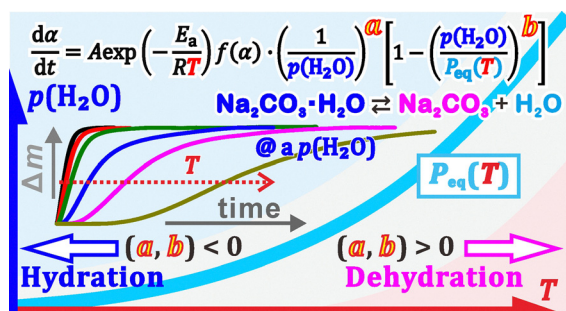
25014



Computational discovery of high-performance B–Al–Ga nanoclusters for oxygen reduction reaction catalysis

Pratik Sarkar, Maya Khatun and Anakuthil Anoop*

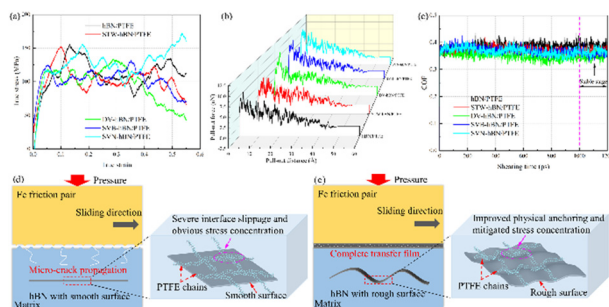
25027



Universal kinetic description for the hydration reaction of sodium carbonate anhydride across different temperatures and water vapor pressures

Mito Hotta and Nobuyoshi Koga*

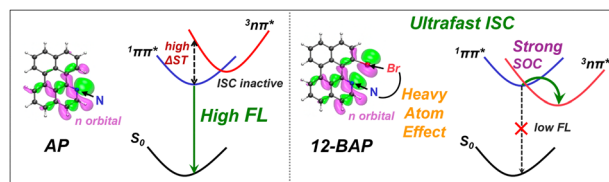
25043



Effect of geometrical defects of hexagonal boron nitride nanosheets on the mechanical and tribological properties of PTFE composites: molecular dynamics simulations

Yadi Yang, Jing Zhao, Jianzheng Cui,* Xiaokun Zhang and Bowen Jiang

25053



Strategic functionalization of bromine and nitrogen at the bay region of perylene induces a heavy atom effect and promotes intersystem crossing

Pandiselvi Durairaj, Sonia Das and Sunandan Sarkar*

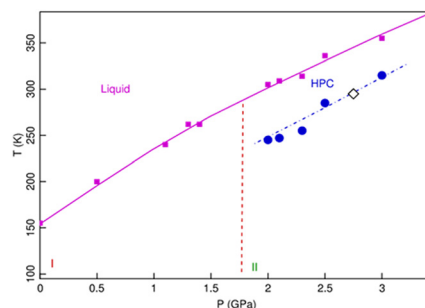


RESEARCH PAPERS

25062

Dielectric relaxation in the high-pressure hindered plastic crystal phase of ethanol

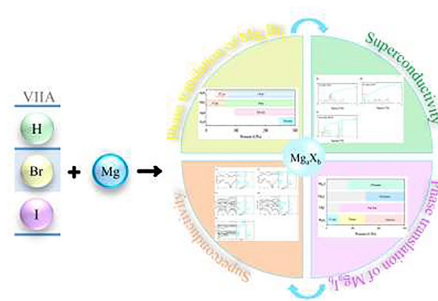
M. V. Kondrin,* A. A. Pronin, Y. B. Lebed and V. V. Brazhkin



25070

Pressure-induced superconductivity in alkaline earth metal halides Mg_aX_b ($\text{X} = \text{Br}, \text{I}$) from first principles calculations

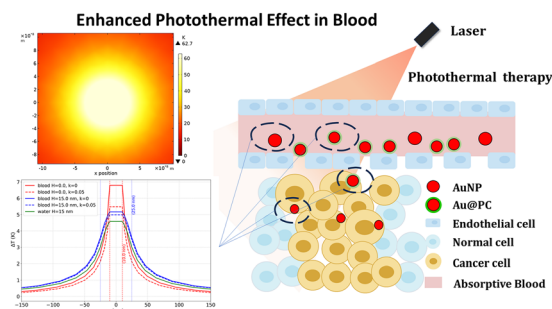
Shuang Zhao, Juan Gao,* Zhen Jiao,* Dai-He Fan, Miao Zhang, Zheng-Tang Liu and Qi-Jun Liu



25087

Research on the impact of blood absorption on the photothermal effect of nanoparticles with protein corona

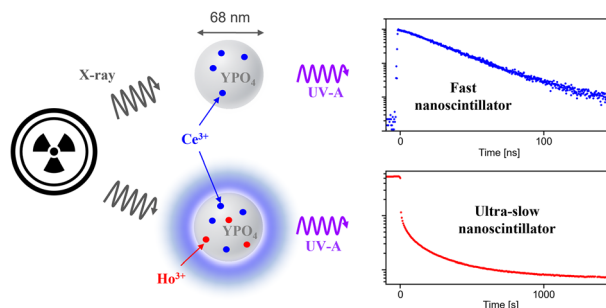
Mingjie Jiang, Xingcai Li,* Juan Wang* and Yunyun Wen



25098

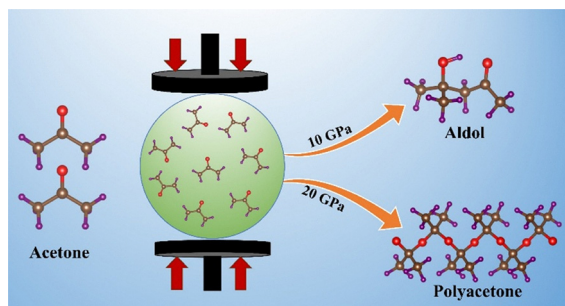
UV-A scintillation and persistent luminescence from Ce- and Ce/Ho-doped YPO_4 nanoparticles

