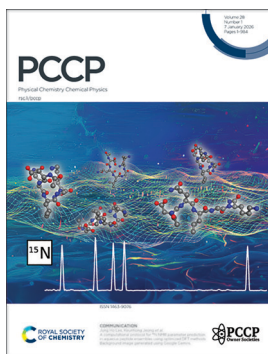


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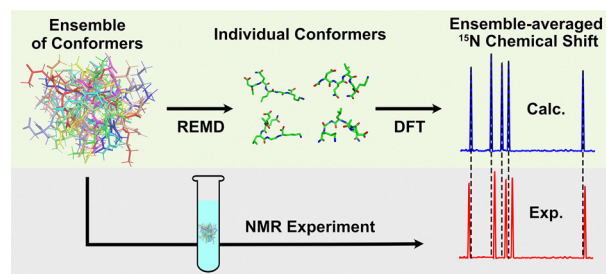
**Inside cover**  
See Vladimir V. Zhivonitko *et al.*, pp. 52–66. Image reproduced by permission of Vladimir V. Zhivonitko from *Phys. Chem. Chem. Phys.*, 2026, 28, 52.

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Minji Kim, Jung Ho Lee\* and Keunhong Jeong\*

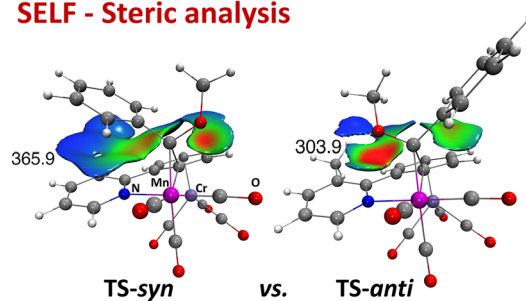


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Sara Figueirêdo de Alcântara Morais, Yann Cornaton, Eric Hénon\* and Jean-Pierre Djukic\*

#### SELF - Steric analysis



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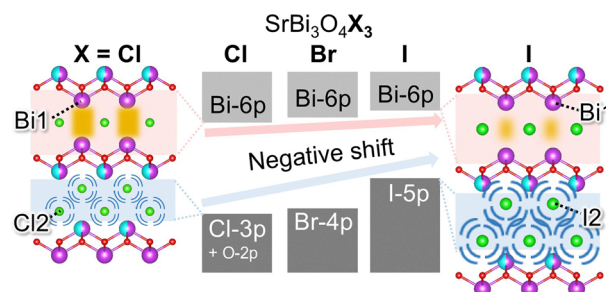
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### Dual halogen layers diversify band engineering in Sillén oxyhalide photocatalysts: electronic structure control of $\text{SrBi}_3\text{O}_4\text{X}_3$ ( $\text{X} = \text{Cl}, \text{Br}, \text{I}$ ) via halogen substitution

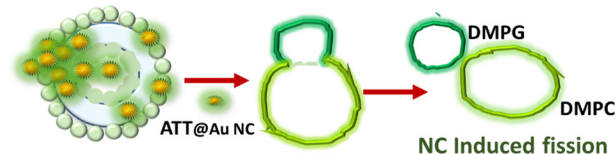
Yusuke Ishii, Hajime Suzuki,\* Osamu Tomita, Akinobu Nakada and Ryu Abe\*



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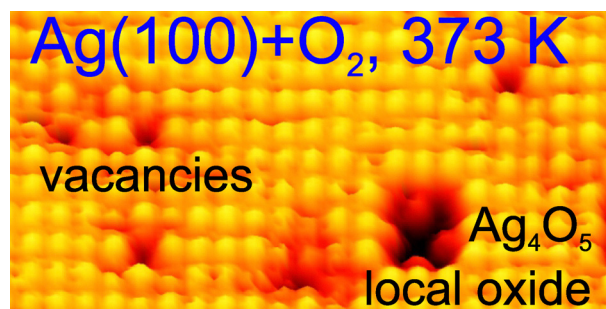
Mallika Mukherjee, Asmita Das and Pradipta Purkayastha\*



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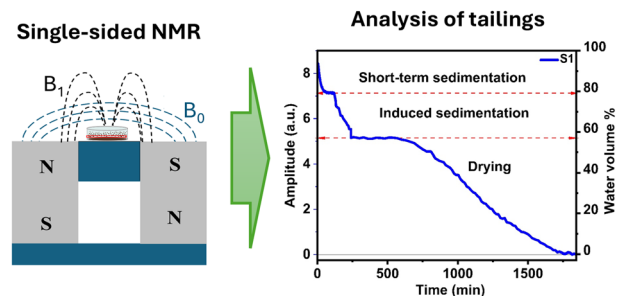


## RESEARCH PAPERS

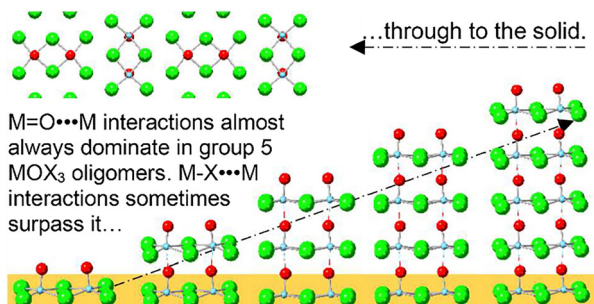
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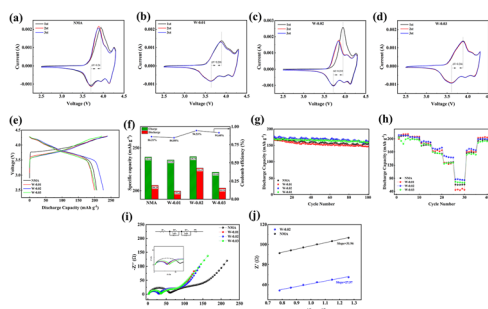
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### Sigma-hole-supported interactions in complexes of group 5 oxyhalides (MOX<sub>3</sub>) with insights for their extended solids

Donovan Hoilette Jr., Gabriel F. Stewart and Kelling J. Donald\*

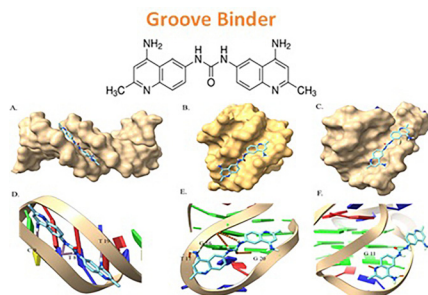
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### W-incorporated high-performance layered cathode materials for advanced lithium-ion batteries

