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#### Inside cover

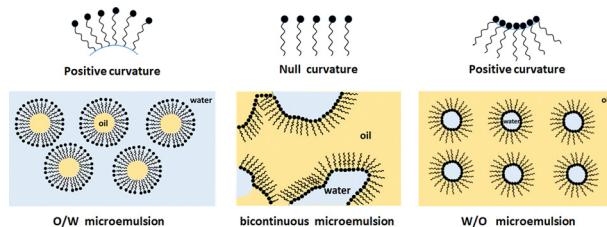
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*Phys. Chem. Chem. Phys.*,  
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#### Effect of polymer addition on the phase behavior of oil–water–surfactant systems of Winsor III type

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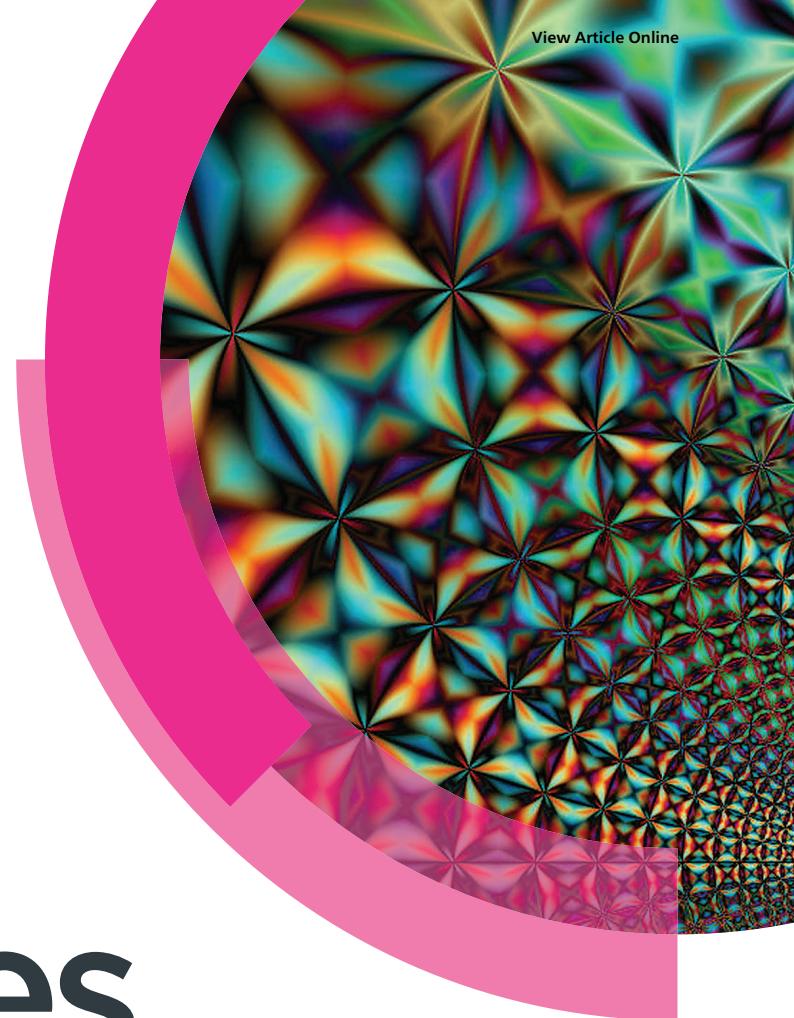
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Krishan Kumar



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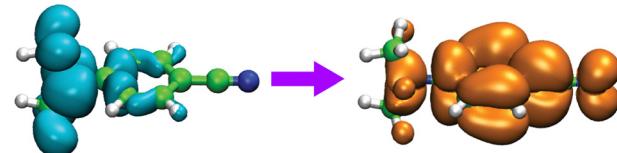
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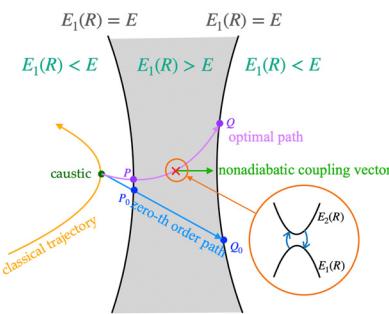


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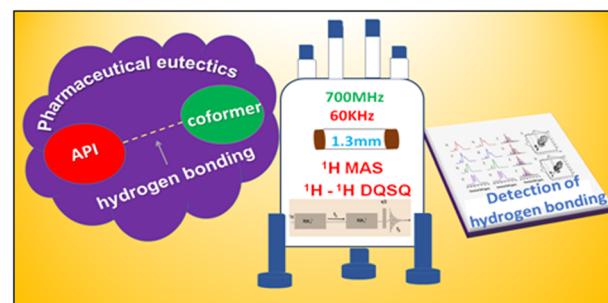
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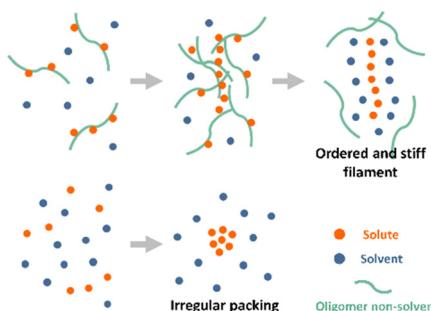
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Abdul Hamid Malhan and Krishnan Thirumoorthy\*



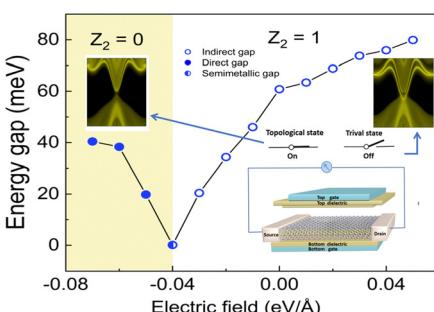
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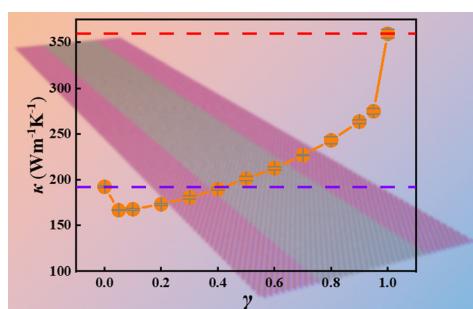
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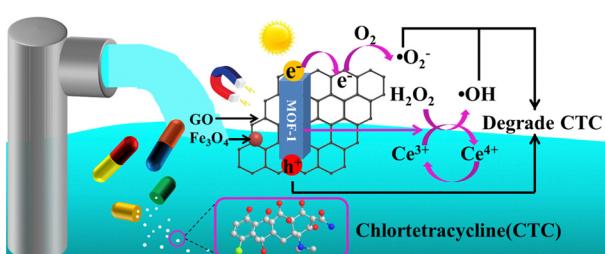
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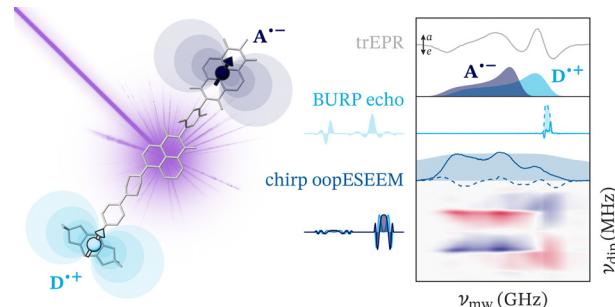


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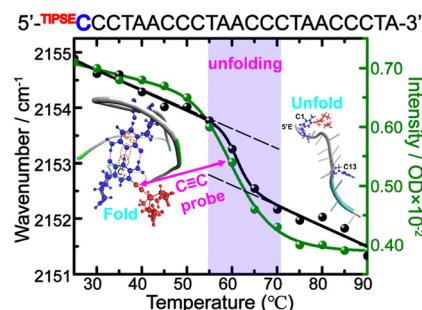
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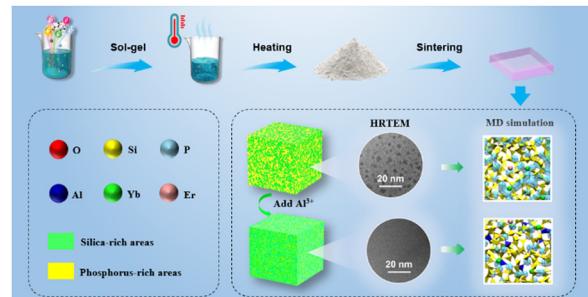
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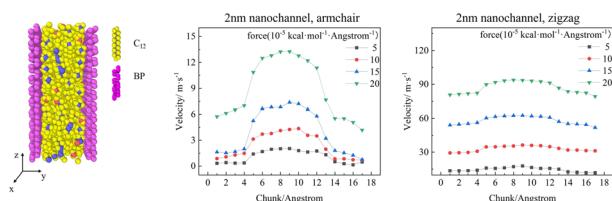
**Te-doped-WSe<sub>2</sub>/W as a stable monolith catalyst for ampere-level current density hydrogen evolution reaction**

