

# PCCP

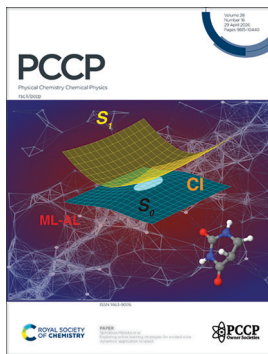
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## IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 28(16) 9815–10440 (2026)



### Cover

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### Inside cover

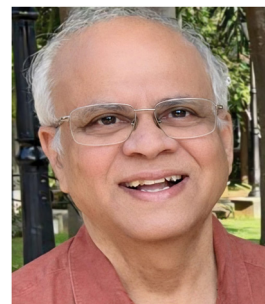
See Osamu Takahashi *et al.*, pp. 9910–9916. Image reproduced by permission of Osamu Takahashi from *Phys. Chem. Chem. Phys.*, 2026, 28, 9910.

## PROFILE

9831

**Atomic and molecular collisions: classical and quantum dynamics, chaos and fractals, periodic orbits, quantum mechanical resonances, gas-surface scattering, atomic and molecular clusters, atoms and molecules under confinement: a kaleidoscopic view**

Narayanasami Sathyamurthy

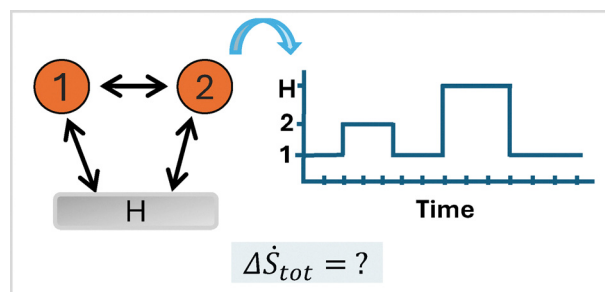


## REVIEWS

9840

**Identification and quantification of irreversibility in stochastic systems**

Aishani Ghosal and Gili Bisker\*



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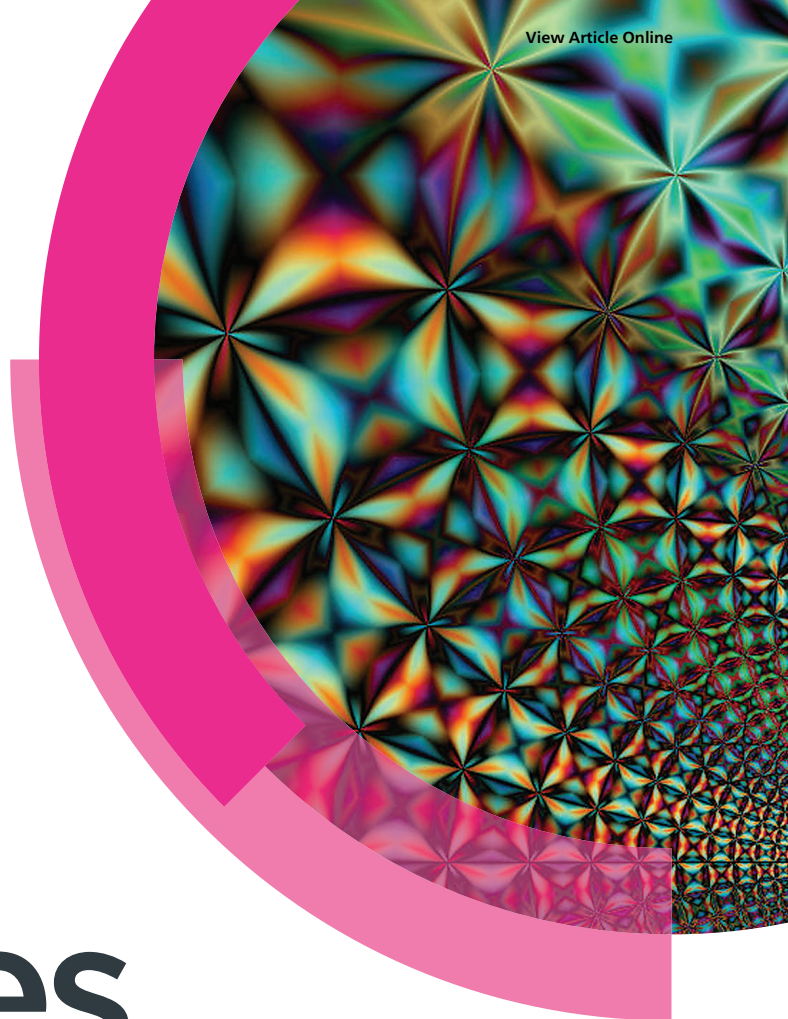


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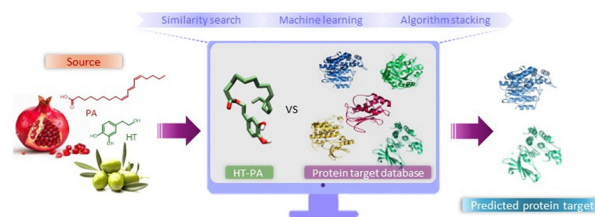


