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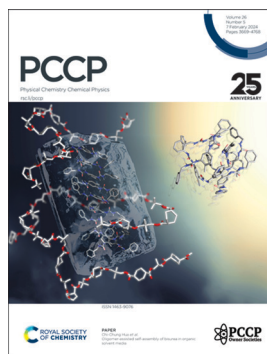
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See Björn Lindman, Krister Holmberg *et al.*, pp. 3699–3710. Image reproduced by permission of Ming Lu from *Phys. Chem. Chem. Phys.*, 2024, 26, 3699.



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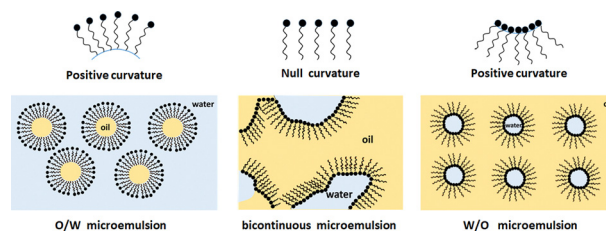
See Chi-Chung Hua *et al.*, pp. 3810–3814. Image reproduced by permission of Ching-Hung Wu and Chi-Chung Hua from *Phys. Chem. Chem. Phys.*, 2024, 26, 3810.

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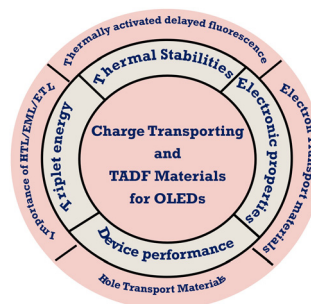
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Krishan Kumar



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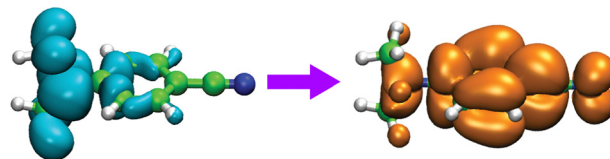


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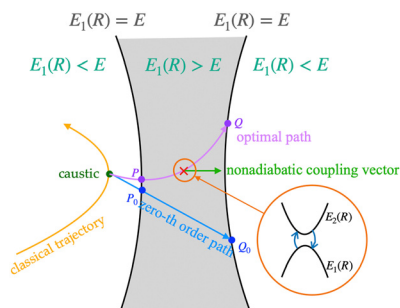


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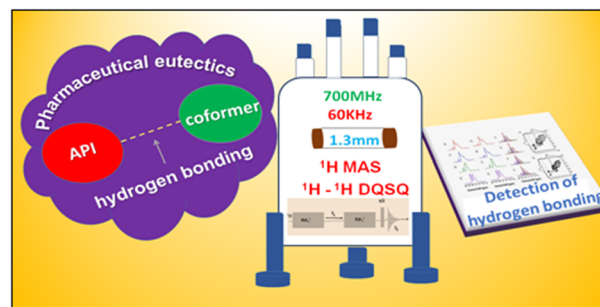
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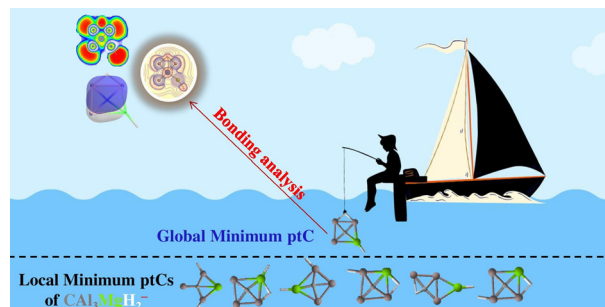
Chaithanya Hareendran, Parth S. Shaligram, Rajesh Gonnade and T. G. Ajithkumar\*



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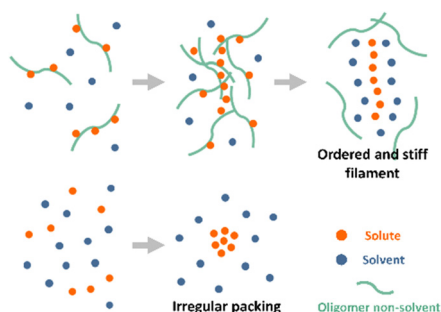
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Abdul Hamid Malhan and Krishnan Thirumoorthy\*



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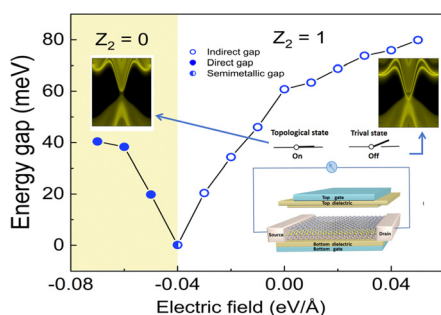
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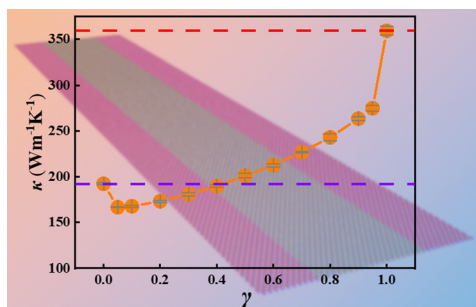
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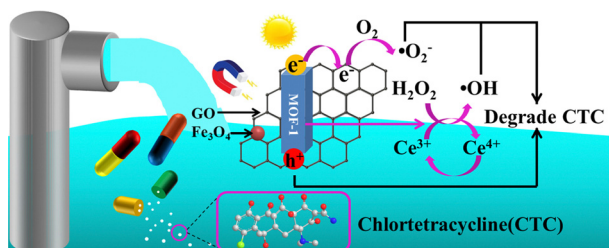
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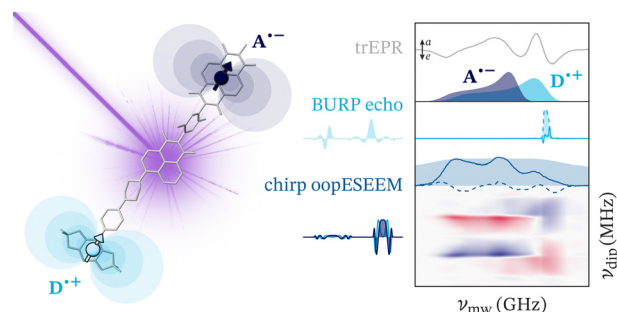


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**Control of excitation selectivity in pulse EPR on spin-correlated radical pairs with shaped pulses**