Xiaoyi Hou,\* Haozhe Wu, Qirongxin Shen, Dengdeng Ai and Xi Wu

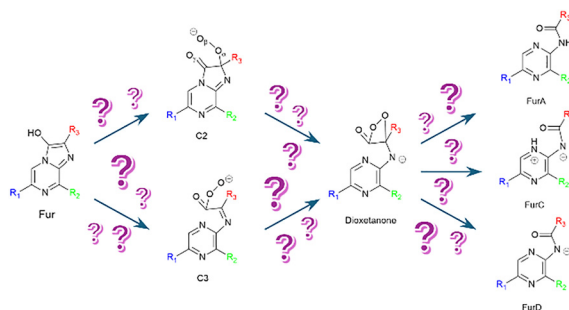
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### Insights on the binding and selectivity of surfen towards different DNA topologies

Laxmi Kashyap, Kritika Varshney and Manoj Munde\*

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### Toward a mechanistic understanding of bioluminescence: a theoretical study of furimazine oxidation and luminescence

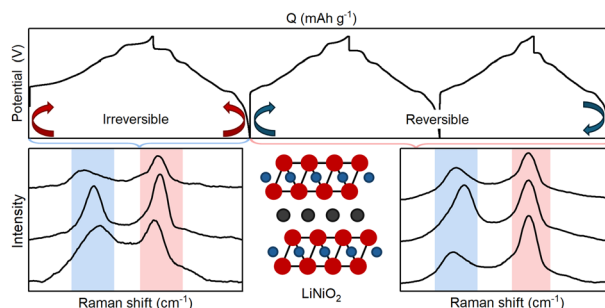
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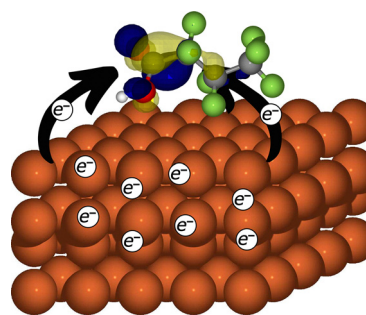
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### Exploring the initial bond activations of PFAS on zero-valent iron

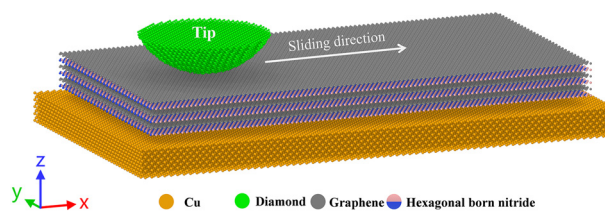
Glen R. Jenness,\* Elizabeth R. Zengel and Manoj K. Shukla\*



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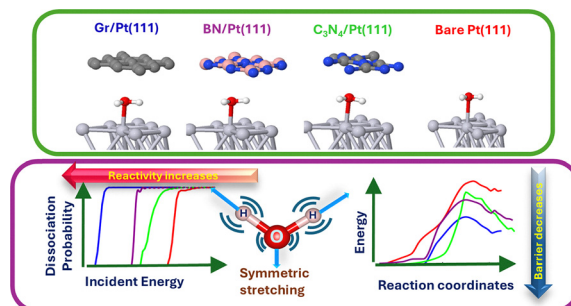
Hao Wang, Lu Chen, Yunxiao Wang, Yongteng Wei, Junqin Shi, Tengfei Cao and Xiaoli Fan\*



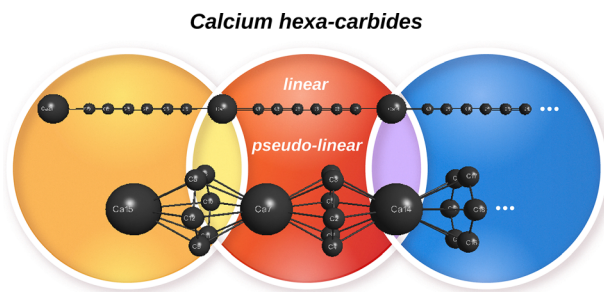
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### Mode-selective H<sub>2</sub>O dissociation on Pt(111) under two-dimensional confinement

Nidhi Tiwari, Sandip Ghosh and Ashwani K. Tiwari\*



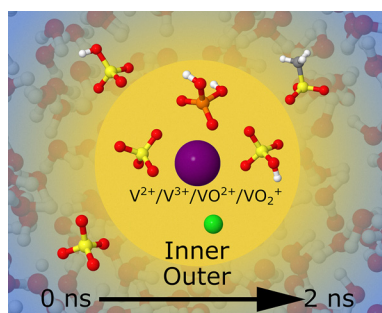
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### Calcium carbides: can hexa-carbides grow unlimitedly? Theoretical perspectives and issues that oppose a definite answer

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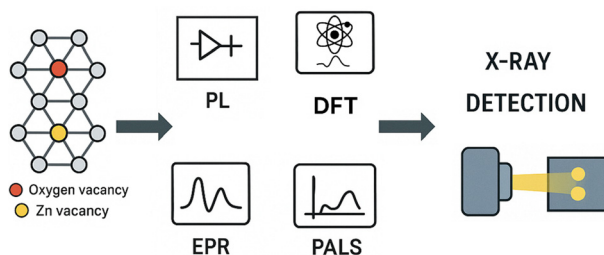
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### Computational investigation of coordinating electrolytes with vanadium ions in redox flow batteries

Christopher S. Mills and Anna L. Garden\*

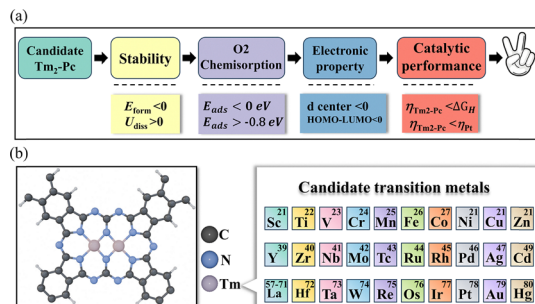
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### Systematic screening of transition metal dual-atom-doped phthalocyanine electrocatalysts for the oxygen reduction reaction

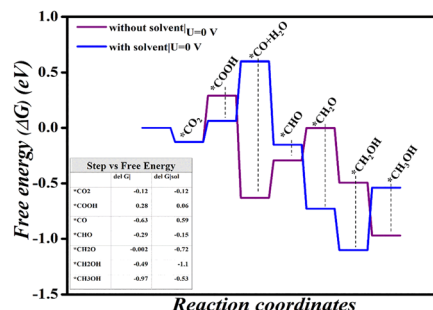
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### Electrochemical CO<sub>2</sub> reduction to methanol over Ni@Ti<sub>3</sub>CN MXene: a first-principles DFT study

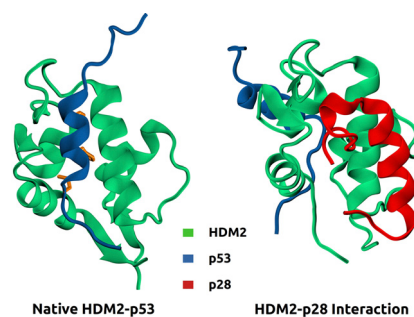
Karthiga Manivannan and Senthilkumar Lakshmiopathi\*