## REVIEWS

9867

### Integrative reverse-screening approaches for target discovery: the case of hydroxytyrosyl punicate

James Stewart, Meriem Chayah and Carmen Domene\*

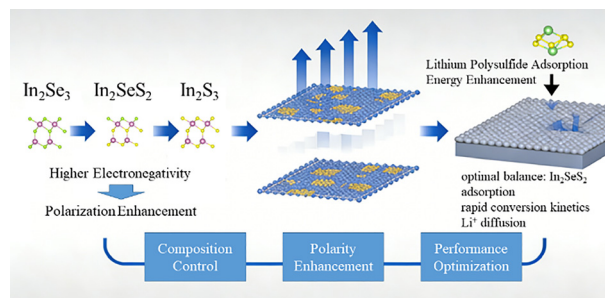


## COMMUNICATIONS

9882

### Tailoring ferroelectric polarization in $\text{In}_2\text{Se}_n\text{S}_{3-n}$ monolayers via Se/S ratio modulation to boost polysulfide electrocatalysis

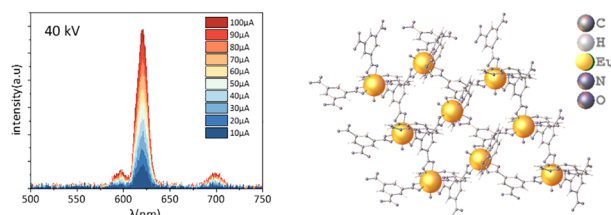
Haoyun Dou, Xuanpan Xu, Rawaid Ali, Hongqing Ma,\* Chen Qing\* and Hong-En Wang\*



9891

### Cathodo- and X-ray excited luminescence of europium tri- and tetracarboxybenzoates and phenanthroline

Yiming Yin, Dmitrii Kopytov, Anastasiya Parashuk, Alexander S. Goloveshkin, Egor Latipov, Guo Zhipeng, Ivan Khanbekov, Yanan Zhu and Valentina V. Utochnikova\*

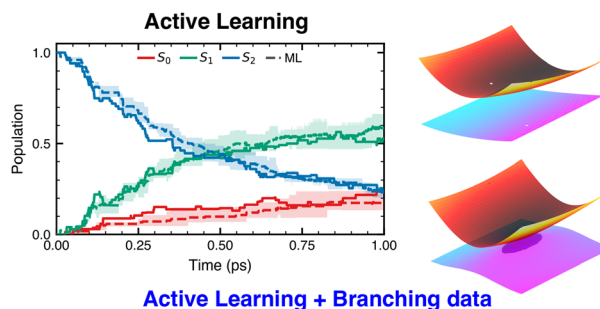


## RESEARCH PAPERS

9897

### Exploring active learning strategies for excited state dynamics: application to uracil

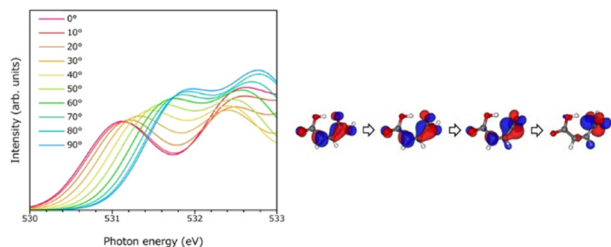
Juan Carlos San Vicente Veliz, Mark DelloStritto and Spiridoula Matsika\*



Active Learning + Branching data



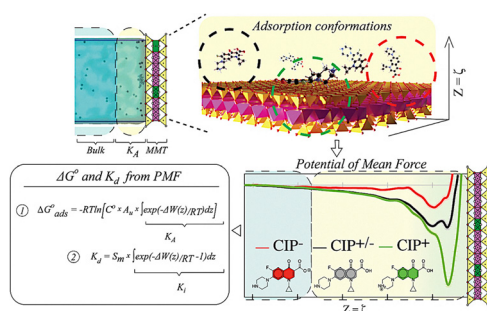
9910



### Controlling the pH of aqueous succinic and maleic acids analyzed by X-ray absorption spectroscopy

Risa Okada, Rikuya Adachi, Ryosuke Yamamura, Taiga Suenaga, Takashi Tokushima, Yuka Horikawa, Masaki Oura and Osamu Takahashi\*

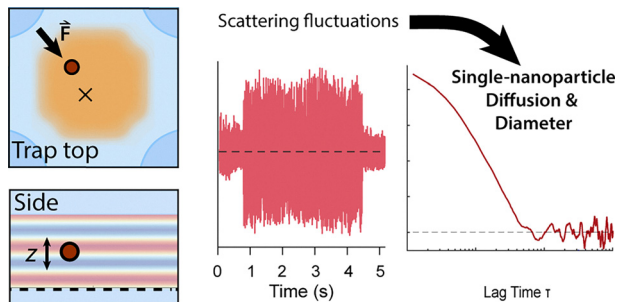
9917



### Molecular dynamics simulations of pH-dependent ciprofloxacin adsorption to Na-montmorillonite

Rogers E. Swai and Michael Holmboe\*

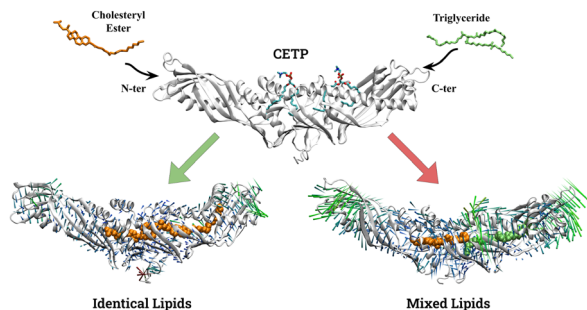
9932



### Sizing single trapped nanoparticles with interferometric scattering fluctuations

Abhijit A. Lavania and William B. Carpenter\*

9944



### Beyond the crystal: molecular dynamics investigations of CESTP with varied lipid substrates reveal asymmetric dominant motions