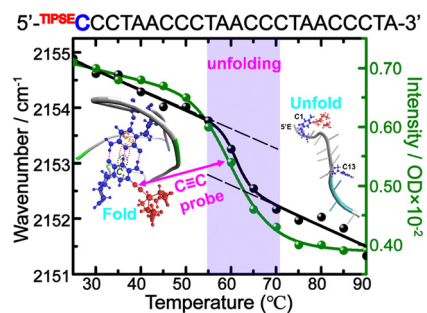
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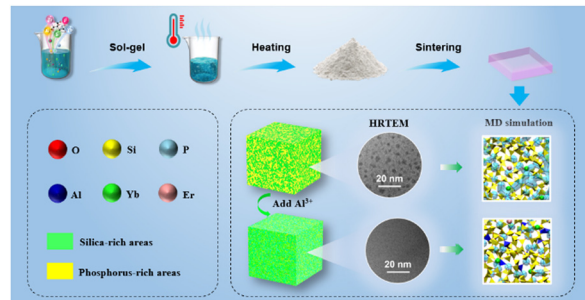
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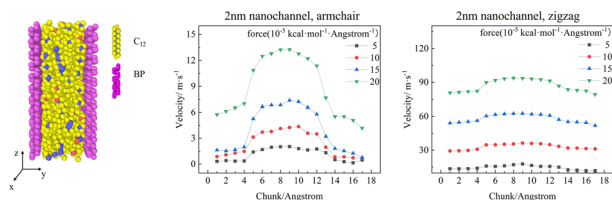
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**Te-doped-WSe<sub>2</sub>/W as a stable monolith catalyst for ampere-level current density hydrogen evolution reaction**

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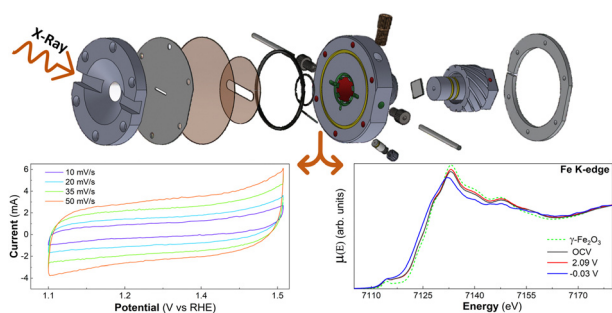
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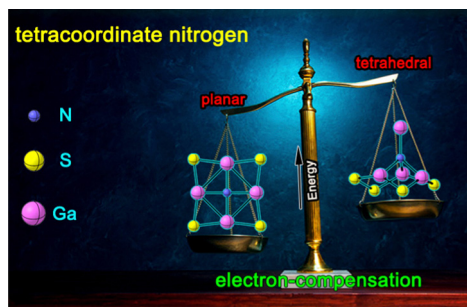
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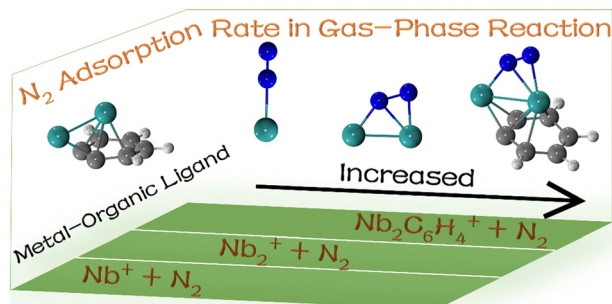
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Feng-Xiang Zhang, Yi-Heng Zhang, Ming Wang and  
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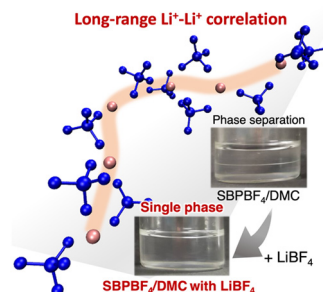


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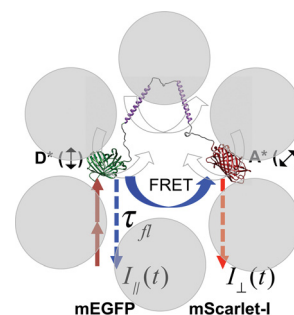
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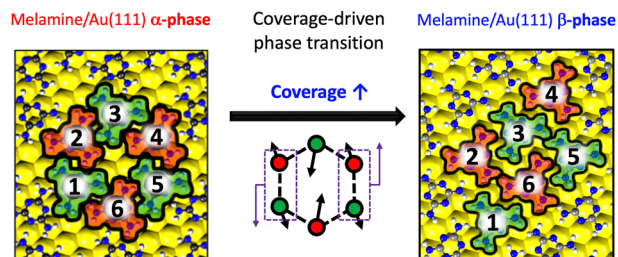
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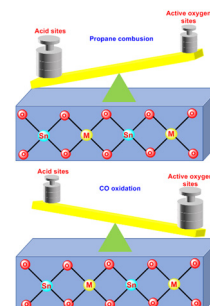
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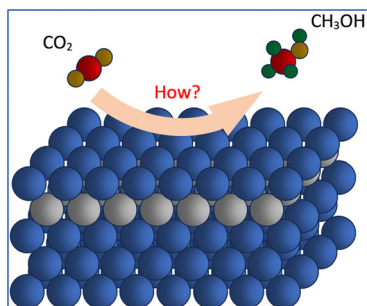
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Haiming Yan, Teng Liu, Yu Lv, Xianglan Xu, Junwei Xu, Xiuzhong Fang and Xiang Wang\*



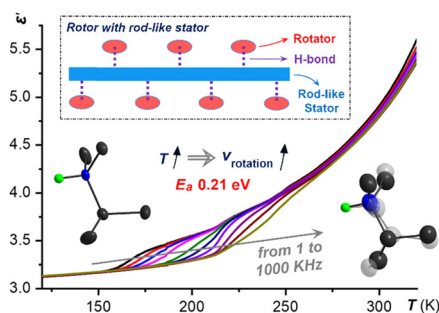
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### Carbon dioxide conversion to methanol on a PdCo bimetallic catalyst

Huynh Tat Thanh, Ong Kim Le, Viorel Chihaiia and Do Ngoc Son\*

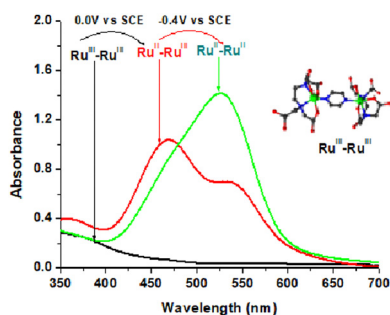
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### Molecular rotators anchored on a rod-like anionic coordination polymer adhered by charge-assisted hydrogen bonds

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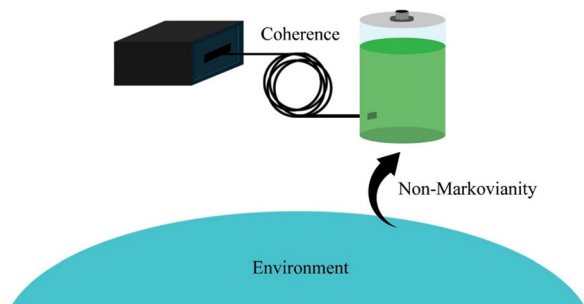
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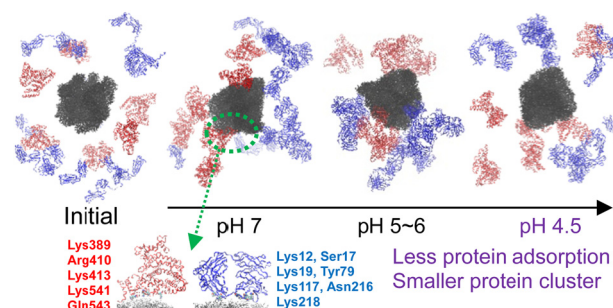
Amin Mohammadi and Afshin Shafiee\*



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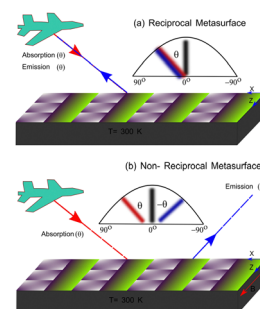
Hwankyu Lee