Xingchen Zhang, Dongfang Zhang, Xinya Chen, Dingyi Zhou, Jinying Zhang and Zhiyong Wang\*



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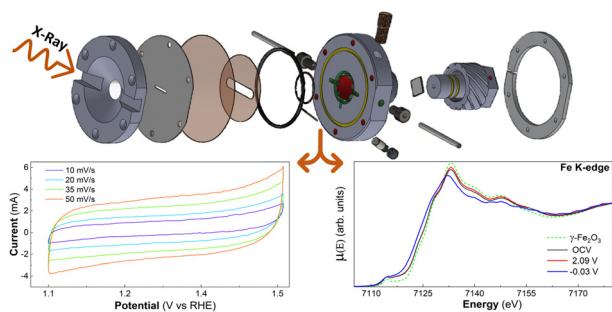
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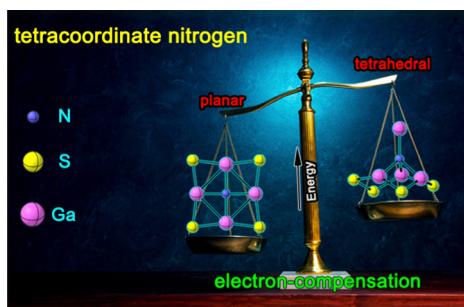
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## A novel electrochemical flow-cell for operando XAS investigations in X-ray opaque supports

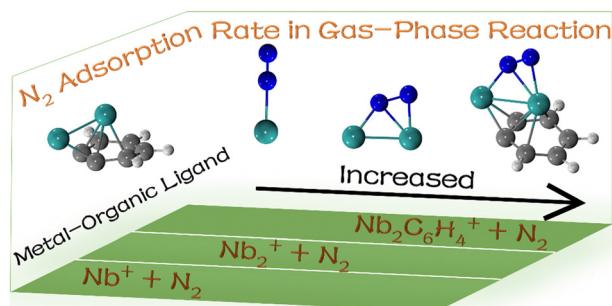
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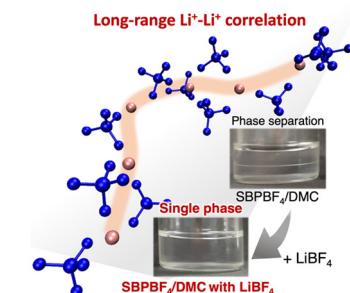


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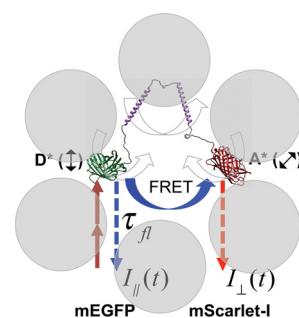
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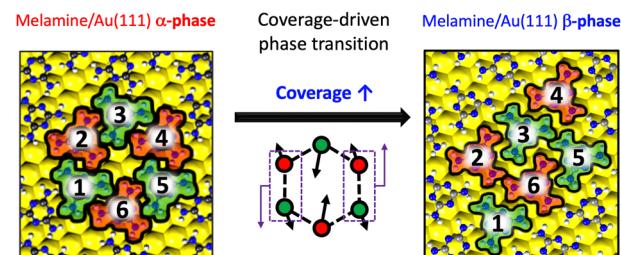
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**Transition mechanism of the coverage-dependent polymorphism of self-assembled melamine nanostructures on Au(111)**

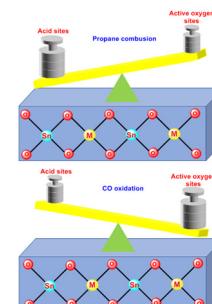
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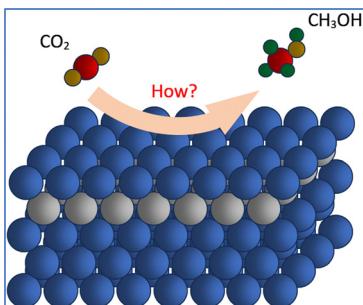
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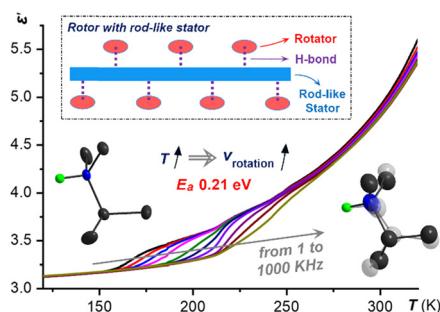
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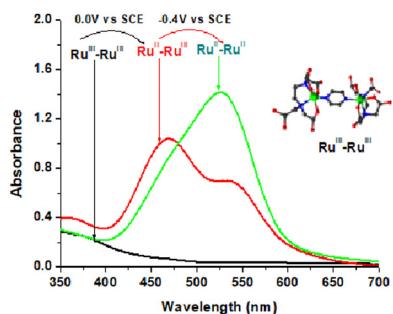
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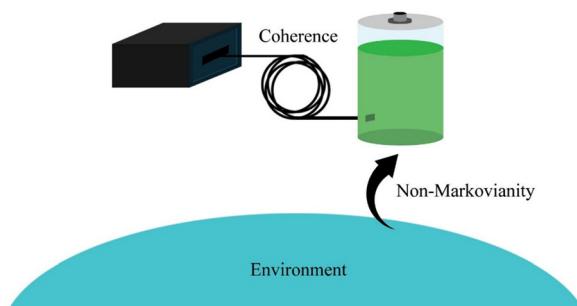
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Amin Mohammadi and Afshin Shafiee\*

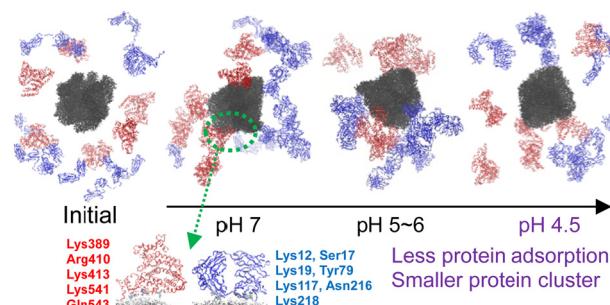


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**Separation of protein corona from nanoparticles under intracellular acidic conditions: effect of protonation on nanoparticle–protein and protein–protein interactions**

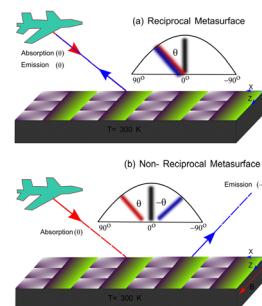
Hwankyu Lee



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**Wide-angle camouflage detectors by manipulating emissivity using a non-reciprocal metasurface array**

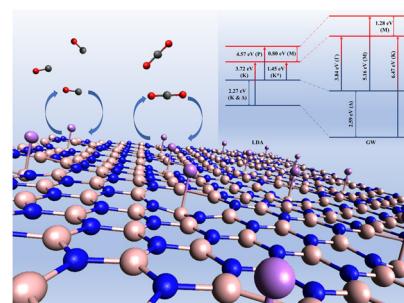
Bowei Zhang, Bin Wang and Sandeep Kumar Chamoli\*



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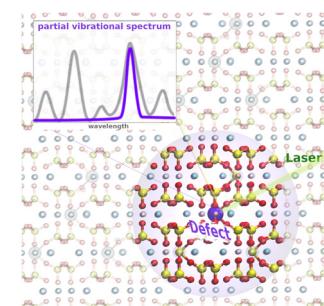
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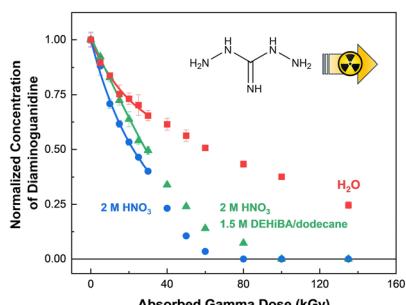
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Luca Bellucci,\* Michele Cassetta, Henrik Skogby and Sabrina Nazzarenii\*