Bharath Raj Parthasarathy and Sanjib Senapati\*

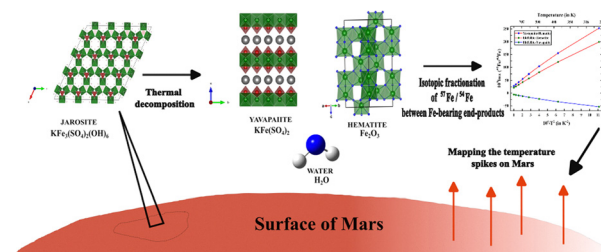


## RESEARCH PAPERS

9955

## Decoding episodes of past temperature spikes on the Martian surface using jarosite

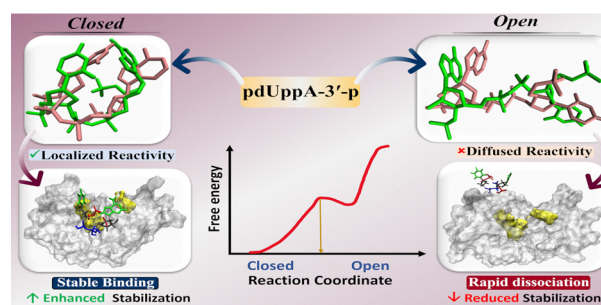
Debdatta Banerjee and Swastika Chatterjee\*



9974

## Exploring the conformation-dependent reactivity and dynamics of a dinucleotide inhibitor of ribonuclease A

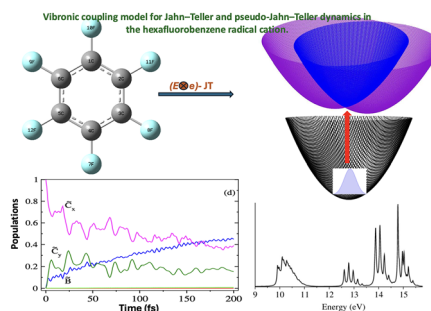
Sudipti Priyadarsinee, Arunendu Das\* and Srabani Taraphder\*



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## The Jahn–Teller and pseudo-Jahn–Teller effects in hexafluorobenzene radical cation: nonradiative decay and radiative emission

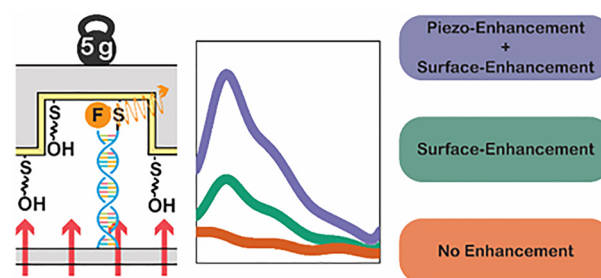
Arun Kumar Kanakati,\* Vadala Jhansi Rani and S. Mahapatra\*



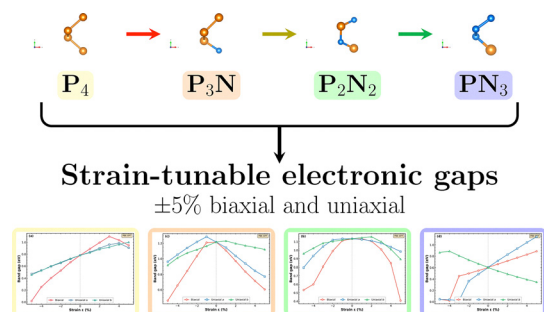
10009

## Dual-enhanced fluorescent biosensors using metal-coated piezoelectric nanoimprinted substrates

Ghadeer Almohammadi, Dominik Duleba, Aeshah F. Alotaibi, Eni Kume, Adrià Martínez-Aviñó, James H. Rice\* and Robert P. Johnson\*



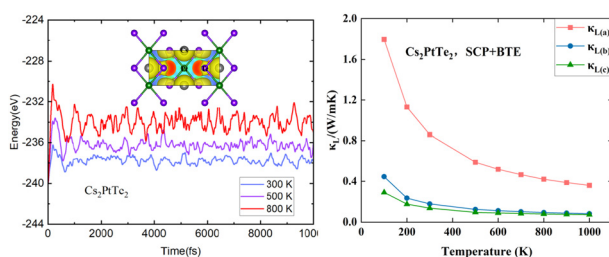
10019



### Electronic tunability and anisotropy in 2D P–N allotropes under strain

Mohammed Benchtaï,\* Abdellah Sellam, Abderrahim Bakak, Driss Lahboub, Abdelaziz Koumina, Mohamed Lotfi and Rodolphe Heyd