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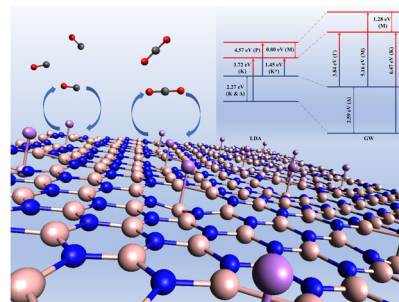
Bowe Zhang, Bin Wang and Sandeep Kumar Chamoli\*



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### Electronic, optical, and adsorption properties of Li-doped hexagonal boron nitride: a GW approach

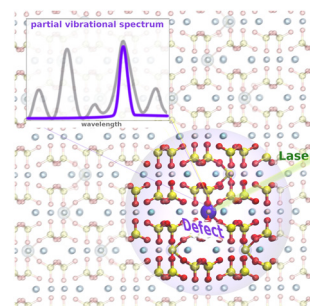
Dhanjit Talukdar,\* Shilpi Stuti Bora and Gazi A. Ahmed



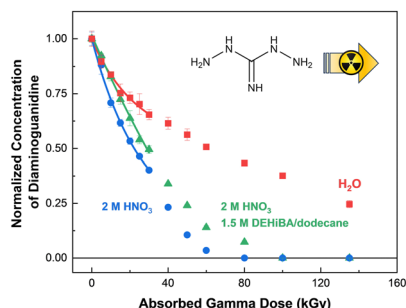
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### Pure and Sc-doped diopside ( $\text{CaMgSi}_2\text{O}_6$ ) vibrational spectra: modelling and experiments

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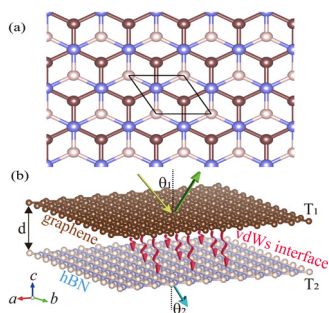
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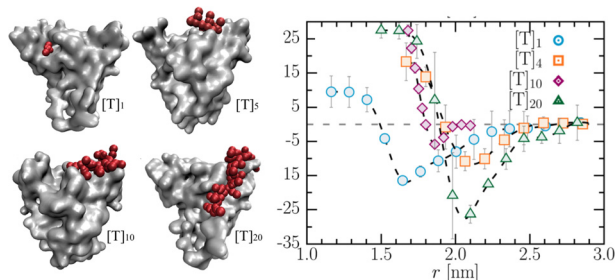
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### Interface thermal conductivities induced by van der Waals interactions

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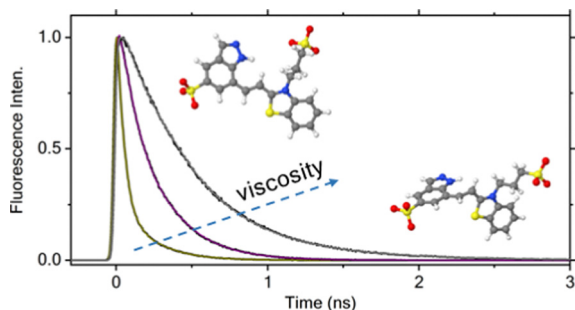
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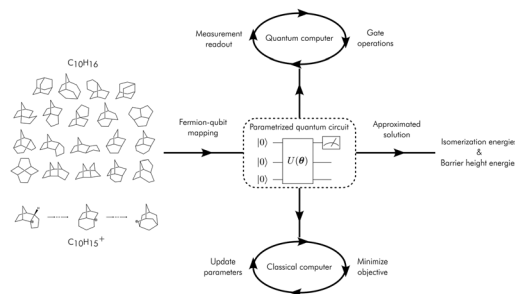


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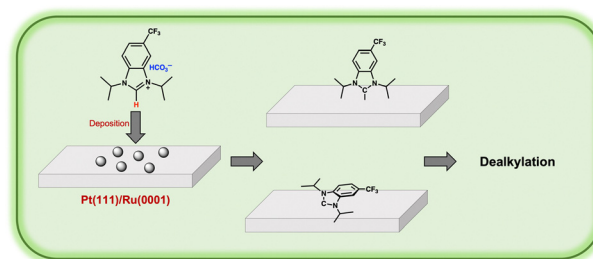
Viki Kumar Prasad, Freeman Cheng, Ulrich Fekl\* and Hans-Arno Jacobsen\*



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### N-heterocyclic carbene adsorption states on Pt(111) and Ru(0001)

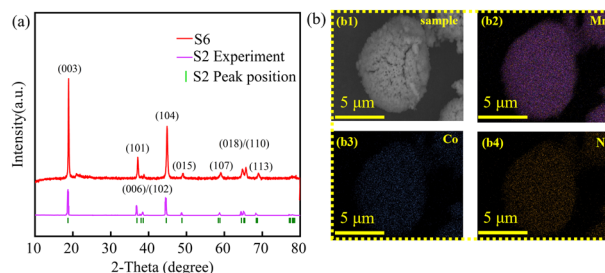
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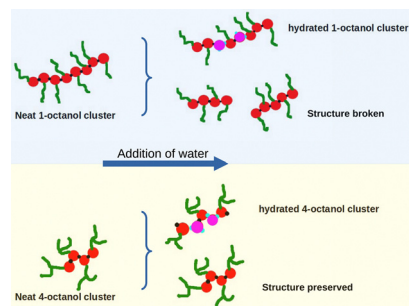
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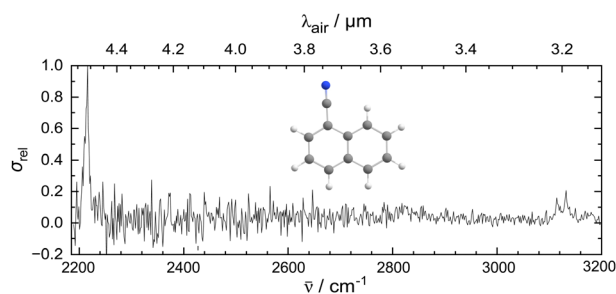
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Martina Požar, Jennifer Bolle, Susanne Dogan-Surmeier, Eric Schneider, Michael Paulus, Christian Sternemann\* and Aurélien Perera



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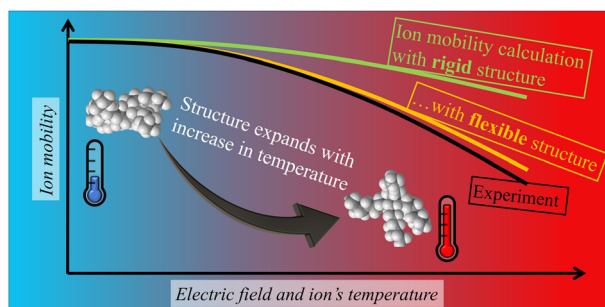
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### Mid-infrared spectroscopy of 1-cyanonaphthalene cation for astrochemical consideration