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### Azurin-based peptide p28 disrupts p53–HDM2 interactions: insights from *in silico* studies

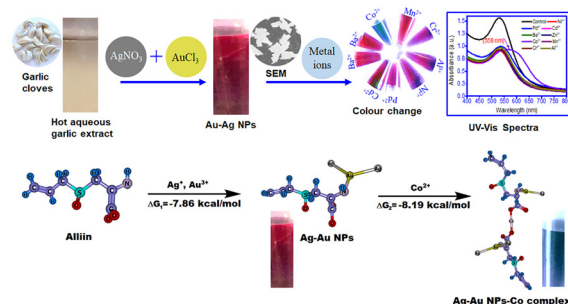
Albin Joy, Anand Srivastava and Rajib Biswas\*



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### Optimized colorimetric detection of cobalt ions (Co<sup>2+</sup>) using alliin–Ag–Au nanoparticles

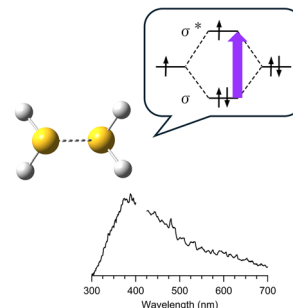
Rintumoni Paw, Kangkan Sarmah, Moushumi Hazarika, Ankur K. Guha and Chandan Tamuly\*



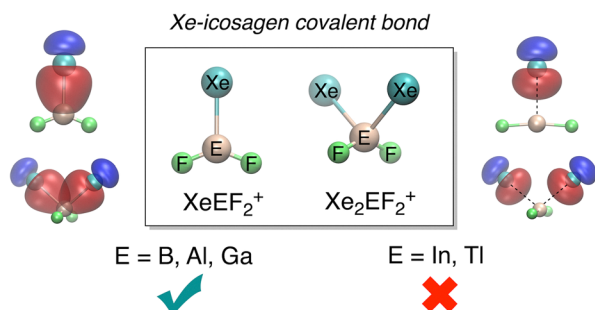
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### Electronic spectra of (H<sub>2</sub>S)<sub>n</sub><sup>+</sup> (n = 2–6) and [(H<sub>2</sub>S)<sub>2</sub>–(H<sub>2</sub>O)<sub>m</sub>]<sup>+</sup> (m = 1–2) in the gas phase

Mitsuaki Shioura, Mizuhiro Kominato and Asuka Fujii\*



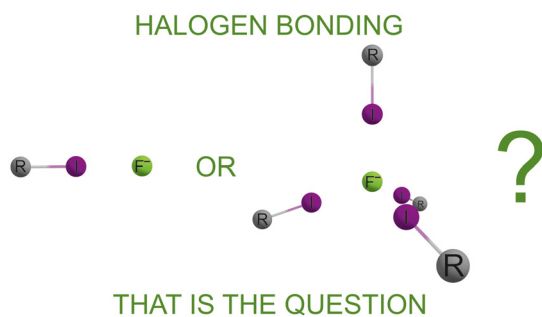
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### Covalent bonding and extreme shielding in xenon–icosagen fluoride cations

Erick Cerpa,\* Jose A. Guerrero-Cruz, Gabriel Merino, J. Oscar C. Jimenez-Halla and Abril C. Castro\*

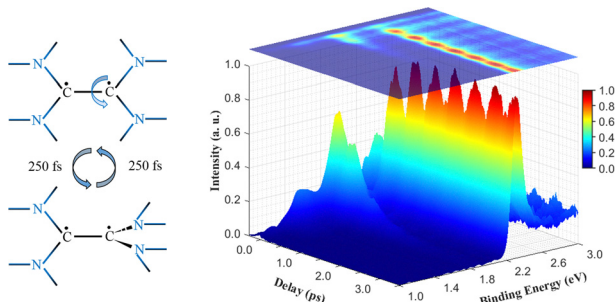
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### Multidentate halogen bond acceptors: from fluorides to iodides. Anticooperativity in halogen-bonded clusters

Justyna Dominikowska\*

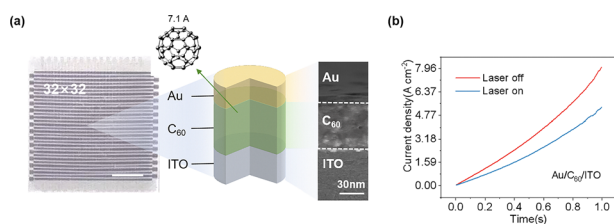
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### A time-, angle- and kinetic-energy-resolved photoelectron spectroscopic study of tetrakis(dimethylamino)ethylene

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### Tunable negative photoconductance states in a C<sub>60</sub> device with optically induced trap center reconfiguration

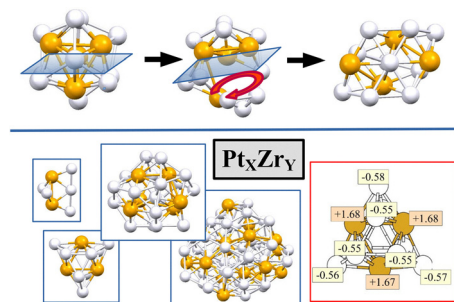
Xiude Yang, Jie Li,\* Zhen Zhang, Xiuxia Wang, Zhonglin Chen, Ping Li, Bo Wu, Guangdong Zhou\* and Jin Ye\*



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### Structural and chemical properties of Pt-rich $\text{Pt}_x\text{Zr}_y$ nanoalloys

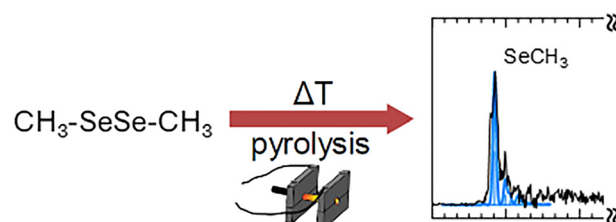
Luis M. Molina\* and Julio A. Alonso



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### Threshold photoelectron spectroscopy of small organo-selenium radicals

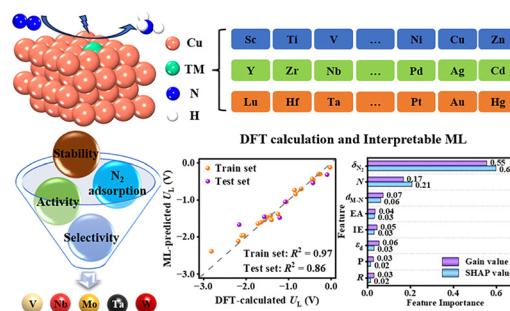
Emil Karaev, Dorothee Schaffner, Marius Gerlach, Sira Grätz, Patrick Hemberger and Ingo Fischer\*



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### Screening copper-based single-atom alloy catalysts for electrochemical nitrogen reduction