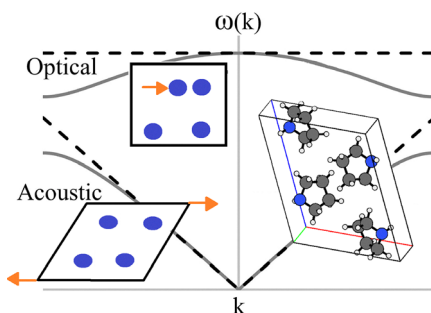
10035



### High thermoelectric performance induced by quasi-one-dimensional structure in $X(\text{Cs} \& \text{Rb})_2\text{PtTe}_2$

Ziyi Pan, Weiyu Zhou, Qinheng Li, Xiang Yan, Jinpeng Yang\* and Shuming Zeng\*

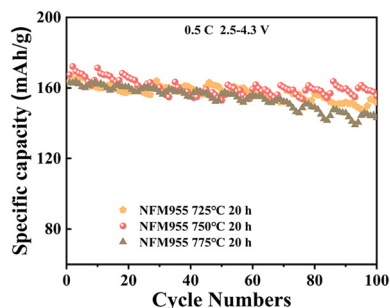
10043



### Einstein–Debye model for density-functional prediction of vibrational free energies of molecular crystals

Cameron J. Nickerson and Erin R. Johnson\*

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### Ultrahigh-Ni cobalt-free ternary cathode $\text{LiNi}_{0.9}\text{Fe}_{0.05}\text{Mn}_{0.05}\text{O}_2$ : synthesis and electrochemical performance for high-energy density lithium-ion batteries

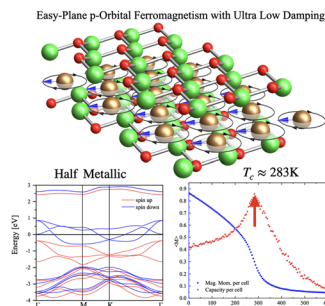
Jiatai Wang,\* Siyu Dong,\* Jiting Li, Cheng Qing, Guibang Zhang and Jian Li



10067

### Near-room-temperature easy-plane p-orbital ferromagnetism in half-metallic monolayer $\text{La}_2\text{CO}_2$

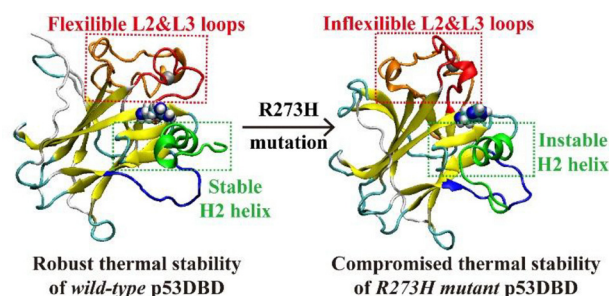
Yang Ou, Feng Tian, Yi Yang, Jianbo Zhang and Yang Zhou\*



10075

### Thermodynamic resilience of wild-type p53 DNA-binding domain and its disruption by the R273H hotspot mutation: insights from REMD simulations

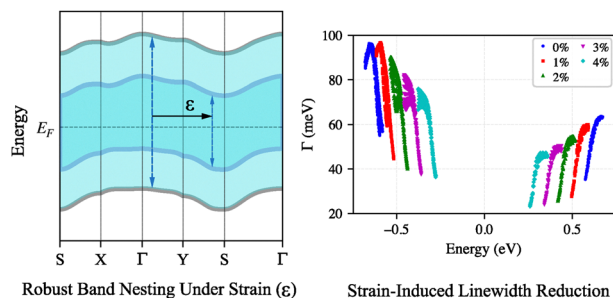
Ziqian Zhao, Gang Wang and Zhenyu Qian\*



10087

### Strain-tunable optoelectronics in a $\text{PdS}_2$ monolayer: the role of band nesting and carrier-phonon scattering

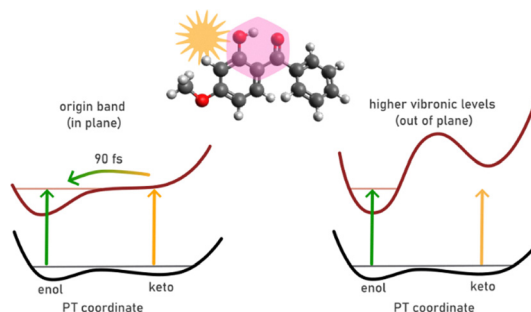
Hongfa Wang, Yancheng Gong, Subrahmanyam Pattamatta, Junwen Li, Hailong Wang\* and Zhizi Guan\*