Julianna Palotás, Francis C. Daly,  
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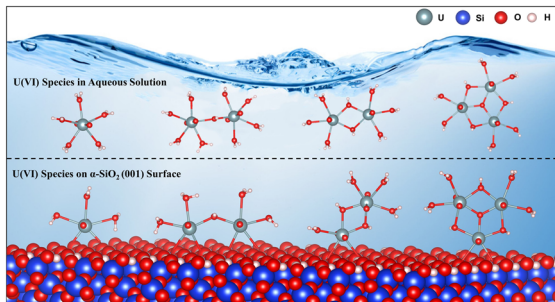
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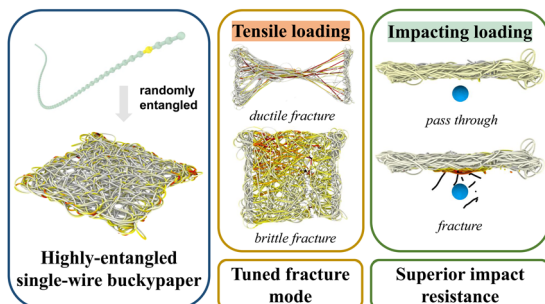
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### Structures of multinuclear U(VI) species on the hydroxylated $\alpha$ -SiO<sub>2</sub>(001) surface: insights from DFT calculations

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

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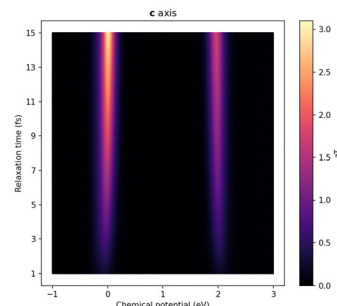


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### Computational prediction of high thermoelectric performance in $\text{As}_2\text{Se}_3$ by engineering out-of-equilibrium defects

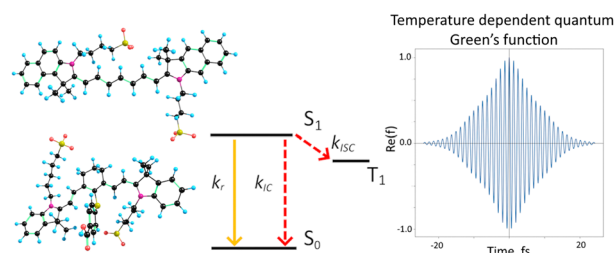
Anderson Silva Chaves, Murilo Aguiar Silva and Alex Antonelli\*



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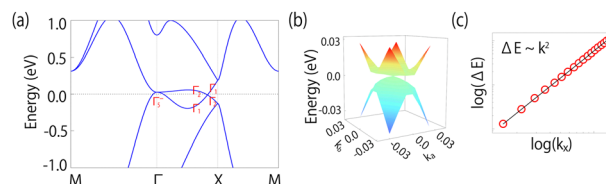
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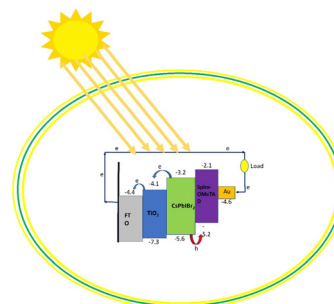
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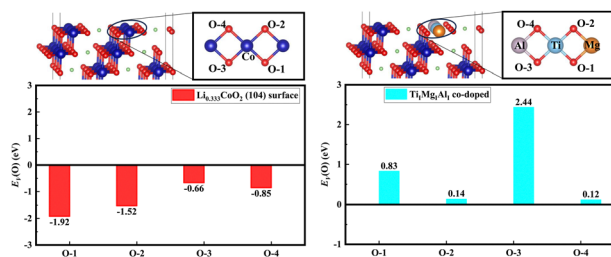
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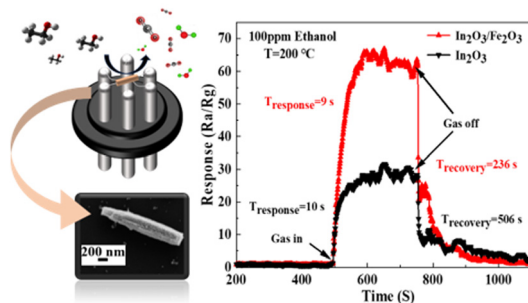
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### A synergetic promotion of surface stability for high-voltage $\text{LiCoO}_2$ by multi-element surface doping: a first-principles study

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

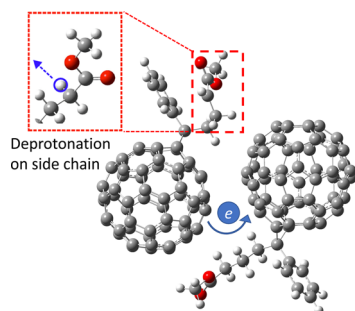
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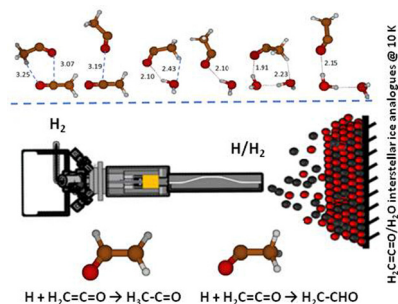
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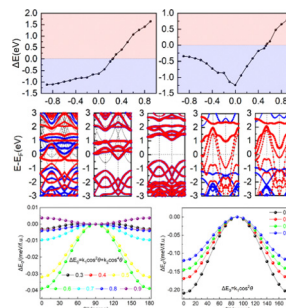
Mohamad Ibrahim, Jean-Claude Guillemin, Patrick Chaquin, Alexis Markovits and Lahouari Krim\*



4208

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

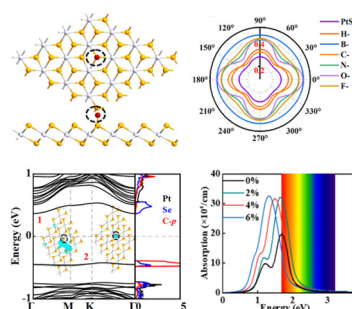
Ziyuan An, Linhui Lv, Ya Su,\* Yanyan Jiang and Zhaoyong Guan\*



4218

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

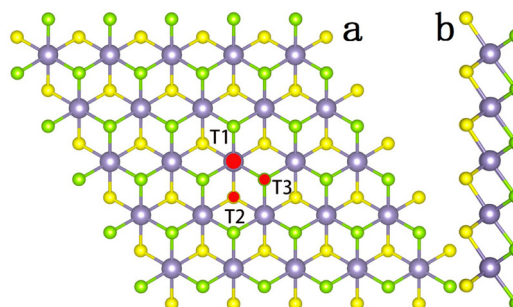
Xinyan Li, Zhanhai Li,\* Jianing Han, Shengguo Cao and Zhenhua Zhang\*



4231

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

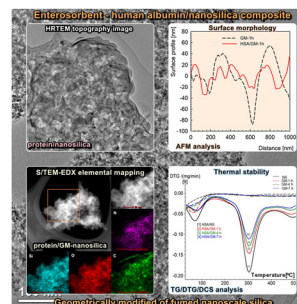
Bin Xu,\* Cheng Qian, Zheng Wang, Jing Zhang, Shanshan Ma, Yusheng Wang and Lin Yi