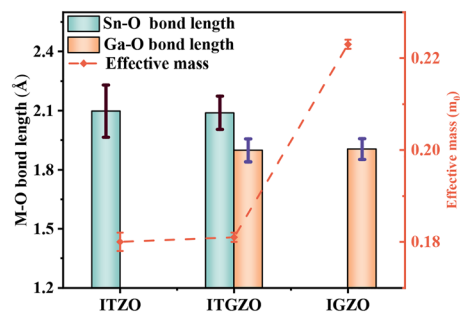
Hengzhi Liu and Yang-Gang Wang\*



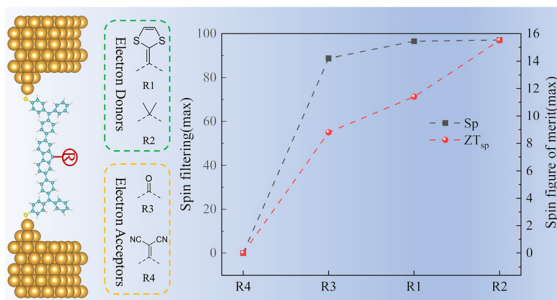
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### Theoretical assessment of multi-doping strategies in amorphous indium oxide for synergistically enhancing carrier mobility and bias stability

Jiejun Pan, Zhibin Liu, Xionghui Tan, Kaixuan Chen, Pingqi Gao\* and Can Han\*



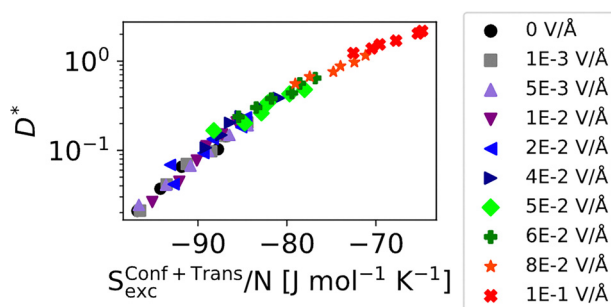
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### Substituent-controlled quantum interference tuning of spin and thermoelectric transport in triphenylmethyl diradical junctions

Zhenhai Cui, Yongfeng Xiong, Qiuming Liu, Ziqiang Liu, Tong Chen and Lin Huang\*

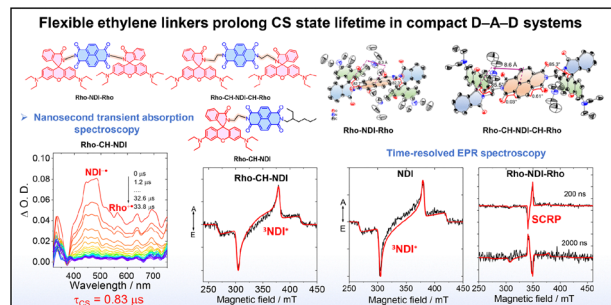
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### Excess entropy scaling explains the enhanced dynamics of the ionic liquid 1-ethyl-3-methylimidazolium chloride in external electric fields

Fernando J. Carmona Esteva, Yong Zhang, Katerina Duncheskie, Edward J. Maginn\* and Yamil J. Colón\*

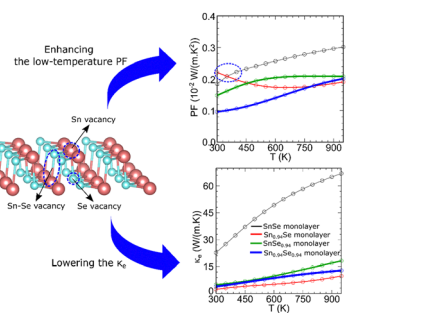
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### Long-lived charge separated states in spiro-compact rhodamine–naphthalenediimide D–A–D systems: synthesis and time-resolved optical and electron paramagnetic resonance spectroscopic studies

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### Tailoring the electronic and thermoelectric properties of the SnSe monolayer via vacancy defects: insights from density functional theory

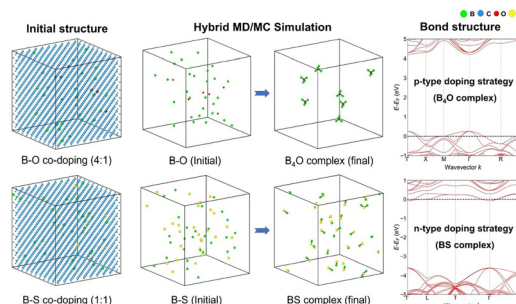
Erik Bhakti Yutomo,\* Suci Faniandari and Muhammad Fahmi



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### Atomistic simulation study of diamond doping based on machine learning potential

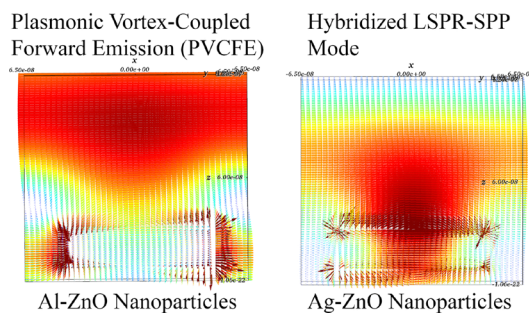
Yiheng Yan, Yaochen Yu, Junwei Hu, Xuecheng Sun, Qinlan Luo, Zengyong Chu,\* Jiayu Dai\* and Haiyang Niu\*



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### Plasmonic vortex-coupled forward emission (PVCFE): a novel light coupling mechanism in aluminium nanostructures for high-efficiency, stable, and cost-effective organic photovoltaics

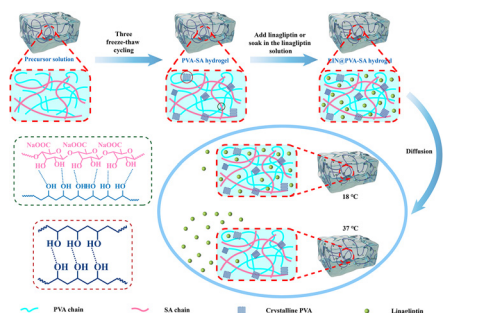
Mahdi Aghlmandi Sadigh Bagheri\*



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### Mechanically robust PVA/SA semi-IPN hydrogels for highly effective temperature-triggered linagliptin delivery

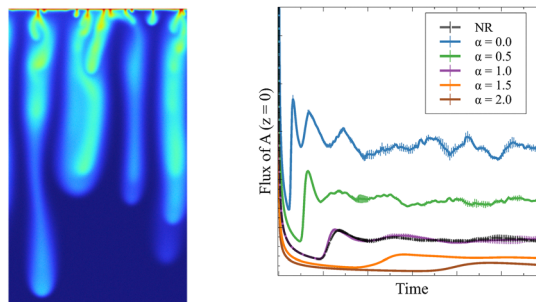
Yue Wang, Guineng Li, Yeying Li, Mutian Yao, Qiaobo Wang, Liang Peng\* and Hua Gu\*