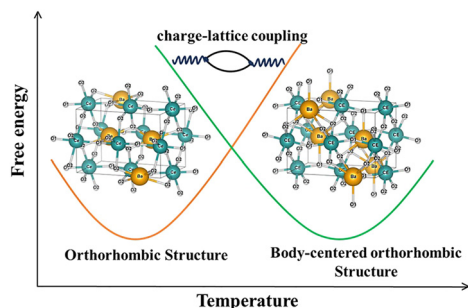
10095

### Unexpected shortening of the excited state lifetime of oxybenzone radical cation upon excitation of the band origin

Juan C. Latorre, Franco L. Molina, Satchin Soorkia, Michel Broquier, Gilles Grégoire\* and Gustavo A. Pino\*



10103

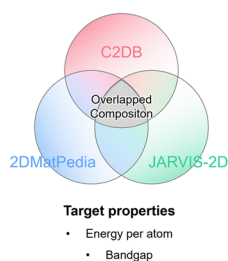


### Exploring the role of charge–lattice coupling in the structural phase transition in BaCeO<sub>3</sub>

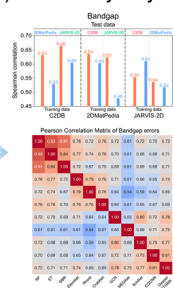
Nikita Jain, Payal Ratnawat, Archana Sagdeo\* and Pankaj R. Sagdeo

10119

#### 1) Practical OOD setting



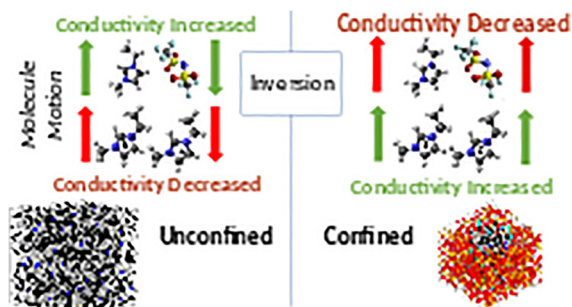
#### 2) Transferability analysis



### Comparative assessment of composition- and structure-based surrogate models across 2D materials databases

Inhyo Lee, Hyeokjae Chae, Jongwon Park, Jihye Shin, Hugon Lee\* and Seunghwa Ryu\*

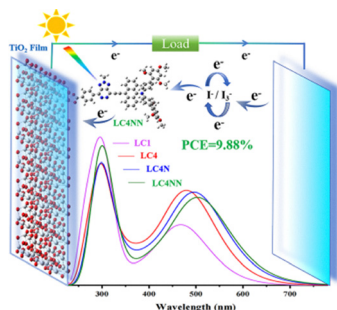
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### Molecular dynamics study of [EMIM][TFSI]/(Li/Na)TFSI ionic liquids confined in silica pores

Samanvitha Kunigal Vijaya Shankar, Chris Ewels, Jean Le Bideau and Yann Claveau\*

10147



### Optoelectronic performance of anthracene-based dyes with modified Hagfeldt donors in dye-sensitized solar cells

Haoyu Fan, Songfeng Li, Xiang Meng, Weiwei Pei, Tao Liu, Minxuan Wang and Yuanzuo Li\*

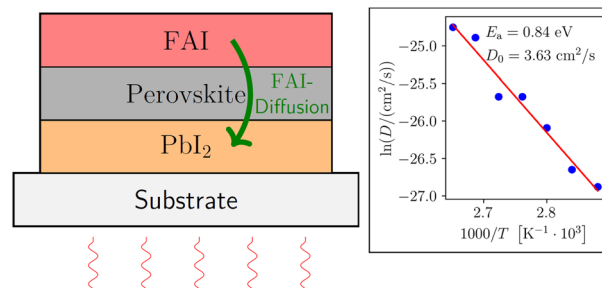


## RESEARCH PAPERS

10169

**Quantitative analysis of FAI-diffusion in sequentially evaporated FAPb<sub>3</sub> perovskite thin films**

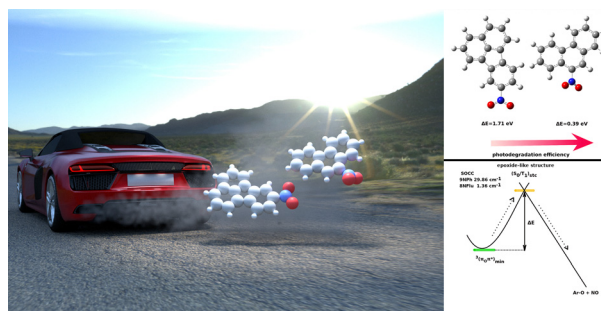
Tobias Schulz, Matthias Maiberg, Marcel Schrader, Roland Scheer and Paul Pistor\*



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**Possible outcome of sunlight-promoted photoinductive reactive pathways for the degradation of environmental pollutants 8-nitrofluoranthrene and 9-nitrophenanthrene**

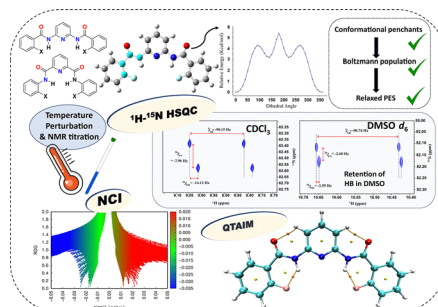
Bojana D. Ostojić,\* Branislav Stanković, Dragana S. Đorđević and Peter Schwerdtfeger