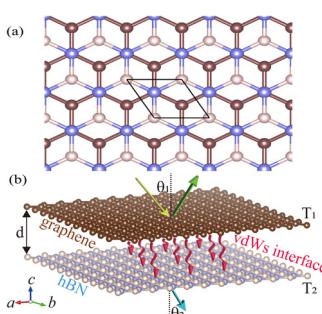
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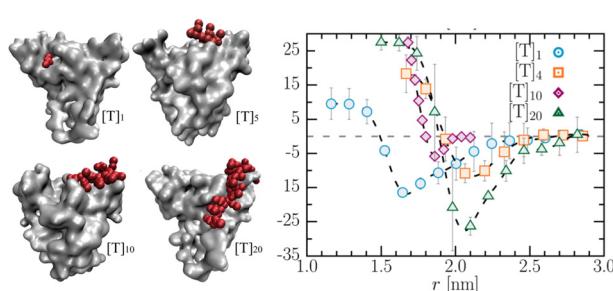
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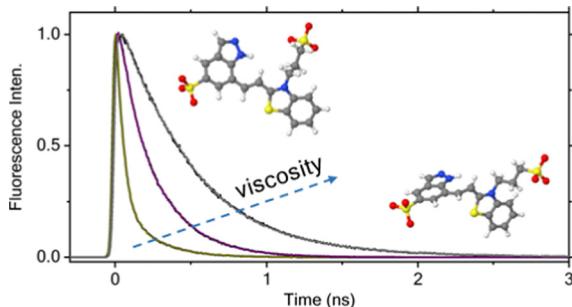
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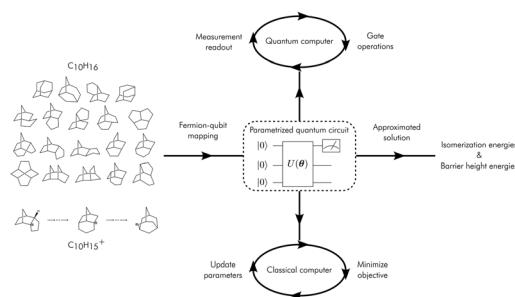


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## Applications of noisy quantum computing and quantum error mitigation to "adamantaneland": a benchmarking study for quantum chemistry

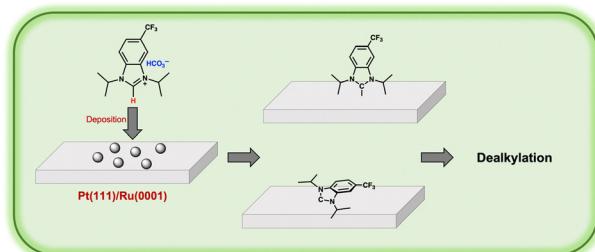
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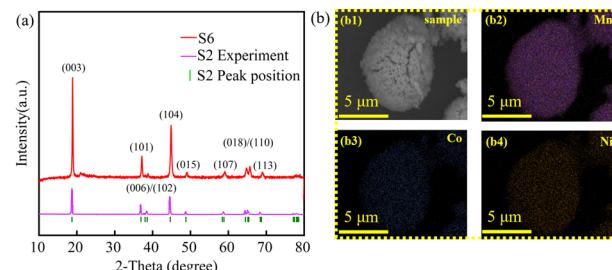
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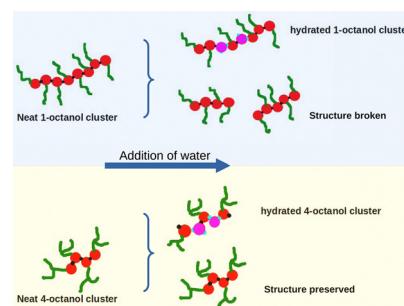
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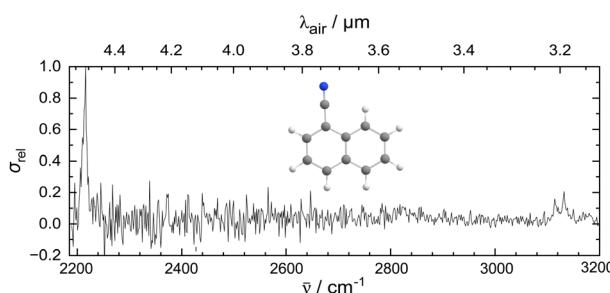
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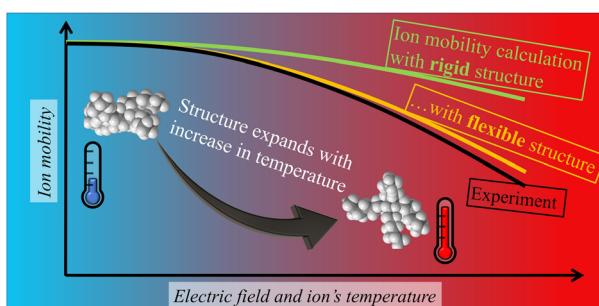
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**Mid-infrared spectroscopy of 1-cyanonaphthalene cation for astrochemical consideration**

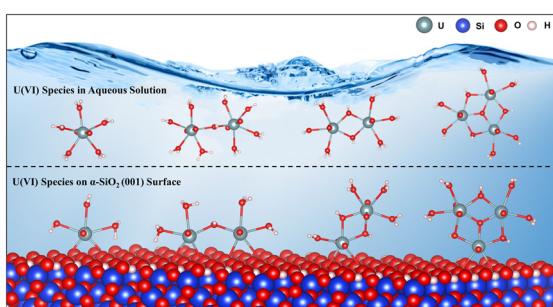
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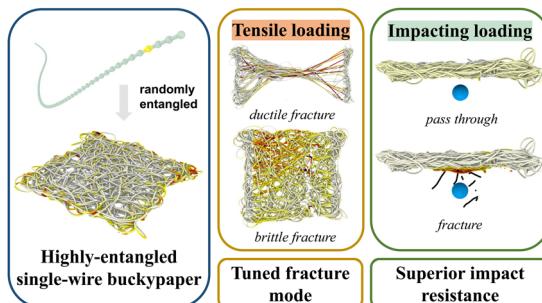
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**A single carbon nanotube-entangled high-performance buckypaper with tunable fracture mode**

Yuna Sang, Chongxiao Cui, Yushun Zhao,\*  
Xiuping Zhang, Zhuochao Zhang, Fei Wang,  
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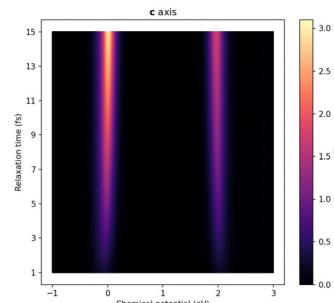


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**Computational prediction of high thermoelectric performance in  $\text{As}_2\text{Se}_3$  by engineering out-of-equilibrium defects**

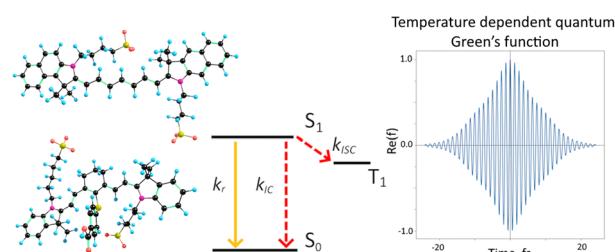
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**Intramolecular rate-constant calculations based on the correlation function using temperature dependent quantum Green's functions**

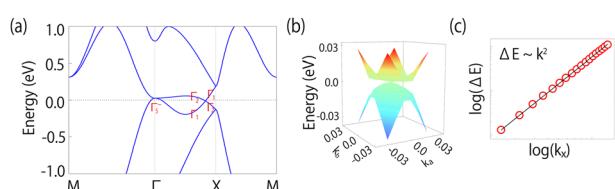
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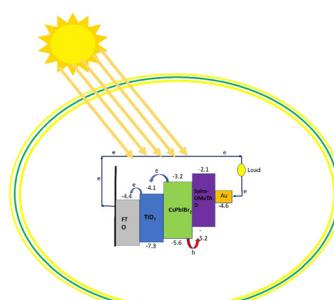
Jin-Yang Li, Xin-Yue Kang, Ying Zhang, Si Li\* and Yugui Yao



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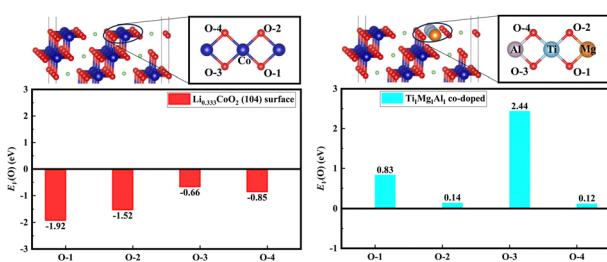
**Impact of Ce doping on the optoelectronic and structural properties of a  $\text{CsPbIBr}_2$  perovskite solar cell**