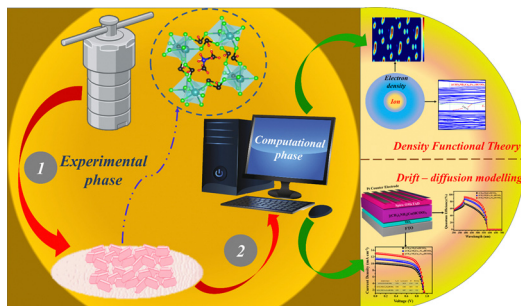
4240

### 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



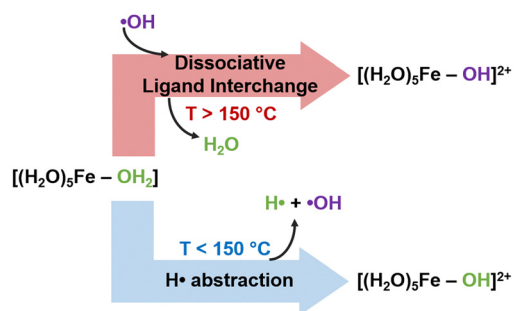
4262



### 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\*

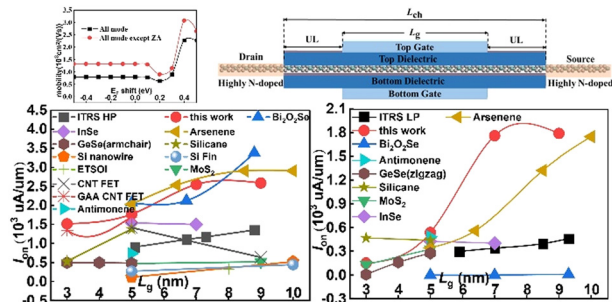
4278



### 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

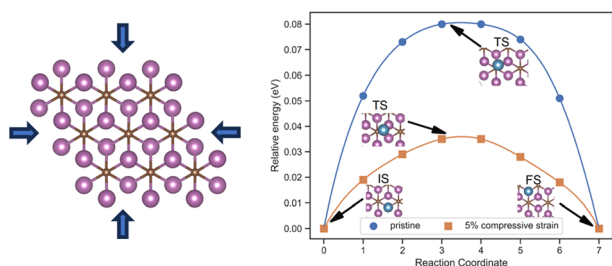
4284



### 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

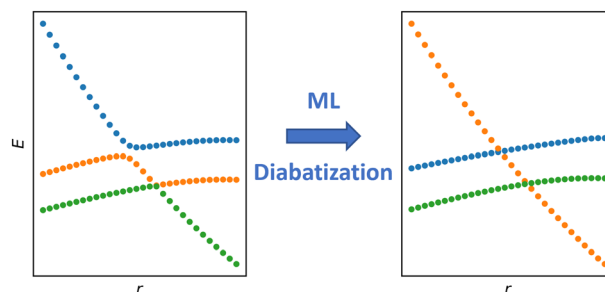


## RESEARCH PAPERS

4306

## Fast and accurate excited states predictions: machine learning and diabaticization

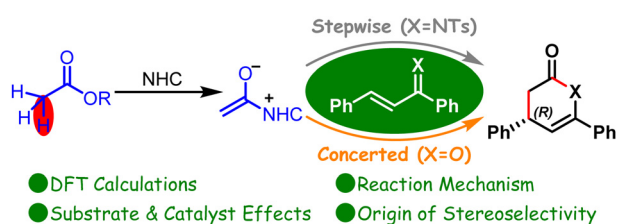
Štěpán Sršeň,\* O. Anatole von Lilienfeld and Petr Slaviček\*



4320

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

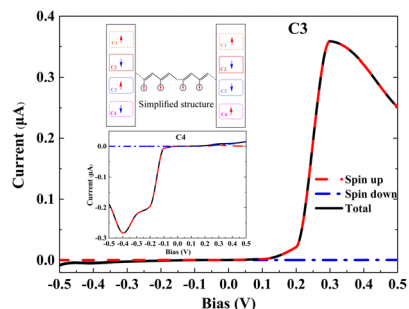
Pingxin Liang, Haoran Yang\* and Yang Wang\*



4329

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

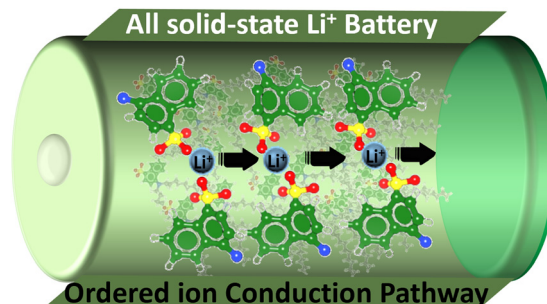
H. Ma, H. X. Li, H. Q. Zhang, Y. Wang, J. T. Li, C. Wang, J. F. Ren and G. C. Hu\*



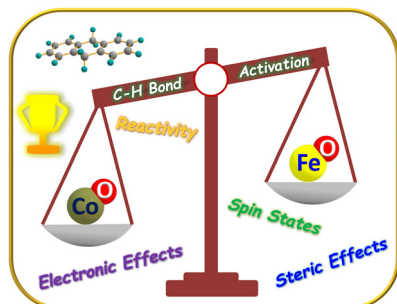
4338

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

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



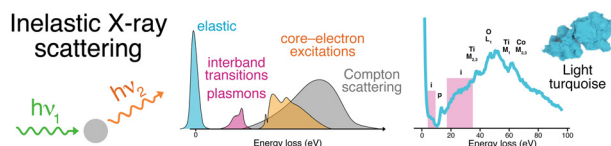
4349



### 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\*

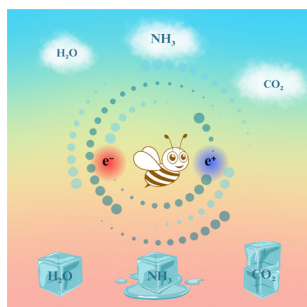
4363



### 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\*

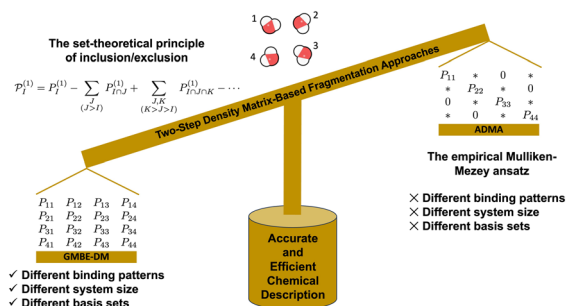
4372



### Electron- and positron-driven molecular processes for H<sub>2</sub>O, CO<sub>2</sub>, and NH<sub>3</sub> 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

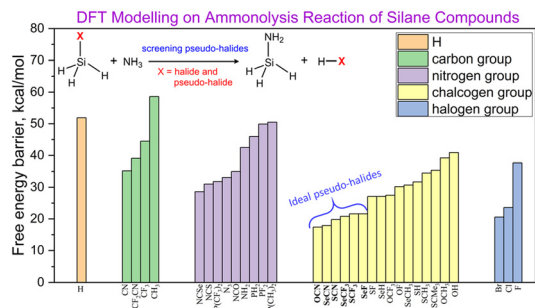
Francisco Ballesteros and Ka Un Lao\*



4395

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

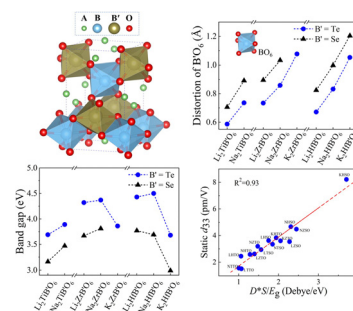
Anil Kumar Tummanapelli, Yingqian Chen and Ming Wah Wong\*