10201

**Intramolecular hydrogen bond-driven conformational preferences in pyridine-containing dibenzamide and dicarboxamide derivatives: evidence from NMR and DFT-based computation**

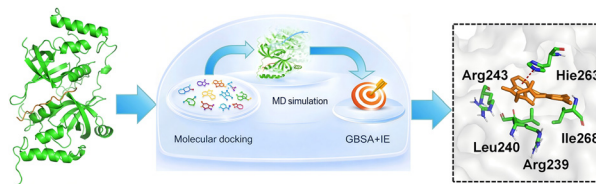
Swaraj Pathak, Sandeep Kumar Mishra\* and Nilamoni Nath\*



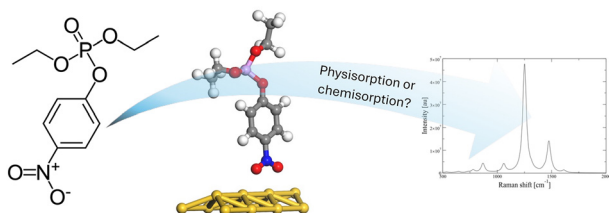
10216

**Comparative binding mechanisms of SND1 with MTDH and small-molecule inhibitors: insights from molecular dynamics simulations and free energy calculations**

Xi Zhu, Jiarui Chang, Min Fang, Xinyu Wu, Zhixiang Yin, John Z. H. Zhang, Fenghua Qi,\* Tong Zhu\* and Ya Gao\*



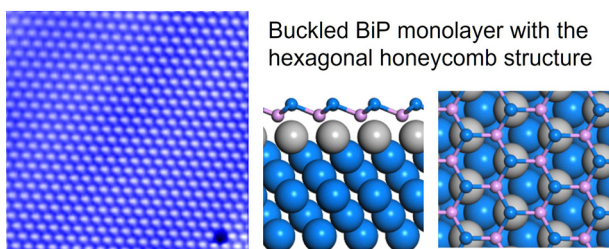
10230



### Organophosphate ethyl paraoxon on Ag and Au surfaces: a density functional theory perspective

Hang Hu,\* Jiří Hostaš,\* Mohammad Sajjad Ghaemi, Junan Lin, Shiliang Wang, Anguang Hu and Hsu Kiang Ooi

10238

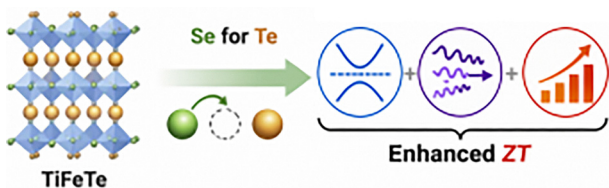


Buckled BiP monolayer with the hexagonal honeycomb structure

### Epitaxial growth of a buckled BiP monolayer on Bi(111)

Ting-Ting Zhang, Gang Yao,\* Xiao-Tian Yang, Kai Sun, Ji-Yong Yang, Min-Long Tao, Hua-Xing Zhu and Jun-Zhong Wang\*

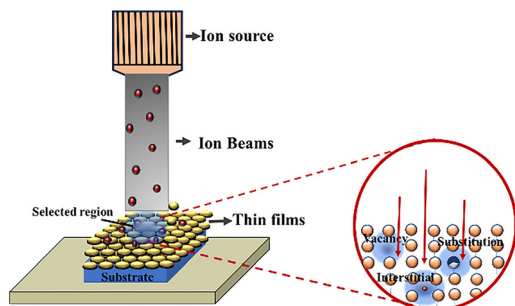
10245



### Alloying-induced reduction of lattice thermal conductivity in TiFeTe

Lei Gao,\* Ruixiu Liu, Yaoyao Chu, Zhen Luan, Yushan Li and Xing Xiong

10255



### Enhancement of the electrochemical properties of BiVO<sub>4</sub>: the role of oxygen vacancies induced by Ag ion implantations

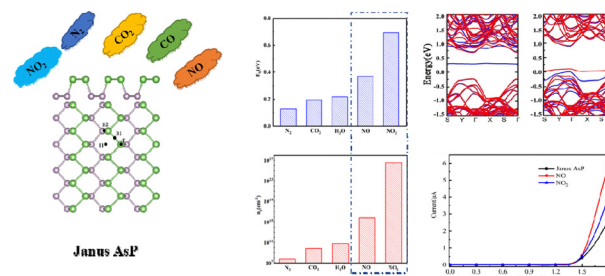
Shilpa Chauhan, Richa Saini, Thanigai Arul Kumaravelu, Chung-Li Dong, K. Deva Rani Devi and Asokan Kandasami\*



10269

### Janus AsP monolayers: a promising 2D platform for NO and NO<sub>2</sub> gas sensing

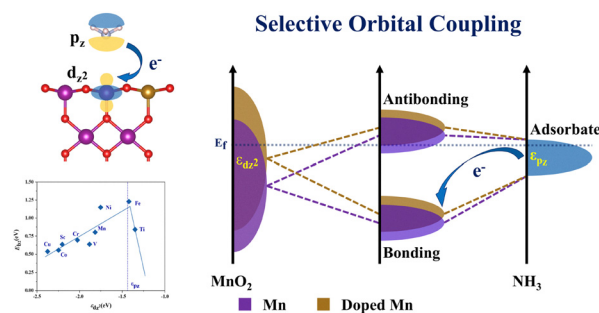
Yuncai Jiang, X. Tao, C. Hung, Shuangying Lei\* and Zaifa Zhou\*