M. I. Khan,\* Ali Mujtaba, Mahvish Fatima, Riadh Marzouki, Saddam Hussain and Tauseef Anwar



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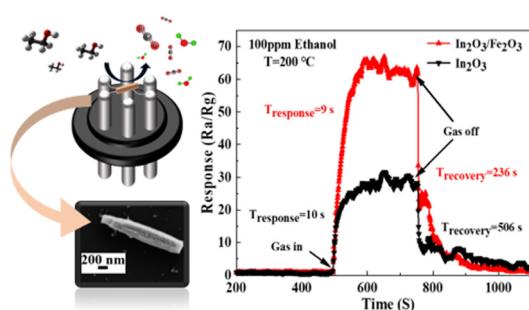
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## A synergistic promotion of surface stability for high-voltage LiCoO<sub>2</sub> by multi-element surface doping: a first-principles study

Hongbin Lin, Xiumei Kang, Guigui Xu,\* Yue Chen, Kehua Zhong, Jian-Min Zhang and Zhigao Huang\*

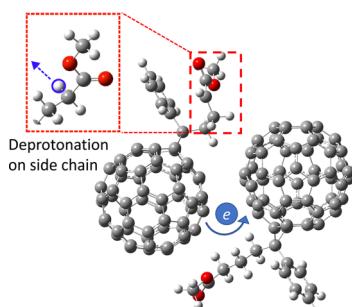
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## In-MIL-68 derived $\text{In}_2\text{O}_3/\text{Fe}_2\text{O}_3$ shuttle-like structures with n-n heterojunctions to improve ethanol sensing performance

Zhenyue Liu, Zhenkai Zhang, Chen Yue, Yang Mu, Zhiguo Yang, Davoud Dastan, Xi-Tao Yin\* and Xiaoguang Ma\*

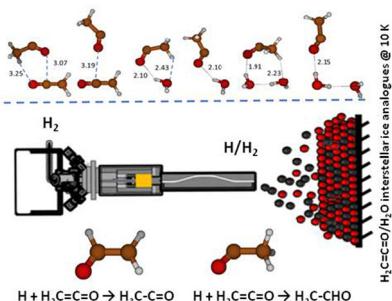
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## The significant role of water in reactions occurring on the surface of interstellar ice grains: Hydrogenation of pure ketene $\text{H}_2\text{C}=\text{C=O}$ ice versus hydrogenation of mixed $\text{H}_2\text{C}=\text{C=O}/\text{H}_2\text{O}$ ice at 10 K

Mohamad Ibrahim, Jean-Claude Guillemin, Patrick Chaquin, Alexis Markovits and Lahouari Krim\*

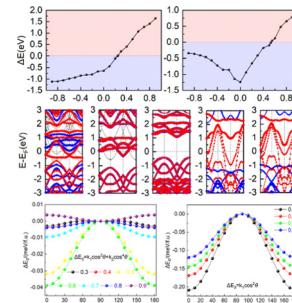


## RESEARCH PAPERS

4208

**Carrier doping modulates the magnetoelectronic and magnetic anisotropic properties of two-dimensional  $\text{MSi}_2\text{N}_4$  ( $\text{M} = \text{Cr}, \text{Mn}, \text{Fe}$ , and  $\text{Co}$ ) monolayers**

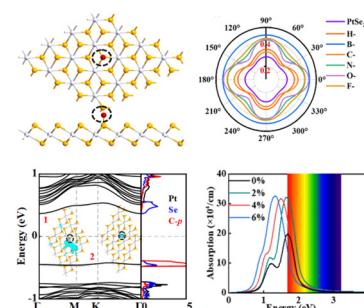
Ziyuan An, Linhui Lv, Ya Su,\* Yanyan Jiang and Zhaoyong Guan\*



4218

**Single-layer  $\text{PtSe}_2$  adsorbed with non-metallic atoms: geometrical, mechanical, electronic and optical properties and strain effects**

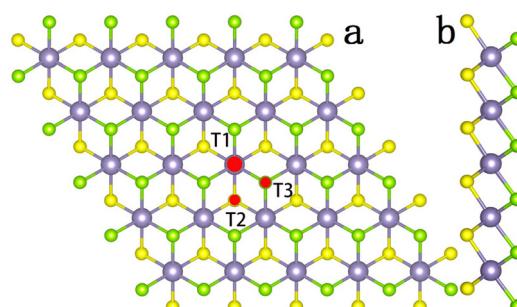
Xinyan Li, Zhanhai Li,\* Jianing Han, Shengguo Cao and Zhenhua Zhang\*



4231

**First-principles study of magnetic properties and electronic structure of 3d transition-metal atom-adsorbed  $\text{SnSSe}$  monolayers**

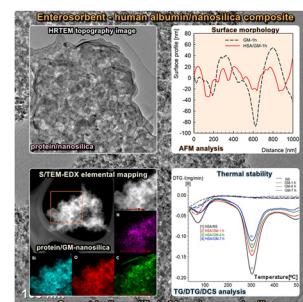
Bin Xu,\* Cheng Qian, Zheng Wang, Jing Zhang, Shanshan Ma, Yusheng Wang and Lin Yi



4240

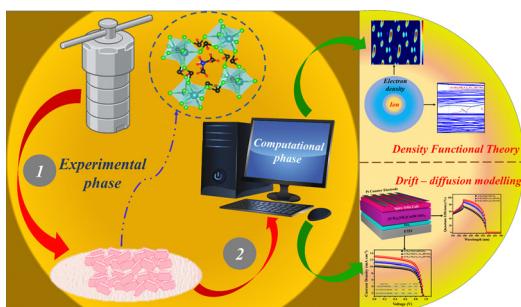
**Nanostructure and thermal characteristics of silica/human serum albumin systems based on a modified nanosilica entero-vulnerosorbent**

Agnieszka Chrzanowska,\* Liudmyla V. Nosach and Anna Derylo-Marczewska



## RESEARCH PAPERS

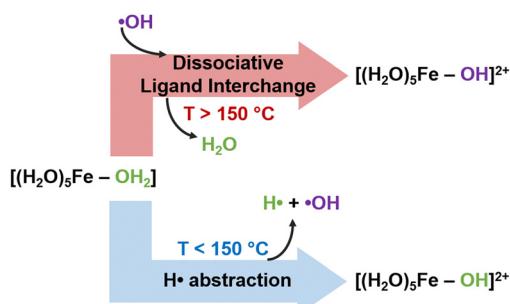
4262



## Experimental and computational DFT, drift-diffusion studies of cobalt-based hybrid perovskite crystals as absorbers in perovskite solar cells

Sathish Marimuthu, Saravanan Pandiaraj, Muthumareeswaran Muthuramamoorthy, Khalid E. Alzahrani, Abdullah N. Alodhayb, Sudhagar Pitchaimuthu and Andrews Nirmala Grace\*

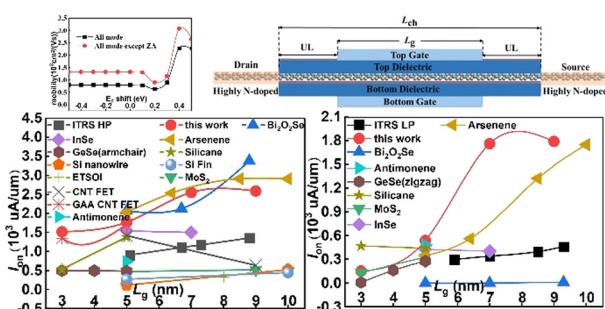
4278



## Kinetics of the reaction of ferrous ions with hydroxyl radicals in the temperature range 25–300 °C

Logan Barr,\* Jacy K. Conrad, Christine McGregor, Randy Perron, Pamela A. Yakabuskie and Craig R. Stuart

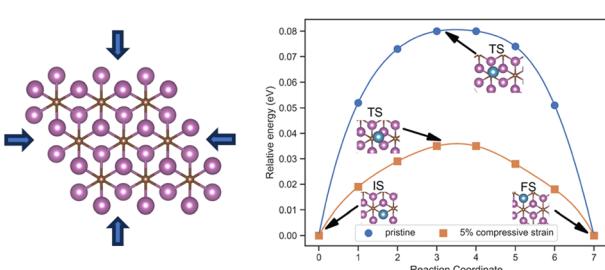
4284



## Comprehensive understanding of electron mobility and superior performance in sub-10 nm DG ML tetrahex-GeC<sub>2</sub> n-type MOSFETs