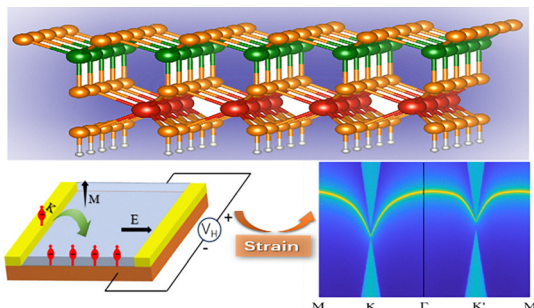
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### Effect of variable solubility on reactive convective dissolution

S. Kabbadj, A. De Wit and L. Rongy\*



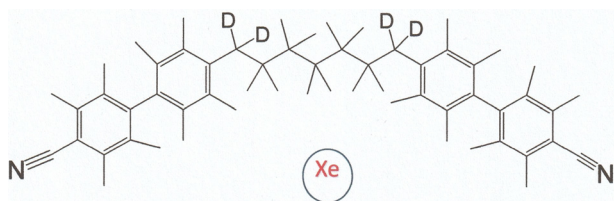
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### Janus VAZ<sub>3</sub>H (A = Si, Ge; Z = N, P) single layers exhibiting valley polarization, magnetic anisotropy, and topological transition

Yang Yang,\* Yanyang Cao, Shao-Jie Zhang, Luogang Xie and Hongyan Lu

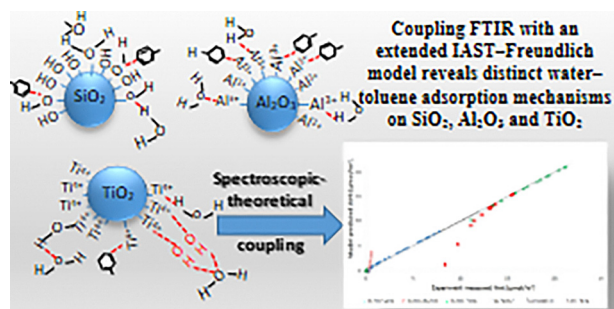
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### Properties of CB7CB-D<sub>4</sub> as derived from <sup>129</sup>Xe and <sup>2</sup>H NMR experiments and computations

Jukka Jokisaari\* and Juha Vaara

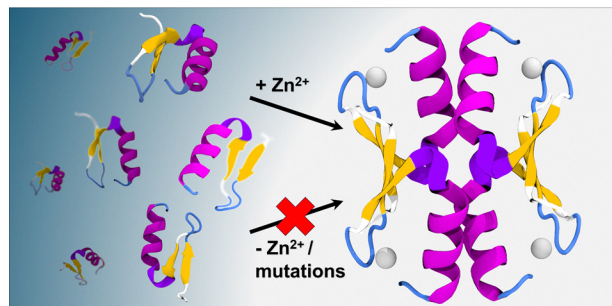
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### Deciphering competitive water–toluene adsorption mechanisms on oxide surfaces

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### Zinc-mediated multimerization of the N-terminal CCHC zinc finger domain of BCL11B: a key to stability and a potential therapeutic target

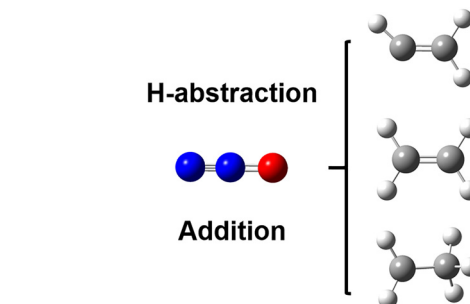
Anne Susemihl, Felix Nagel, Piotr Grabarczyk, Christian Andreas Schmidt and Mihaela Delcea\*



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### A theoretical study on the mechanism of $C_2H_3-5$ oxidation by $N_2O$

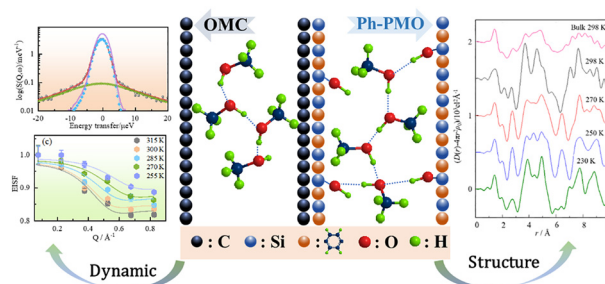
Huanhuan Wang, Long Qin, Bingzhi Liu, Shaohua Zhu, Zhandong Wang and Ran Sui\*



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### An X-ray scattering and quasielastic neutron scattering study on the structure and dynamic properties of low-temperature methanol confined in ordered microporous carbon and mesoporous organosilica pores

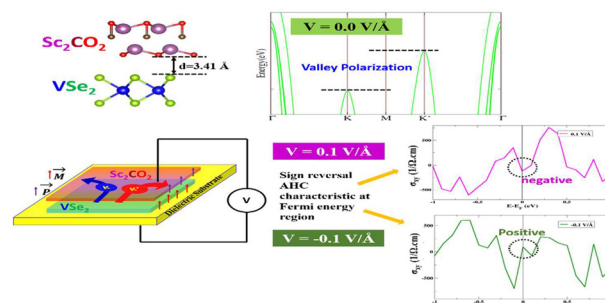
Hongyan Liu, Zhuanfang Jing, Keke Chai, Yongquan Zhou,\* Koji Yoshida, Takeshi Yamada and Toshio Yamaguchi\*



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### Electrically tunable anomalous Hall conductivity in ferrovalley–ferroelectric heterostructure $VSe_2/Sc_2CO_2$

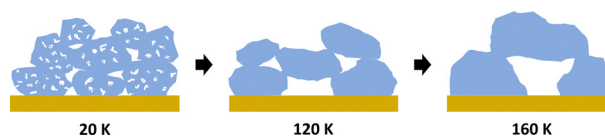
Mayuri Bora,\* Himangshu Sekhar Sarmah\* and Subhradip Ghosh



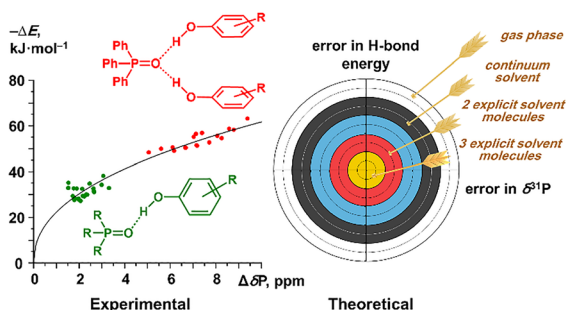
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### Molecular and pore-scale structure evolution in amorphous solid water