4403

### Investigation of nonlinear optical properties in $\alpha$ - $A_2BB'O_6$ ( $A = Li, Na, K; B = Ti, Zr, Hf; B' = Se, Te$ ) by first-principles calculations

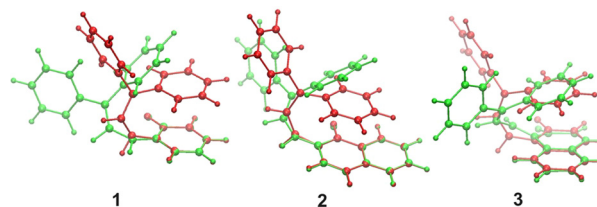
Gaojing Fang, Xiaojun Teng, Luo Yan, Yu Wu, Kui Xue, Xiaofeng Zhang, Yi-min Ding,\* Liujiang Zhou\* and Qiye Wen\*



4412

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

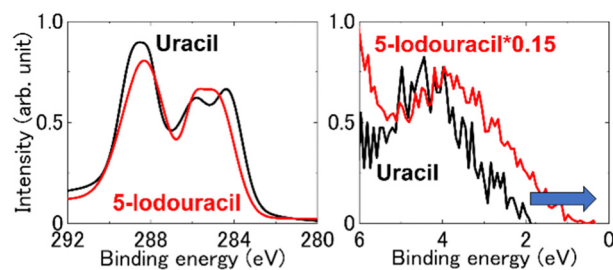
Daiana S. Tabirja and Victor V. Kostjukov\*



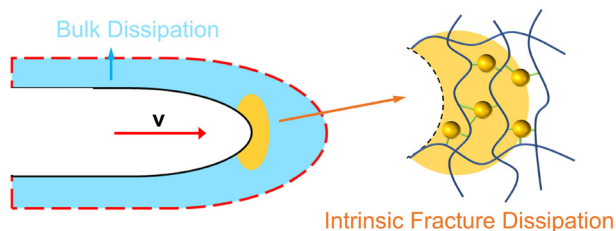
4422

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

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



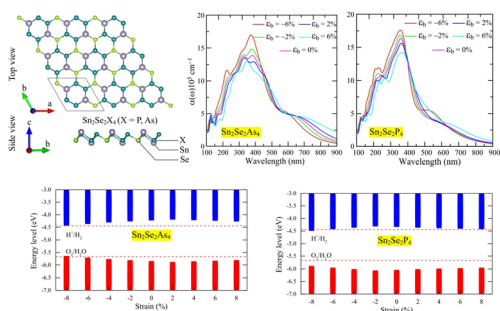
4429



### 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

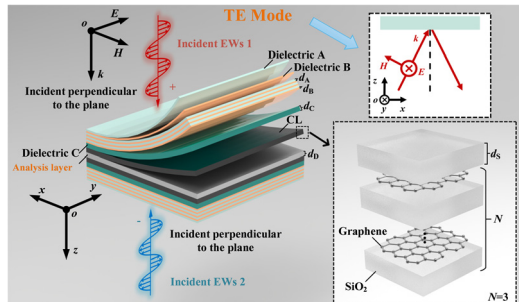
4437



### First principles study of strain effects on prospective 2D photocatalysts $\text{Sn}_2\text{Se}_2\text{X}_4$ (X = P, 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



### $\text{TiB}_4$ and $\text{SrB}_8$ 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\*

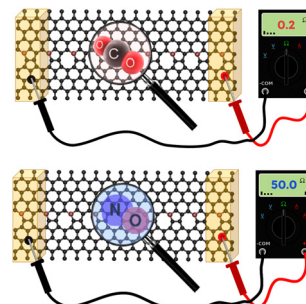


## RESEARCH PAPERS

4466

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

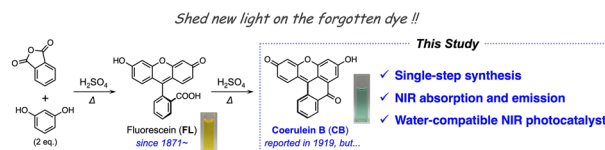
B. Keshav Rao, Tadeu Luiz Gomes Cabral, Debora Carvalho de Melo Rodrigues, Fábio A. L. de Souza, Wanderlã L. Scopel, Rodrigo G. Amorim\* and Ravindra Pandey



4474

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

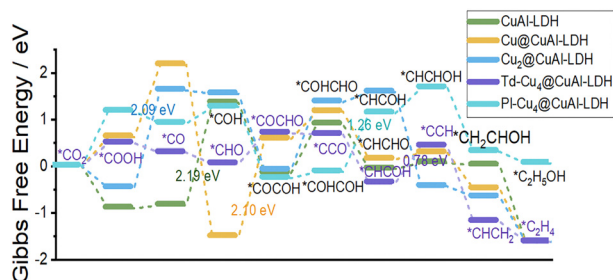
Masaru Tanioka,\* Masaya Oyama, Kaito Nakajima, Minori Mori, Mei Harada, Yuji Matsuya\* and Shinichiro Kamino\*



4480

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

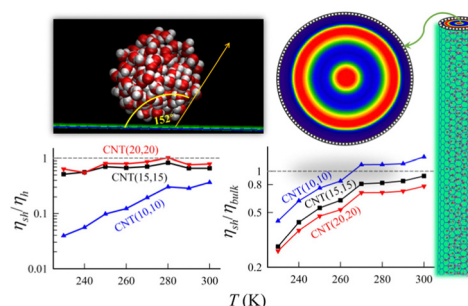
Xin-Yu Xu, Jing-Yi Guo, Wei Zhang, Yao Jie, Hui-Ting Song, Hao Lu, Yi-Fan Zhang, Jia Zhao, Chen-Xu Hu and Hong Yan\*