10280

### Elucidating d–d orbital hybridization in metal-doped MnO<sub>2</sub> for the inhibition of N<sub>2</sub>O formation in NH<sub>3</sub>–SCR

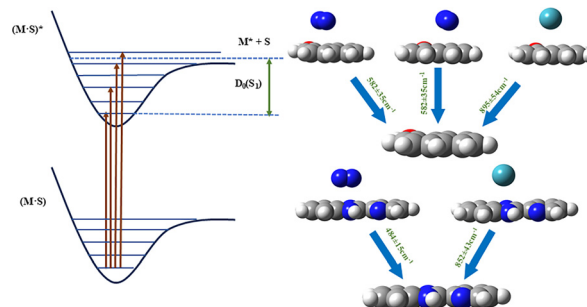
Kai Xie, Ying Wang, Fenghui Li, Haiqiao Wei and Lei Zhou\*



10291

### Determination of the intermolecular dissociation energies in the dispersion-bound N<sub>2</sub> and Xe complexes of 2-(2'-pyridyl)benzimidazole and 1-naphthol

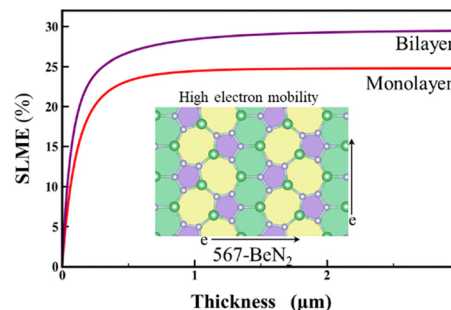
Bhavika Kalal, Simran Baweja, Satish Bhusan Panda and Surajit Maity\*



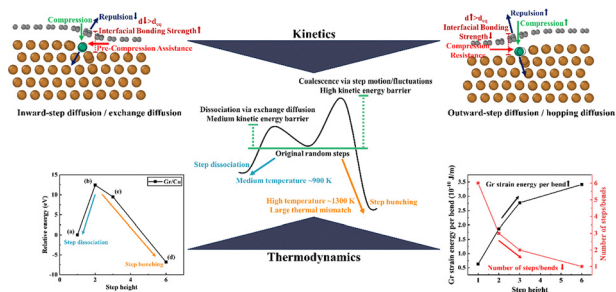
10300

### A direct-band-gap planar BeN<sub>2</sub> monolayer with high mobility and bilayer-enhanced photovoltaic efficiency

Changping Sun, Renyu Duan, Hongzhe Pan, Zhaoxin Lu, Caoping Niu,\* Meiling Xu\* and Yinwei



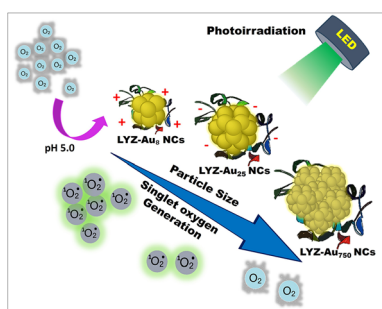
10309



## Surface diffusion of Cu mediated by graphene coverage

Haitao Zhang, Qi Zhang, Baixue Bian,\* Yue Liu,\*  
Tongxiang Fan\* and Mingyu Gong

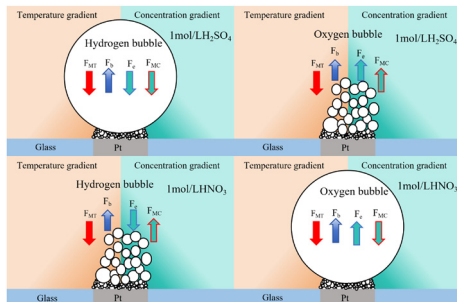
10320



## Size-dependent properties of gold nanoclusters in photoirradiation-mediated singlet oxygen generation

S Santhoshkumar, Yan-Ru Liu and Wei-Lung Tseng\*

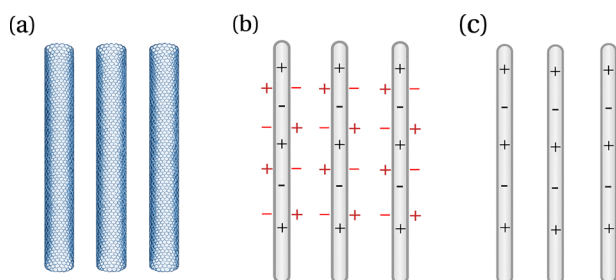
10329



## Experimental investigation of hydrogen and oxygen bubble growth on platinum microelectrodes of different sizes

Peng Kong, Liang Hao, Ming Gao,\* Wu-han Dong and  
Qi-rong Zuo

10339



## Do 1-dimensional metals prefer to form even-numbered van der Waals clusters?

S. Pal\* and John F. Dobson\*

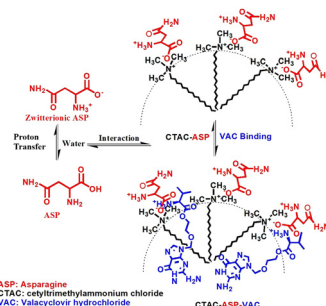


## RESEARCH PAPERS

10350

## Zwitterionic asparagine as a molecular modulator of cetyltrimethylammonium chloride micellization and drug–micelle interactions: a detailed study