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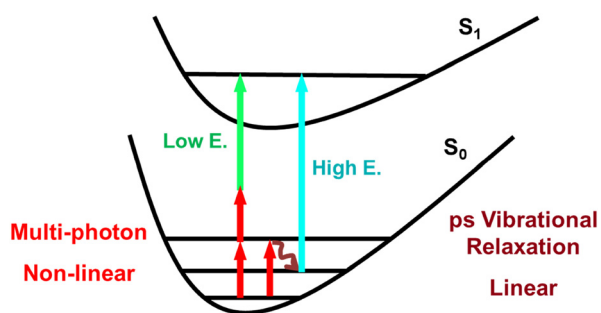
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### $^{31}\text{P}$ NMR chemical shift of phosphine oxides measures the total strength of multiple anticooperative H-bonds formed between the P=O group and proton donors

Omar Alkhuder, Mikhail A. Kostin and Peter M. Tolstoy\*

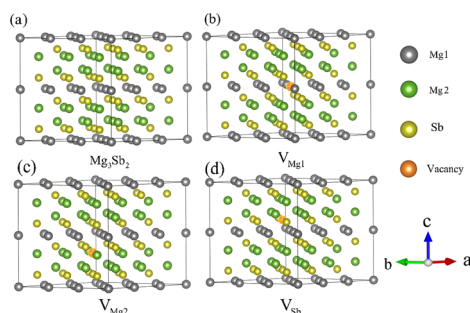
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### The interplay of nonlinear multi-photon processes and vibrational population effect on vibration-modulated fluorescence

Qirui Yu, Yuanzhou Shi, Jianxin Guan, Xinmao Li, Zhihao Yu and Junrong Zheng\*

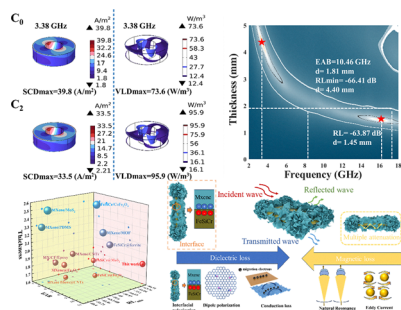
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### Vacancy-induced phonon localization and lattice softening for reduced thermal conductivity in $\text{Mg}_3\text{Sb}_2$

Sheng Zhang, Jinbao Zhang, Liqi Ren, Yijing Shao, Wanyue Yan, Meng Tian, Kunling Peng,\* Ping Lin\* and Yunzhen Du\*

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### Research on two-dimensional FeSiCr/mesoporous MXene composites and their absorption properties

Zhengxing Li, Quan Fang, Zhongyue Song, Juan Liu,\* Honghui Jiang\* and Tongxiang Liang\*

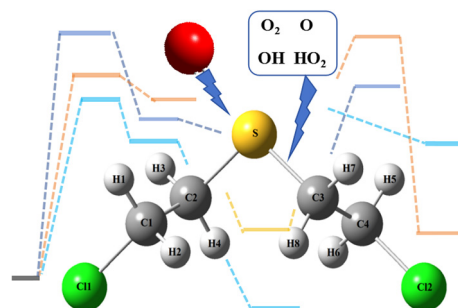


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### High-accuracy theoretical studies on the gas-phase reaction mechanisms of sulfur mustard with reactive oxygen species (OH/O<sub>2</sub>/HO<sub>2</sub>/O)

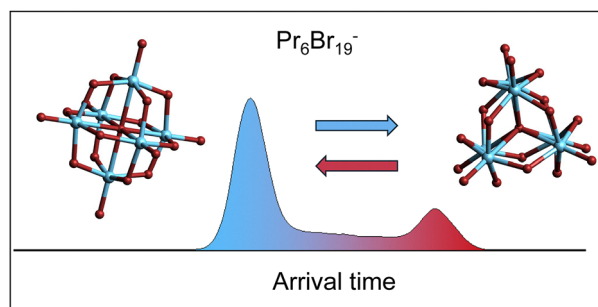
Xuefeng Liu, Shangpeng Hao, Xin Gao, Lin Yang, Huanhuan Wang\* and Haitao Wang\*



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### A cyclic ion mobility and DFT study of the structures, isomer space and isomer interconversion of lanthanide bromide clusters, Ln<sub>x</sub>Br<sub>3x+1</sub><sup>-</sup>, x = 1–6

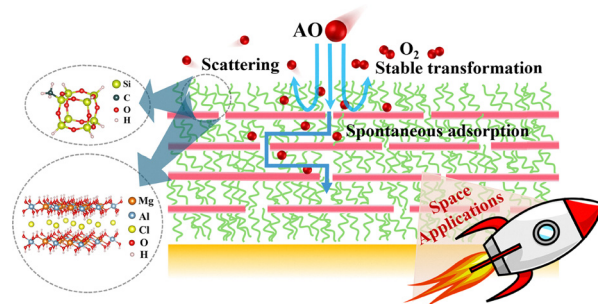
Yuto Nakajima, Patrick Weis,\* Florian Weigend,\* Marcel Lukanowski, Fuminori Misaizu and Manfred M. Kappes\*



613

### First-principles insights into atomic oxygen protection coatings composed of scale-like layered double hydroxide nanosheets

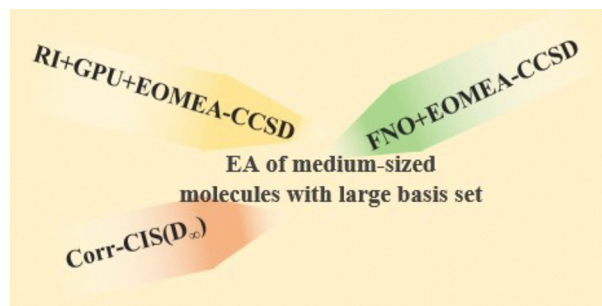
Denghang Tang, Rui Sun, Jiayu Zheng, Mengyun Xu, Haogeng Li, Hongyu Gu,\* Yuzhi Zhang,\* Yi-Yang Sun and Lixin Song



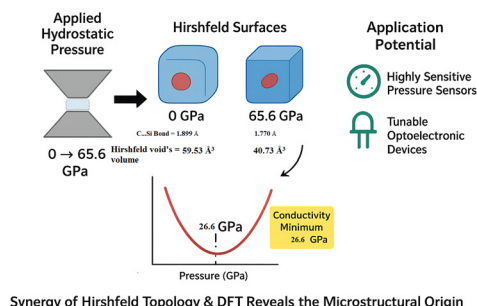
620

### Electron affinities with GPU-accelerated density-fitting EOM-CCSD, approximate EOM-CCSD methods and EOM-CCSD with frozen natural orbitals