Yuehua Xu,\* Daqing Li, He Sun, Haowen Xu and Pengfei Li

4298



## Biaxial compressive strain enhances calcium binding and mobility on two-dimensional Sc<sub>2</sub>C: a density functional theory investigation

Darwin B. Putungan,\* Christian Loer T. Llemit, Alexandra B. Santos-Putungan, Roland V. Sarmago and Ralph Gebauer

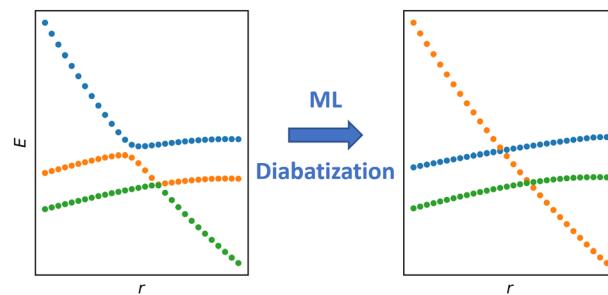


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4306

**Fast and accurate excited states predictions: machine learning and diabatization**

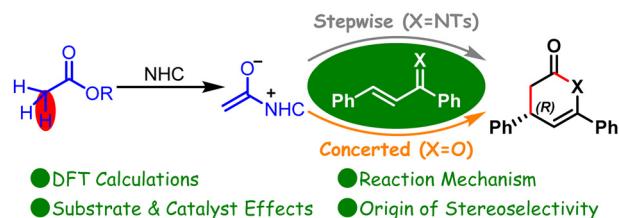
Štěpán Sršen,\* O. Anatole von Lilienfeld and Petr Slavíček\*



4320

**Elucidating the mechanism and origin of stereoselectivity in the activation/ transformation of an acetic ester catalyzed by an N-heterocyclic carbene**

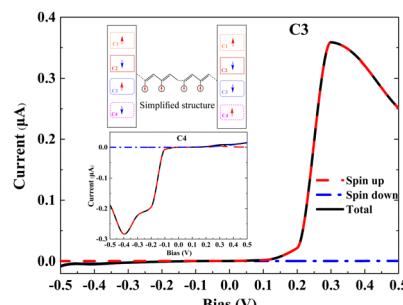
Pingxin Liang, Haoran Yang\* and Yang Wang\*



4329

**Molecular rectification induced by magnetization alignment in organic-ferromagnetic devices**

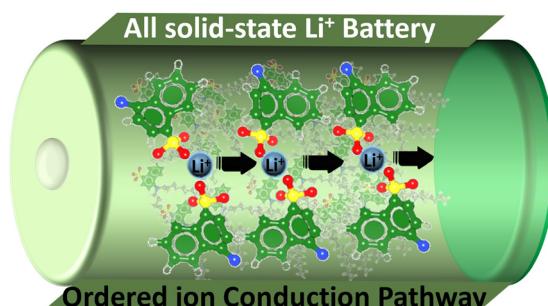
H. Ma, H. X. Li, H. Q. Zhang, Y. Wang, J. T. Li, C. Wang, J. F. Ren and G. C. Hu\*



4338

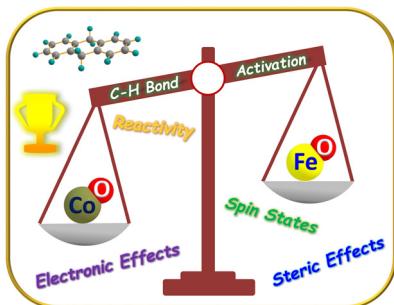
**Modelling structure and ionic diffusion in a class of ionic liquid crystal-based solid electrolytes**

Md Sharif Khan,\* Ambroise Van Roeghem, Stefano Mossa, Flavien Ivol, Laurent Bernard, Lionel Picard and Natalio Mingo\*



## RESEARCH PAPERS

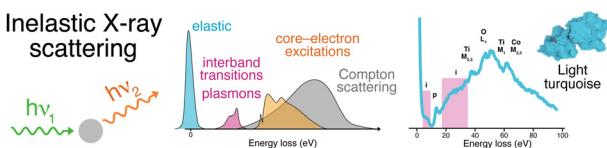
4349



## C–H bond activation by high-valent iron/cobalt–oxo complexes: a quantum chemical modeling approach

Manjeet Kumar, Manoj Kumar Gupta, Mursaleem Ansari\* and Azaj Ansari\*

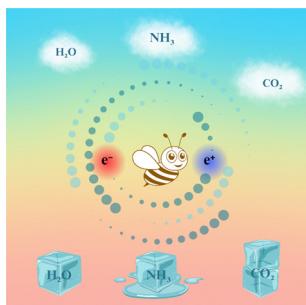
4363



## Non-resonant inelastic X-ray scattering for discrimination of pigments

Lauren Dalecky, Francesco Sottile, Linda Hung, Laure Cazals, Agnès Desolneux, Aurélia Chevalier, Jean-Pascal Rueff and Loïc Bertrand\*

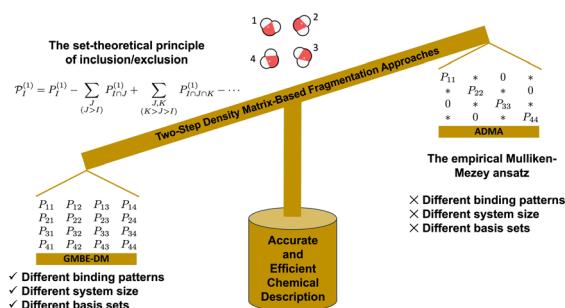
4372



## Electron- and positron-driven molecular processes for H₂O, CO₂, and NH₃ in their gas and ice phases

Neha Barad and Chetan Limbachiya\*

4386



## Analysis of two overlapping fragmentation approaches in density matrix construction: GMBE-DM vs. ADMA

Francisco Ballesteros and Ka Un Lao\*

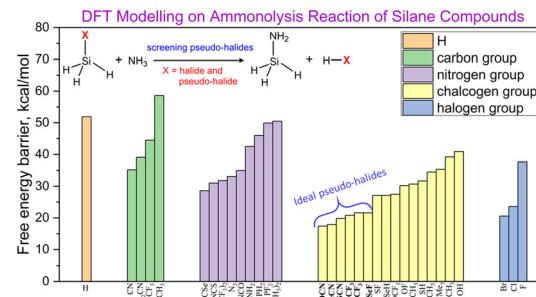


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4395

## Enhancing silicon-nitride formation through ammonolysis of silanes with pseudo-halide substituents

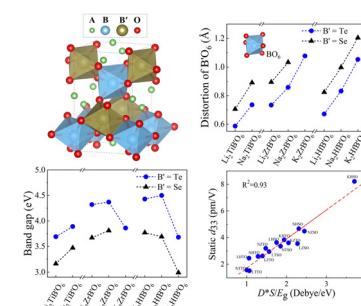
Anil Kumar Tummanapelli, Yingqian Chen and Ming Wah Wong\*



4403

## Investigation of nonlinear optical properties in $\alpha$ -A<sub>2</sub>BB'O<sub>6</sub> (A = Li, Na, K; B = Ti, Zr, Hf; B' = Se, Te) by first-principles calculations

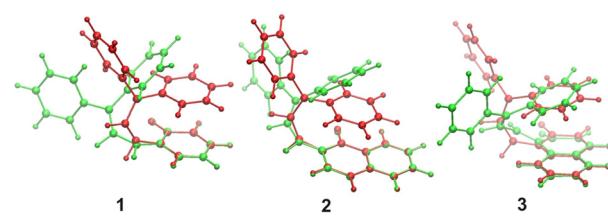
Gaojing Fang, Xiaojun Teng, Luo Yan, Yu Wu, Kui Xue, Xiaofeng Zhang, Yi-min Ding,\* Liujiang Zhou\* and Qiye Wen\*



4412

## Intramolecular excimers of open forms of 2H-benzopyran, 2H- and 3H-naphthopyrans in solution: TD-DFT/DFT analysis

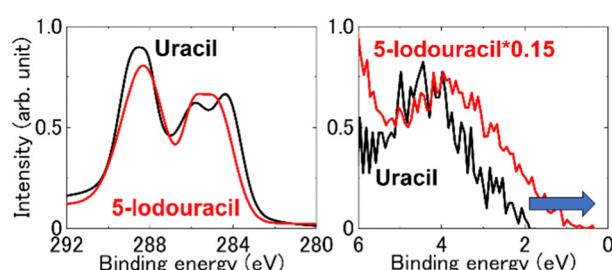
Daiana S. Tabirja and Victor V. Kostjukov\*