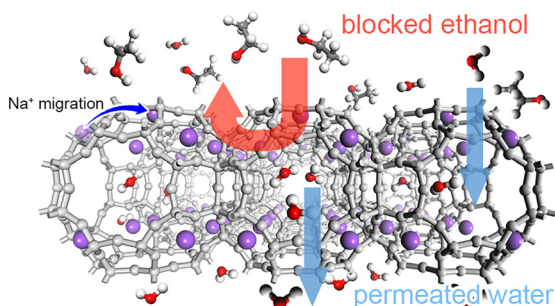
4492

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

Golam Rosul Khan and Snehasis Daschakraborty\*



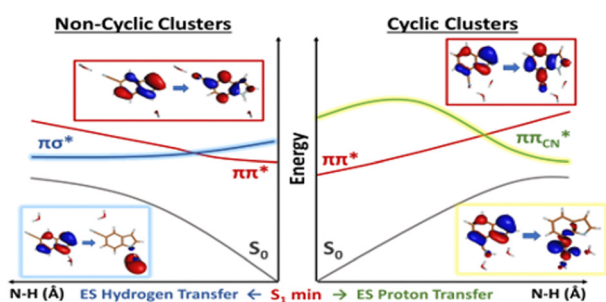
4505



### Computational understanding of Na-LTA for ethanol–water separation

Zicheng Wan, Chen Zhou, Yichao Lin,\*  
Liang Chen and Ziqi Tian\*

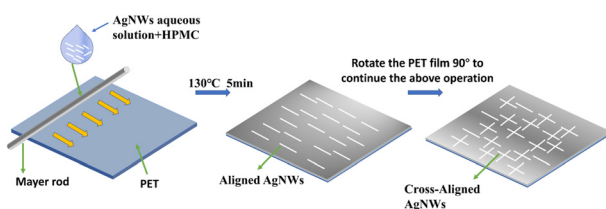
4511



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

Salsabil Abou-Hatab and Spiridoula Matsika\*

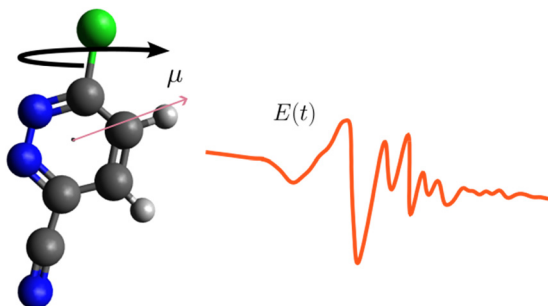
4524



### 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\*

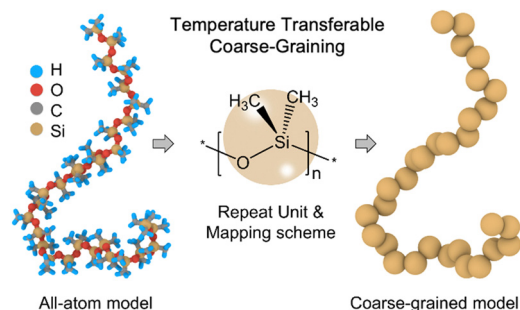


## RESEARCH PAPERS

4541

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

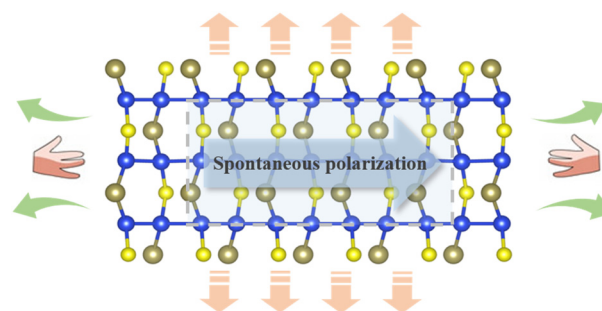
Dawei Zhang, Yang Wang, Maryam Safaripour, Daniel A. Bellido-Aguilar, Kurt R. Van Donselaar, Dean C. Webster, Andrew B. Croll and Wenjie Xia\*



4555

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

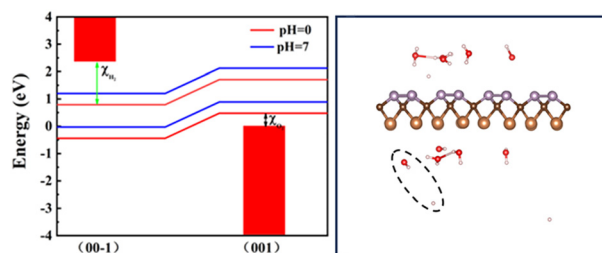
Yunlai Zhu, Zihan Qu, Jishun Zhang, Xiaoteng Wang, Shuo Jiang, Zuyu Xu, Fei Yang, Zuheng Wu\* and Yuehua Dai\*



4564

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

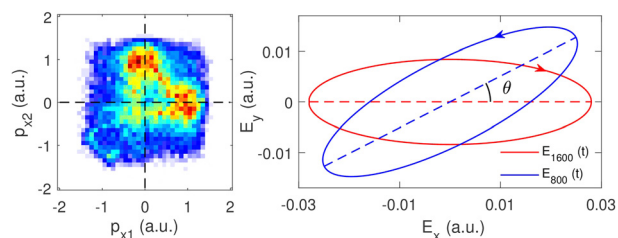
Yunlai Zhu, Shuo Jiang, Jishun Zhang, Zihan Qu, Zuheng Wu, Zuyu Xu, Wei Hu, Yuehua Dai and Fei Yang\*



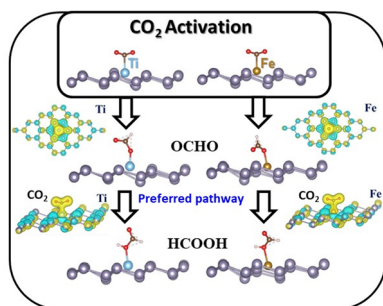
4572

**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



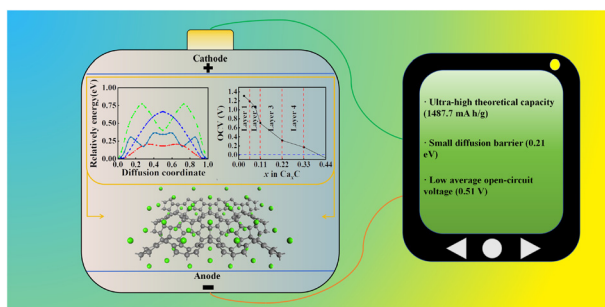
4579



### A first-principles study of electro-catalytic reduction of CO<sub>2</sub> on transition metal-doped stanene

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

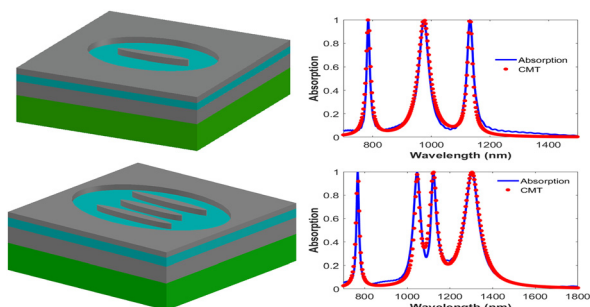
4589



### 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\*

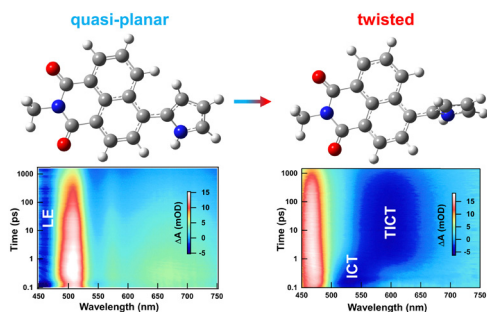
4597



### 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

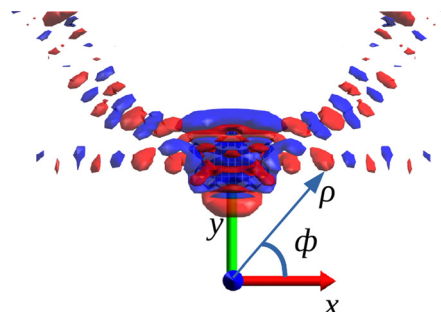
Wei Zhang, Yalei Ma, Hongwei Song, Rong Miao,\* Jie Kong\* and Meng Zhou\*