Yanmei Hu, Zhifan Wang and Fan Wang\*



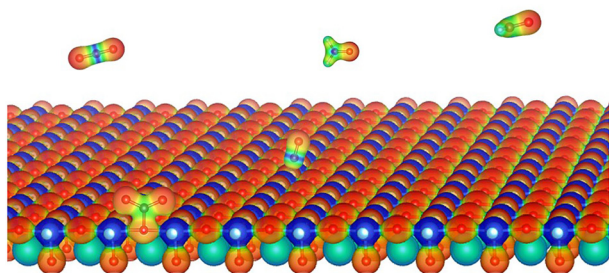
632



## Pressure-induced tunability and conductivity minimum in 3C-SiC for optoelectronic applications

Z. Y. Khattari\* and M. Albaddawi

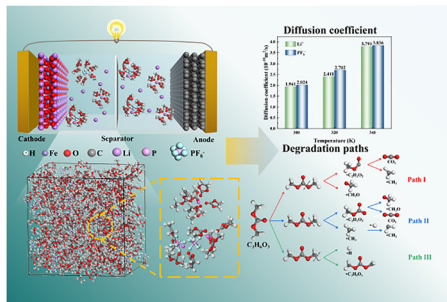
644



## The adsorption characteristics and mechanism of C1 molecules on two-dimensional SrTiO<sub>3</sub> films

Yuanbin Xue, Cuihuan Geng, Xiaojing Bai and Huali Hao\*

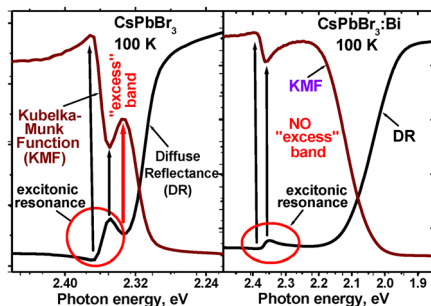
651



## Thermal runaway mechanism of LiFePO<sub>4</sub> battery electrolytes: a molecular dynamics and density functional theory simulation study

Jun Xie,\* Ping Huang, Guowei Xia, Yixiao Zhang, Yutong Zhang, Kun Tian and Qing Xie

662



## Manifestation of excitonic resonance in diffuse reflectance spectra of halide perovskites

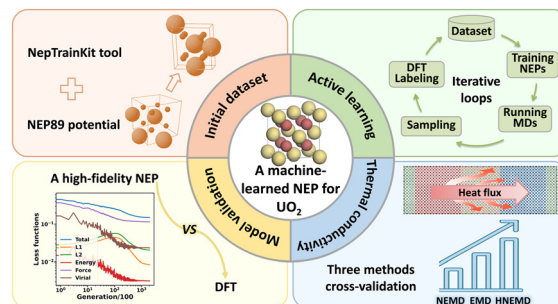
Vyacheslav N. Kuznetsov,\* Yuri V. Chizhov, Nadezhda I. Glazkova, Galina V. Kataeva, Ruslan V. Mikhaylov, Vladimir K. Ryabchuk, Alexei V. Emeline and Nick Serpone\*



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## Active learning-enhanced neuroevolution potential for predictive modeling of $\text{UO}_2$ thermophysical properties

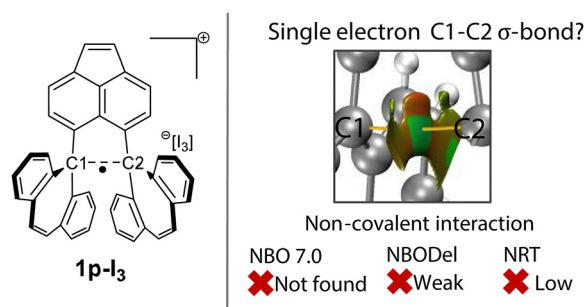
Junying Zhong, Lei Zhang and Tao Bo\*



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## Dissecting the single-electron C–C bond: NBO and AIM perspectives

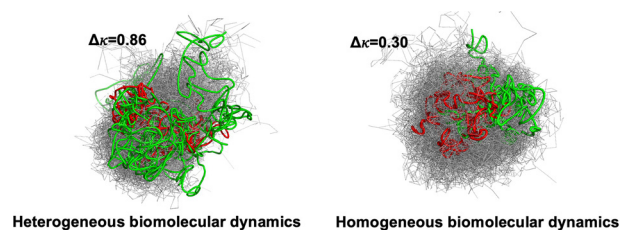
Leonardo I. Lugo-Fuentes, Darien I. Martínez-Valencia, J. Oscar C. Jiménez-Halla and Joaquín Barroso-Flores\*



692

## Differential sequence charge clustering and mixing ratio affect stability and dynamics of heterotypic peptide condensates

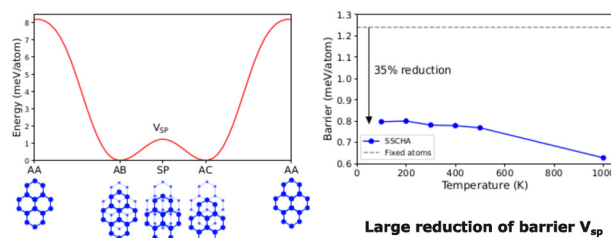
Milan Kumar Hazra



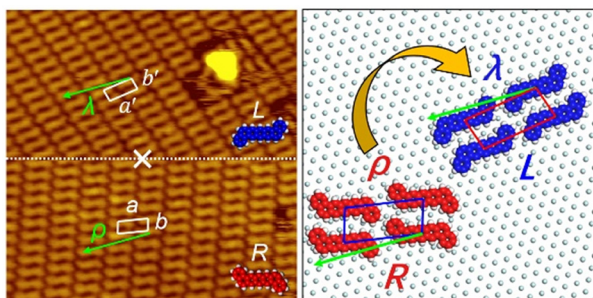
707

## Free energy barrier and thermal-quantum behavior of sliding bilayer graphene

Jean Paul Nery,\* Lorenzo Monacelli and Francesco Mauri\*



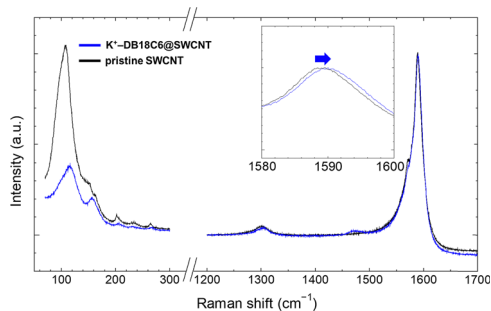
715



### Collective chirality flipping of dibenzopentacene molecules induced by an electric field

Li-Ting Yuan, Chen-Yu Hu, Ji-Yong Yang, Gang Yao, Ming-Long Tao, Kai Sun and Jun-Zhong Wang\*

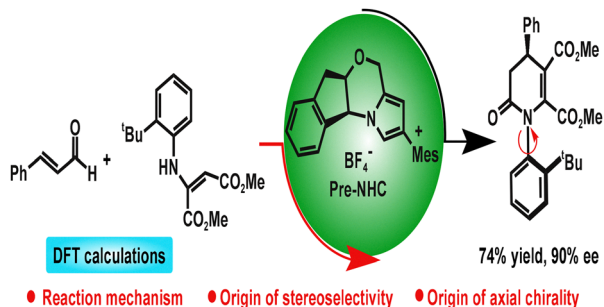
721



### Enhancement of oxygen reduction activity of iron phthalocyanine electrocatalyst supported on carbon nanotubes through molecular encapsulation