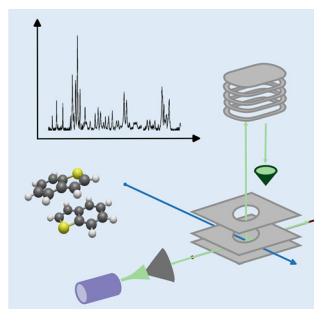
Malik Abdul Rub,\* Anirudh Srivastava,\* Naved Azum and Khalid A. Alzahrani



10364

## Elucidating the structure and binding nature of thianaphthene dimers using gas-phase infrared spectroscopy

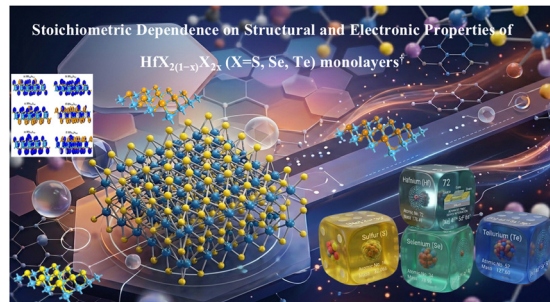
Gaia Zucali, Vincent J. Esposito, Sandra Brünken and Piero Ferrari\*



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Stoichiometric dependence of the structural and electronic properties of  $\text{HfX}_{2(1-x)}\text{X}_{2x}$  ( $X = \text{S}, \text{Se}, \text{Te}$ ) monolayers

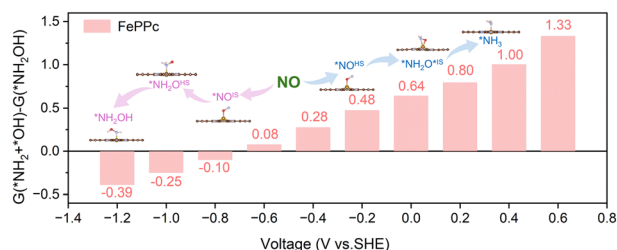
Vivek Mahajan\* and Hitesh Sharma



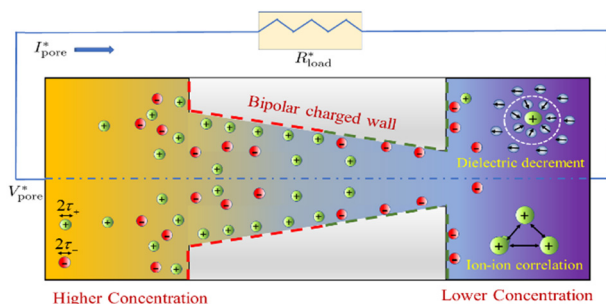
10385

## A spin-crossover-mediated potential-dependent selective NO reduction reaction on iron-polyphthalocyanine: a DFT study

Ya Jin, Mingyuan Yu, Erjun Kan and Cheng Zhan\*



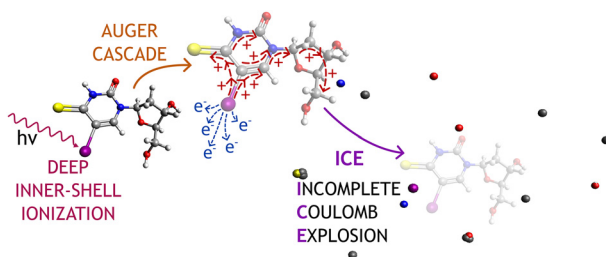
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### Impact of multivalent ions on osmotic power generation in a bipolar conical pore: a numerical analysis based on modified electrokinetic models

Shakyajit Paik and Somnath Bhattacharyya\*

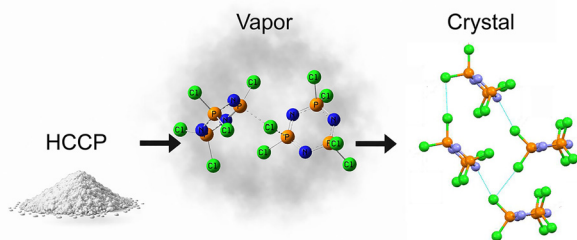
10414



### Dissociation of halogenated deoxyridines as potential radiosensitizers, induced by deep inner-shell photoionization – experiment and modeling

Kerttu-Inkeri Pusa,\* Edwin Kukk, Marta Berholts, Tatiana Marchenko, Iyas Ismail, Denis Céolin, Marc Simon and Oksana Travnikova\*

10428



### Hexachlorocyclotriphosphazene: macromolecular assemblies in vapor and crystalline phases. experimental and computational approach

Semyon S. Egorov,\* Elena Yu. Tupikina and Artem A. Selyutin