4422

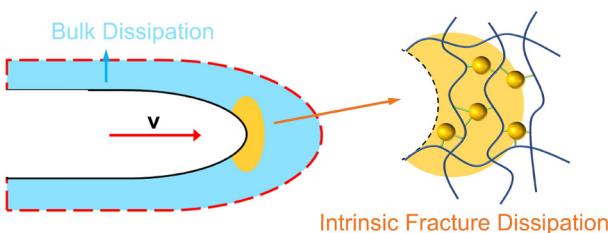
## Comparison of core and valence band electronic structures of bulk uracil and 5-halouracils

Yudai Izumi,\* Maki Ohara, Yuji Baba and Akinari Yokoya



## RESEARCH PAPERS

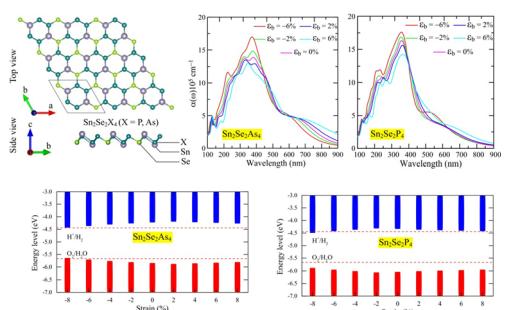
4429



### Insight into the fracture energy dissipation mechanism in elastomer composites via sacrificial bonds and fillers

Dongyi He, Xiaxia Cheng, Chunyu Wong, Xiangliang Zeng, Linling Li, Chao Teng,\* Guoping Du, Chenxu Zhang,\* Linlin Ren, Xiaoliang Zeng\* and Rong Sun

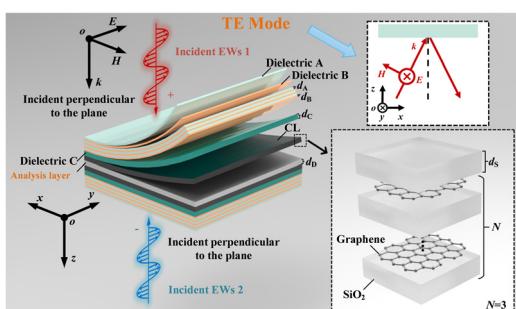
4437



### First principles study of strain effects on prospective 2D photocatalysts $\text{Sn}_2\text{Se}_2\text{X}_4$ ( $\text{X} = \text{P}, \text{As}$ ) with ultra-high charge carrier mobility

Pham D. Trung\* and Hien D. Tong\*

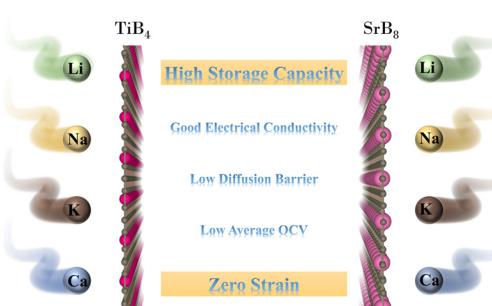
4447



### A multiple cancer cell optical biosensing metastructure realized by CPA

Jia-Hao Zou, Jun-Yang Sui, You-Ran Wu and Hai-Feng Zhang\*

4455



### TiB<sub>4</sub> and SrB<sub>8</sub> monolayers: high capacity and zero strain-like anode materials for Li/Na/K/Ca ion batteries

Yunxin Wang, Sisi Liang, Juncheng Tian, Huixian Duan, Ying Lv, Lijia Wan, Chunlai Huang, Musheng Wu, Chuying Ouyang and Junping Hu\*

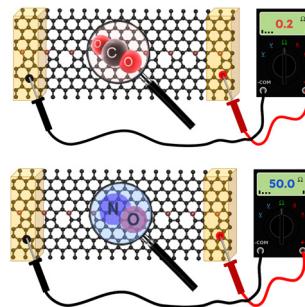


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4466

## Boron-doped graphene topological defects: unveiling high sensitivity to NO molecule for gas sensing applications

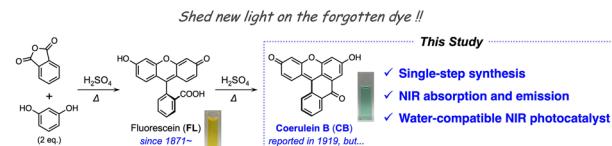
B. Keshav Rao, Tadeu Luiz Gomes Cabral, Debora Carvalho de Melo Rodrigues, Fábio A. L. de Souza, Wanderlã L. Scopel, Rodrigo G. Amorim\* and Ravindra Pandey



4474

## Coerulein B: a water-soluble and water-compatible near-infrared photoredox catalyst

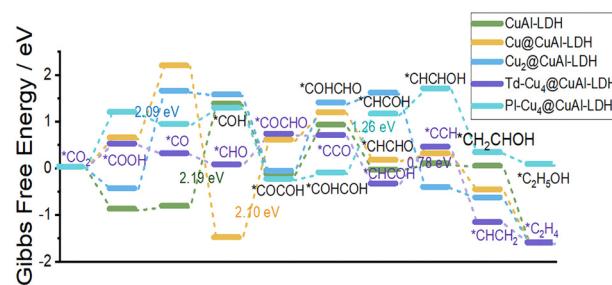
Masaru Tanioka,\* Masaya Oyama, Kaito Nakajima, Minori Mori, Mei Harada, Yuji Matsuya\* and Shinichiro Kamino\*



4480

## Theoretical study on electrocatalytic carbon dioxide reduction over copper with copper-based layered double hydroxides

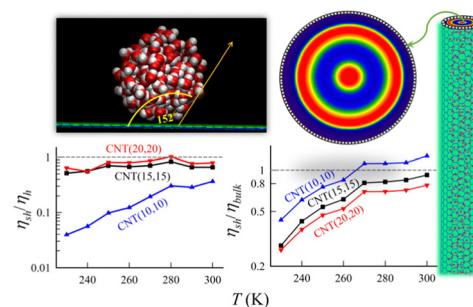
Xin-Yu Xu, Jing-Yi Guo, Wei Zhang, Yao Jie, Hui-Ting Song, Hao Lu, Yi-Fan Zhang, Jia Zhao, Chen-Xu Hu and Hong Yan\*



4492

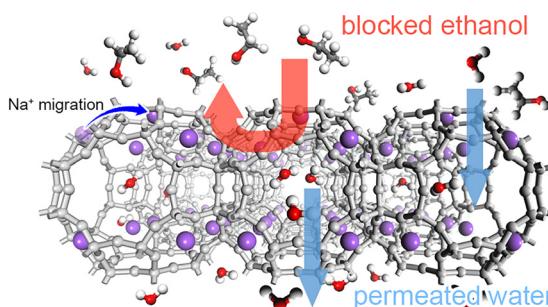
## Enhanced fluidity of water in superhydrophobic nanotubes: estimating viscosity using jump-corrected confined Stokes–Einstein approach

Golam Rosul Khan and Snehasis Daschakraborty\*

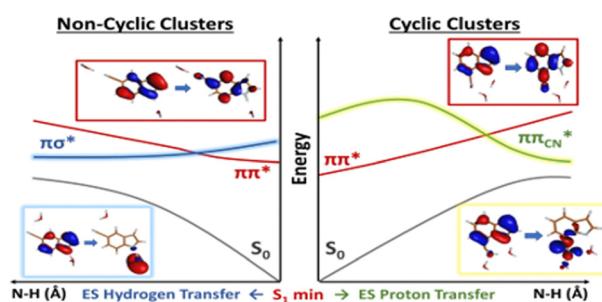


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4505

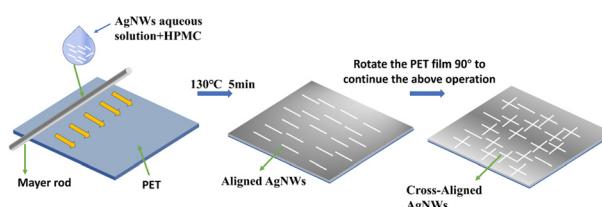
**Computational understanding of Na-LTA for ethanol–water separation**Zicheng Wan, Chen Zhou, Yichao Lin,\*  
Liang Chen and Ziqi Tian\*

4511

**Excited state hydrogen or proton transfer pathways in microsolvated *n*-cyanoindole fluorescent probes**

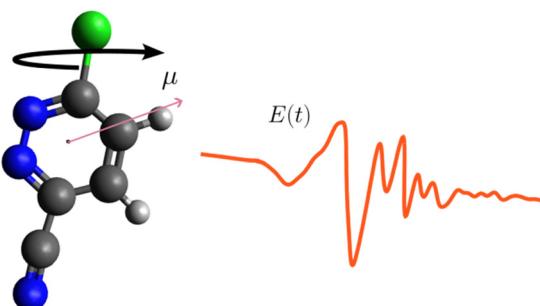
Salsabil Abou-Hatab and Spiridoula Matsika\*