4614

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

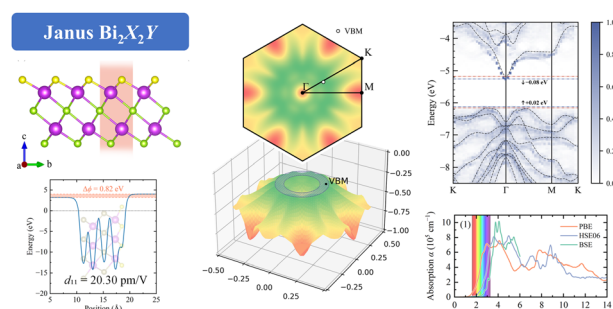
Viatcheslav Kokoouline,\* Alexander Alijah and Vladimir Tyuterev



4629

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

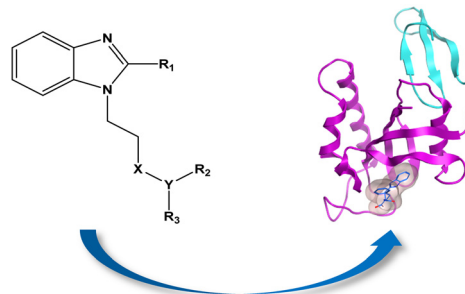
Shu-Hao Cao, Tian Zhang,\* Hua-Yun Geng and Xiang-Rong Chen\*



4643

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

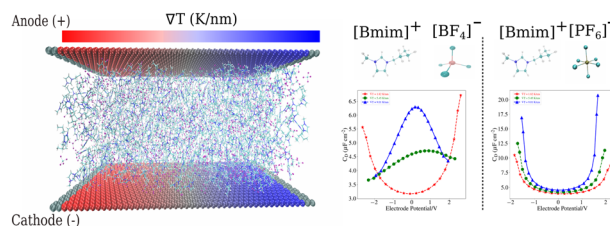
Min Liu, Bingli Wang, Huan Liu, Haolun Xia and Lina Ding\*



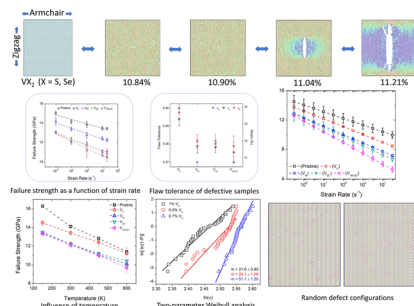
4657

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

Kiran Prakash and Sarith P. Sathian\*



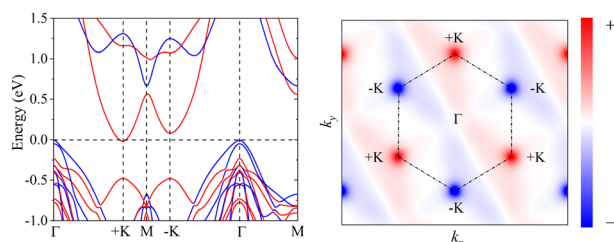
4668



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

Akash Baski, Zimmi Singh and Sankha Mukherjee\*

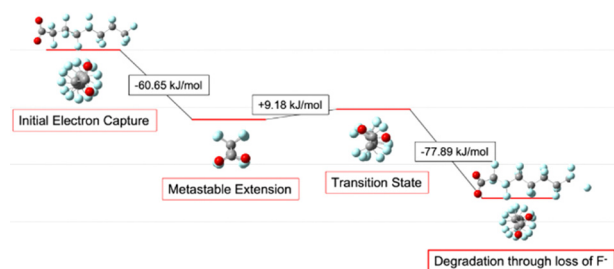
4683



### Novel valley character and tunable quasi-half-valley metal state in Janus monolayer VSIGeP<sub>4</sub>

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

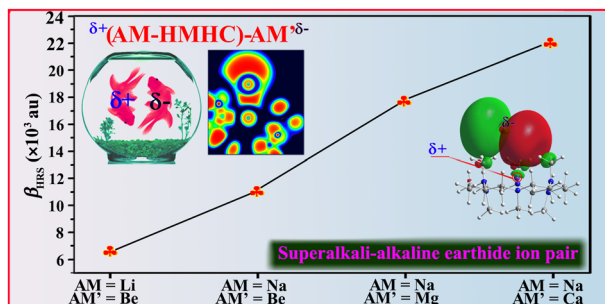
4692



### 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 alkali characteristics: a DFT study

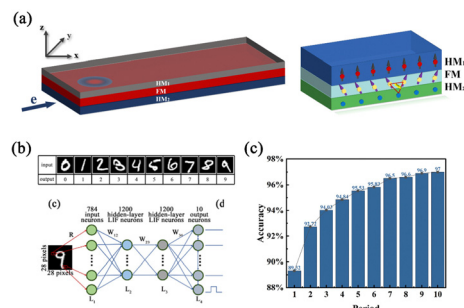
Jianguan Huang, Yin-Feng Wang,\* Kai Yang, Wen Zhang, Zhi-Jun Wang, Xuexia Liu\* and Zhi-Ru Li\*



4716

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

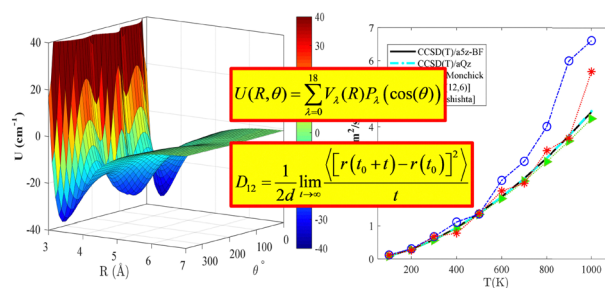
Bin Gong, Luowen Wang, Sunan Wang, Ziyang Yu,\*  
Lun Xiong, Rui Xiong, Qingbo Liu\* and Yue Zhang



4724

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

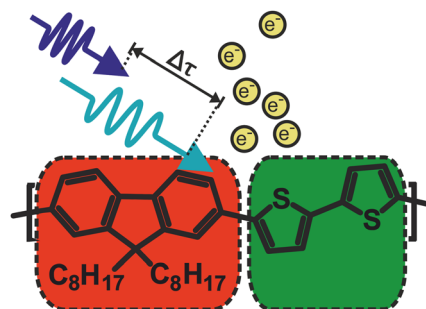
Fatemeh Aghababaei and Ebrahim Nemati-Kande\*



4736

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

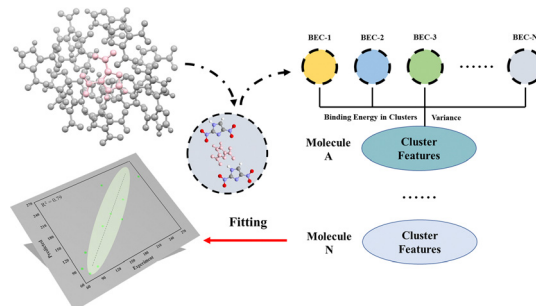
T. Reiker,\* Z. Liu, C. Winter, M. V. Cappellari,  
D. Gonzalez Abradelo, C. A. Strassert, D. Zhang and  
H. Zacharias



4752

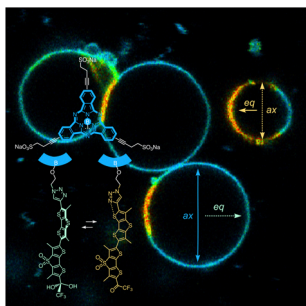
### Insight into melting point differences of dinitroimidazoles and dinitropyrazoles from the perspective of intermolecular interactions

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



## RESEARCH PAPERS

4759

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

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

## CORRECTION

4766

**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