Paul Ganigal, David Van der Heggen, Philippe F. Smet, Christophe Dujardin, Mathilde Ménard, Christophe Dorandeu, Jean-Olivier Durand and Aurélie Bessière*



RESEARCH PAPERS

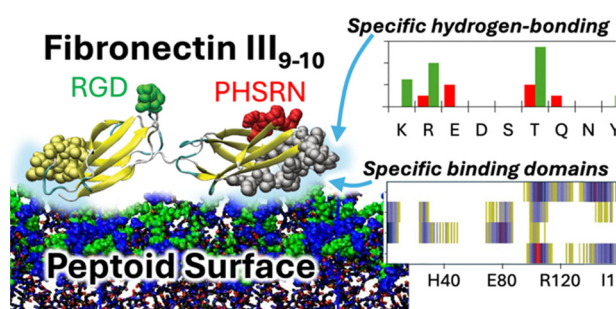
25110



Additive-free formation of aldol and polyacetone from acetone under pressure

Adrish Das, Shovan Das and Ayan Datta*

25116

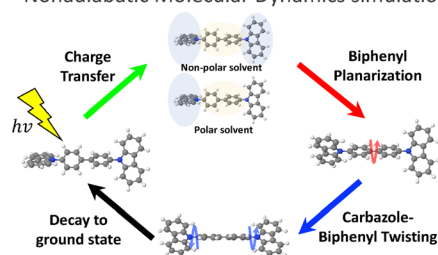


Specific and non-specific interactions of fibronectin with zwitterionic peptoid brushes studied by molecular dynamics simulation

David L. Cheung,* Phillip B. Messersmith and King Hang Aaron Lau*

25127

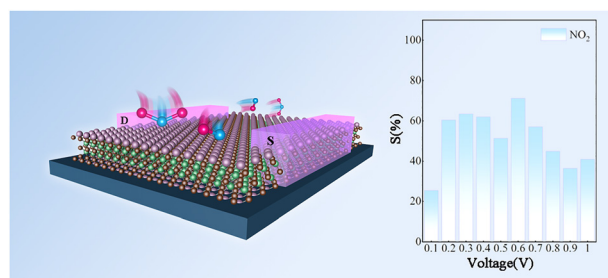
- ✓ Ultrafast Spectroscopy
- ✓ Nonadiabatic Molecular Dynamics simulations



Uncovering elusive ultrafast charge transfer-driven structural changes in 4,4'-bis(9-carbazol-9-yl)-1,1'-biphenyl, a paradigmatic molecular triad

Jungkweon Choi, Donghwan Im, Jeong Hoon Lee, Alekos Segalina and Hyotcherl Ihee*

25137



Study on the superior gas adsorption and sensing properties of $M_2Nb_2C_3$ ($M = Mo, V, \text{ and } Cr$) MXene based sensors in the detection of NO and NO_2 molecules

Shuo Ruan, Luzhen Xie, Jiaqi Xie, Lin Huang, Yun Liu,* Qiuming Liu,* Mengqiu Long and Tong Chen*

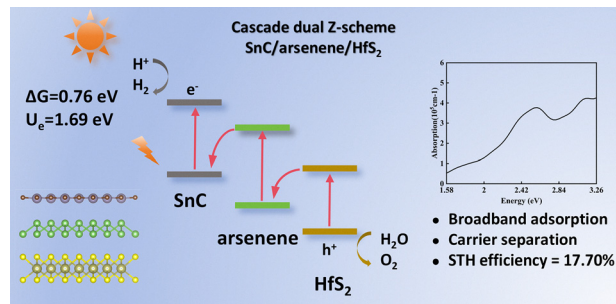


RESEARCH PAPERS

25148

Stable cascade dual Z-scheme SnC/arsenene/HfS₂ trilayer heterojunction for high-efficiency photocatalytic water splitting: a first-principles study

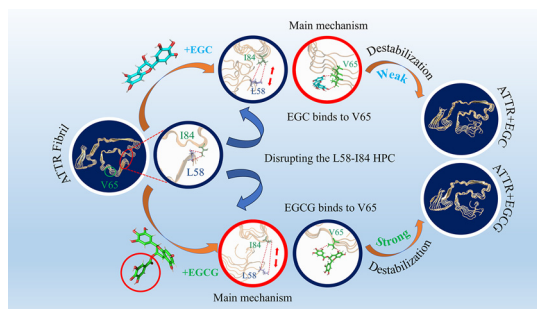
Zhengdong Sun, Jiaxin Ma, Junhao Zhu, Yifei Shen, Zhuyuan Sheng, Yiqing Liu, Weide Liu, Minwei Zhang and Meng Zhang*



25163

Distinct disruption mechanisms of green tea extracts EGC and EGCG on ATTR fibrils: a molecular simulation study

Xingke Yan, Yuanming Cao, Zihan Xu, Yanyan Zhu, Qingjie Zhao, Huiyu Li* and Yujie Chen*



25179

Dynamics of lifting the Au(111) reconstruction in perchloric acid electrolyte

Gary S. Harlow,* Weronica Linpé, Sebastian Pfaff, Ziyang Yang, Leon Jacobse, Vedran Vonk, Giuseppe Abbondanza, Marina Peña-Díaz, S. Barja, Ann-Christin Dippel, Olof Gutowski, Alfred Larsson, Lisa Rämisch, Johan Zetterberg, Lindsay R. Merte, Andreas Stierle and Edvin Lundgren*