4524

**Silver nanowires/cellulose flexible transparent conductive films for electromagnetic interference shielding and electrothermal conversion**

Zhijiang Guo, Xiaoli Li, Ning Li, Xuanji Liu, Longhui Hao, Yuxuan Wang, Wei Deng, Haoxuan Bai, Jianguo Liang\* and Zhanchun Chen\*

4533

**Full control of the orientation of non-symmetric molecules using weak and moderate electric fields**

Rosario González-Férez and Juan J. Omiste\*

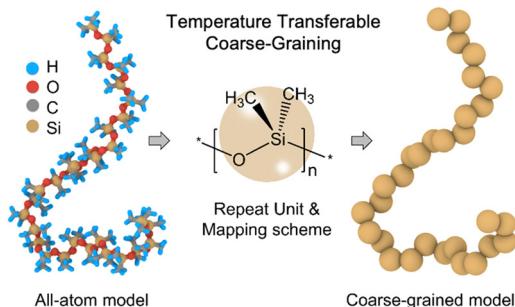


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4541

**Energy renormalization for temperature transferable coarse-graining of silicone polymer**

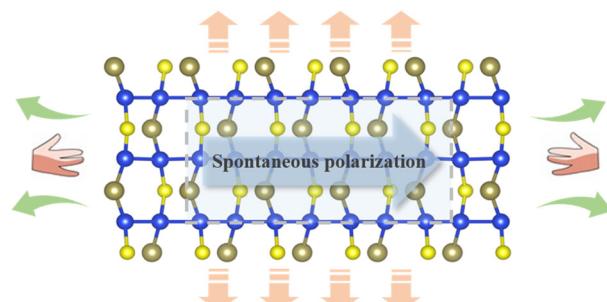
Dawei Zhang, Yang Wang, Maryam Safaripour, Daniel A. Bellido-Aguilar, Kurt R. Van Donselaar, Dean C. Webster, Andrew B. Croll and Wenjie Xia\*



4555

**First-principles prediction of ferroelectric Janus  $\text{Si}_2\text{XY}$  ( $\text{X}/\text{Y} = \text{S}/\text{Se}/\text{Te}$ ,  $\text{X} \neq \text{Y}$ ) monolayers with negative Poisson's ratios**

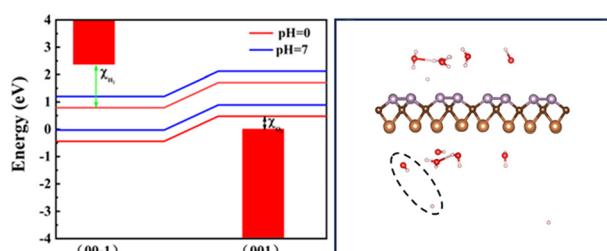
Yunlai Zhu, Zihan Qu, Jishun Zhang, Xiaoteng Wang, Shuo Jiang, Zuyu Xu, Fei Yang, Zuheng Wu\* and Yuehua Dai\*



4564

**Janus monolayer PXC ( $\text{X} = \text{As}/\text{Sb}$ ) for photocatalytic water splitting with a negative Poisson's ratio**

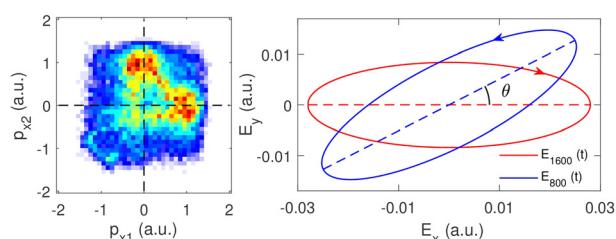
Yunlai Zhu, Shuo Jiang, Jishun Zhang, Zihan Qu, Zuheng Wu, Zuyu Xu, Wei Hu, Yuehua Dai and Fei Yang\*



4572

**The Coulomb effect in nonsequential double ionization by counter-rotating two-color elliptical polarization fields**

Zichao Liu, Cheng Huang,\* Tongtong He, Jianying Liao, Yingbin Li and Benhai Yu



## RESEARCH PAPERS

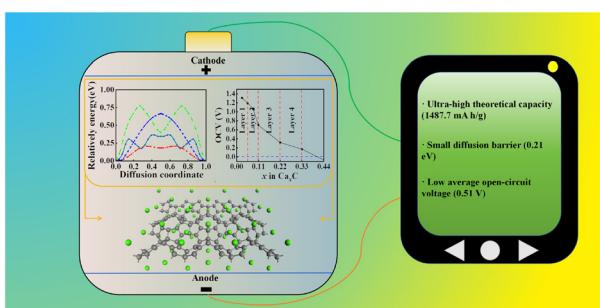
4579



### A first-principles study of electro-catalytic reduction of $\text{CO}_2$ on transition metal-doped stanene

Sudatta Giri, Satyesh K. Yadav and Debolina Misra\*

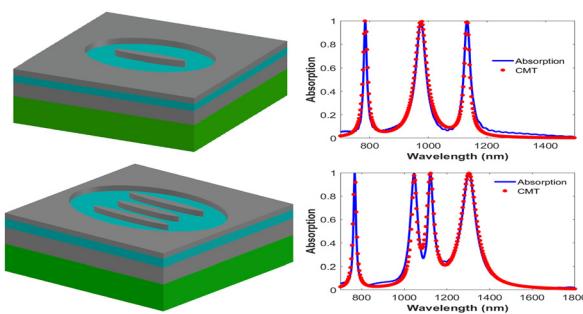
4589



### Two-dimensional graphene+ as an anode material for calcium-ion batteries with ultra-high capacity: a first-principles study

Tao Yang, Tian-Ci Ma, Xiao-Juan Ye,\* Xiao-Hong Zheng, Ran Jia, Xiao-Hong Yan and Chun-Sheng Liu\*

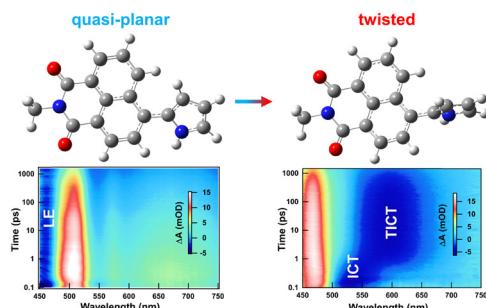
4597



### Multi-band perfect absorber based on an elliptical cavity coupled with an elliptical metal nanorod

Yizhao Pan, Yuchang Li, Fang Chen,\* Shubo Cheng, Wenxing Yang, Boyun Wang and Zao Yi

4607



### Deciphering the photophysical properties of naphthalimide derivatives using ultrafast spectroscopy

Wei Zhang, Yalei Ma, Hongwei Song, Rong Miao,\* Jie Kong\* and Meng Zhou\*

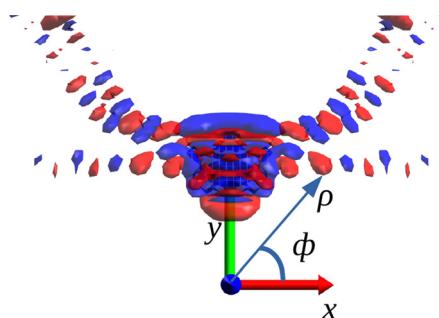


## RESEARCH PAPERS

4614

**Lifetimes and decay mechanisms of isotopically substituted ozone above the dissociation threshold: matching quantum and classical dynamics**

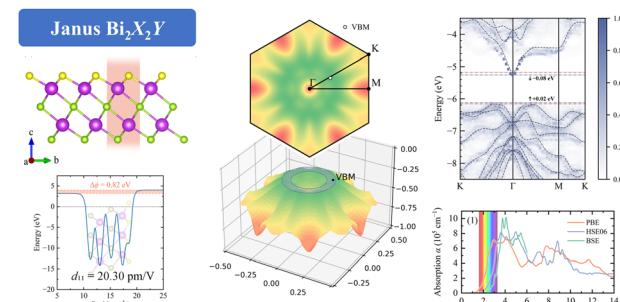
Viatcheslav Kokoouline,\* Alexander Alijah and Vladimir Tyuterev



4629

**The coexistence of high piezoelectricity and superior optical absorption in Janus  $\text{Bi}_2\text{X}_2\text{Y}$  ( $\text{X} = \text{Te}, \text{Se}; \text{Y} = \text{Te}, \text{Se}, \text{S}$ ) monolayers**

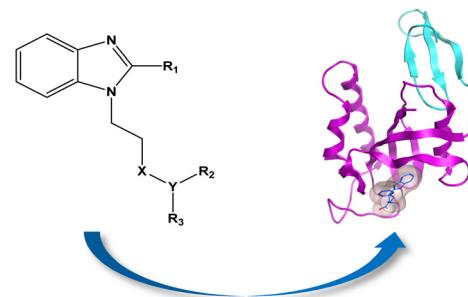
Shu-Hao Cao, Tian Zhang,\* Hua-Yun Geng and Xiang-Rong Chen\*



4643

**Molecular docking, 3D-QASR and molecular dynamics simulations of benzimidazole Pin1 inhibitors**

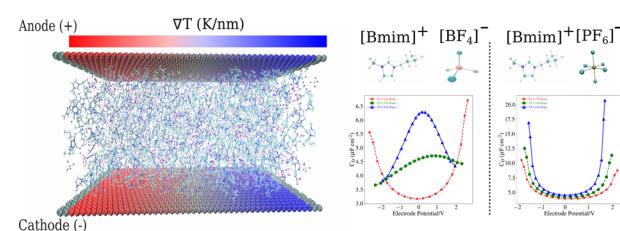
Min Liu, Bingli Wang, Huan Liu, Haolun Xia and Lina Ding\*



4657

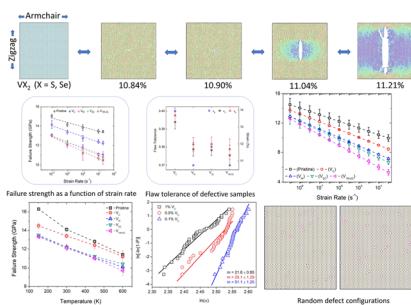
**Temperature-dependent differential capacitance of an ionic liquid-graphene-based supercapacitor**

Kiran Prakash and Sarith P. Sathian\*



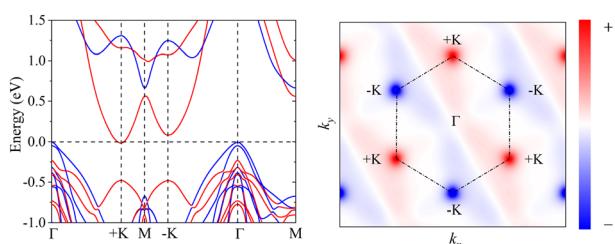
## RESEARCH PAPERS

4668

**Vacancy-mediated inelasticity in two-dimensional vanadium-based dichalcogenides**

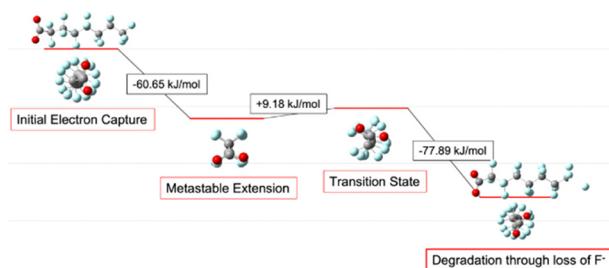
Akash Baski, Zimmi Singh and Sankha Mukherjee\*

4683

**Novel valley character and tunable quasi-half-valley metal state in Janus monolayer  $VSiGeP_4$** 

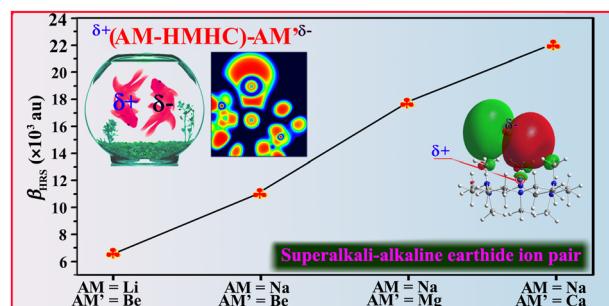
Kang Jia, Xiao-Jing Dong, Sheng-Shi Li, Wei-Xiao Ji and Chang-Wen Zhang\*

4692

**The role of helicity in PFAS resistance to degradation: DFT simulation of electron capture and defluorination**

Matt McTaggart and Cécile Malardier-Jugroot\*

4702

**Superalkali-alkaline earthide ion pairs of  $\delta^+$ -(AM-HMHC)-AM' $\delta^-$  (AM = Li, Na and K; AM' = Be, Mg and Ca) possessing large NLO responses and excellent electronic stabilities and alkalide characteristics: a DFT study**

Jiangen Huang, Yin-Feng Wang,\* Kai Yang, Wen Zhang, Zhi-Jun Wang, Xuexia Liu\* and Zhi-Ru Li\*

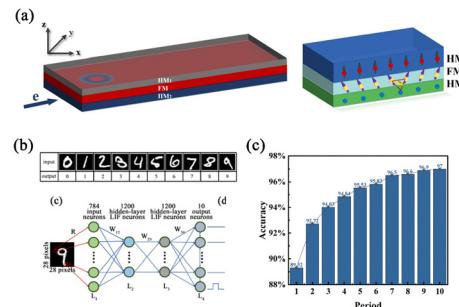


## RESEARCH PAPERS

4716

**Optimizing skyrmionium movement and stability via stray magnetic fields in trilayer nanowire constructs**

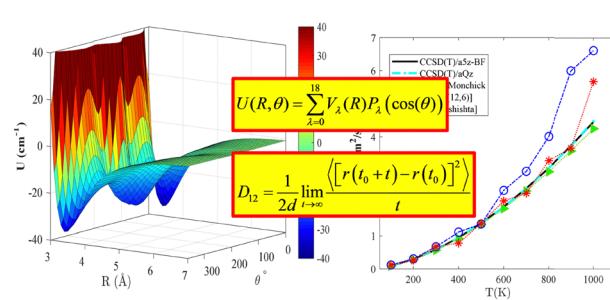
Bin Gong, Luowen Wang, Sunan Wang, Ziyang Yu,\* Lun Xiong, Rui Xiong, Qingbo Liu\* and Yue Zhang



4724

**PES and transport properties of the He··HBr complex from kinetic theory and molecular dynamics simulations**

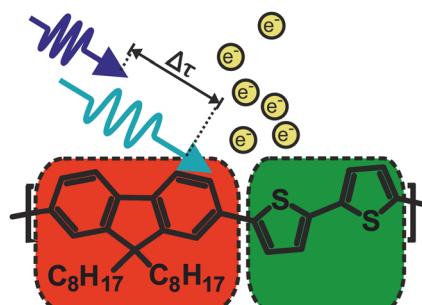
Fatemeh Aghababaei and Ebrahim Nemati-Kande\*



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**Ultrafast electron dynamics in excited states of conjugated thiophene-fluorene organic polymer (pF8T2) thin films**

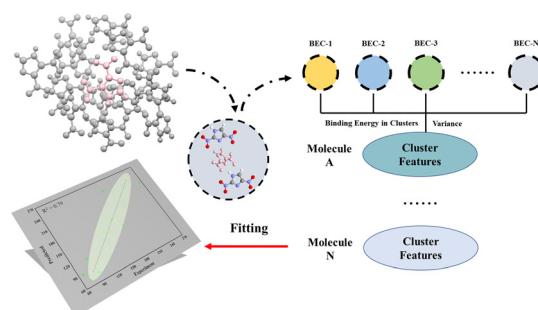
T. Reiker,\* Z. Liu, C. Winter, M. V. Cappellari, D. Gonzalez Abradello, C. A. Strassert, D. Zhang and H. Zacharias



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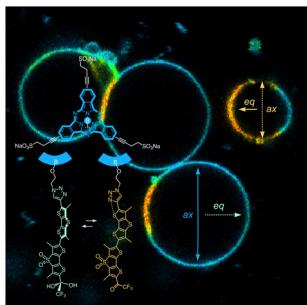
**Insight into melting point differences of dinitroimidazoles and dinitropyrazoles from the perspective of intermolecular interactions**

Junnan Wu, Siwei Song, Xiujuan Qi,\* Haijun Yang\* and Yi Wang\*



## RESEARCH PAPERS

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**Subphthalocyanine-flipper dyads for selective membrane staining**

José García-Calvo,\* Xiao-Xiao Chen, Naomi Sakai, Stefan Matile and Tomás Torres\*

## CORRECTION

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**Correction: Optical bands of dodecanuclear compounds  $H_4PvMo_{11}O_{40}\cdot yH_2O$  with Keggin structure. Semiclassical vibronic model**

S. Klokishner,\* J. Melsheimer, F. C. Jentoft and R. Schlögl