Tatsuya Akiyama,\* Yosuke Ishii\* and Shinji Kawasaki\*

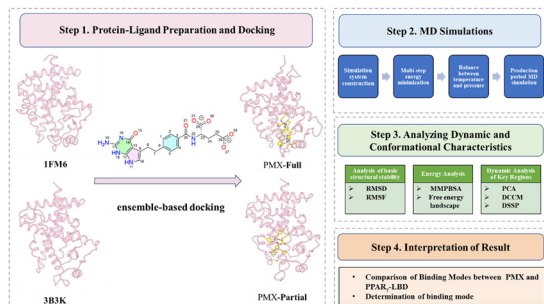
730



### Mechanisms and regio- and stereoselectivities in NHC-catalyzed [3+3] annulations for the synthesis of axially and centrally chiral dihydropyridinones

Yanlong Kang, Mingchao Zhang, Yan Li\* and Zhiqiang Zhang

742



### Molecular insight into pemetrexed as a partial agonist of PPAR $\gamma$ through molecular dynamics simulations

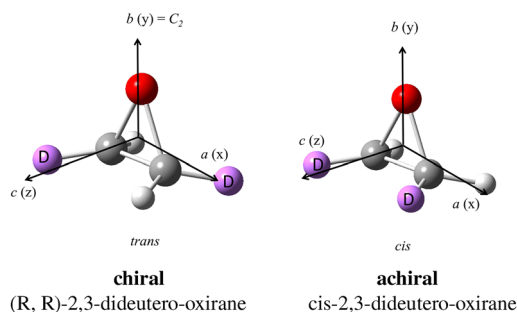
Yifan She, Jiasheng Zhao, Shunlin Ren, Lei Zhang, Shengli Zhang and Zhiwei Yang\*



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### Isotopic chirality and high-resolution gigahertz and terahertz spectroscopy of *trans*-2,3-dideutero-oxirane (*tc*-CHDCHDO)

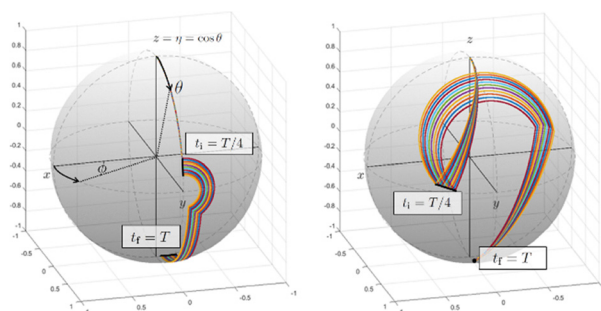
Ziqiu Chen,\* Sieghard Albert, Karen Keppler, Gunther Wichmann, Martin Quack,\* Volker Schurig and Oliver Trapp



764

### The robustness of composite pulses elucidated by classical mechanics: stability around the globe

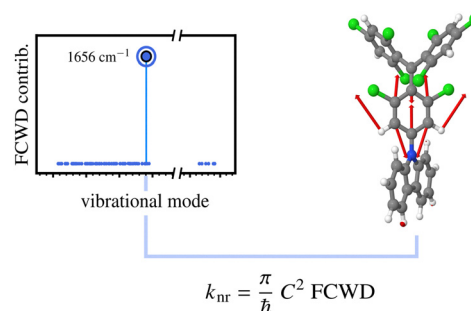
Jonathan Berkheim\* and David J. Tannor



776

### Dissecting non-radiative decay in donor-functionalized radicals with a mode-resolved model

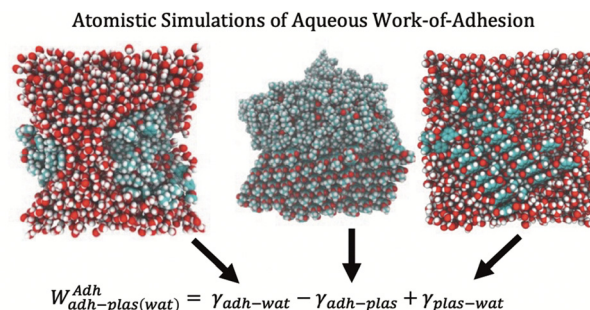
Robert Toews\* and Andreas Köhn



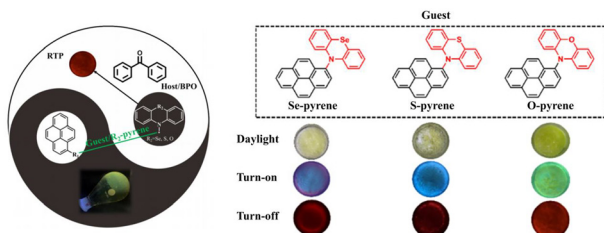
790

### Predicting polyacrylate–microplastic interactions with atomistic simulation

Timothy M. E. Jugovic, Henry E. Thurber, Michael T. Robo, Woojung Ji, Madeline E. Clough, Anne J. McNeil and Paul M. Zimmerman\*



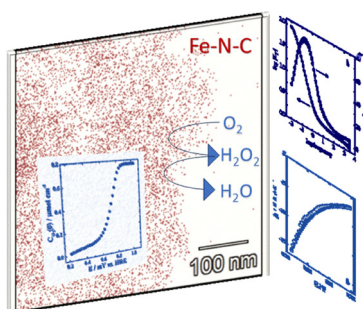
798



### Buchwald–Hartwig aminated pyrene-heterocycles with host–guest-enhanced NIR phosphorescence: DFT-guided design toward breast cancer imaging probes

Kaixuan Hu, Shufeng Chen, Xinmin Wang, Lingkai Tang, Yan Cheng, Yuting Song, Hubing Shi, Jing Jing, Jianping Hu\* and Ting Luo\*

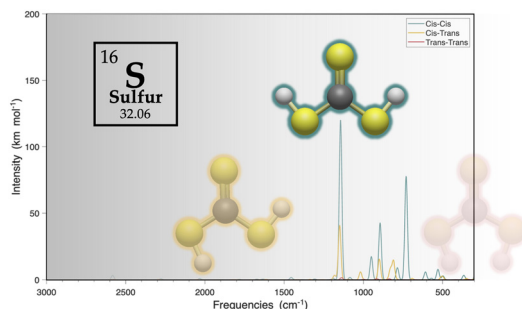
811



### Fe–N–C electrocatalysts derived from a 1,10-phenanthroline–iron complex: kinetic insights into the acidic oxygen reduction reaction

Matheus Martins, Bianca Tainá Ferreira, Carlos Sant'ana Vasconcellos, Nelson A. Galote, Fabio Henrique Barros Lima and Fritz Huguenin\*

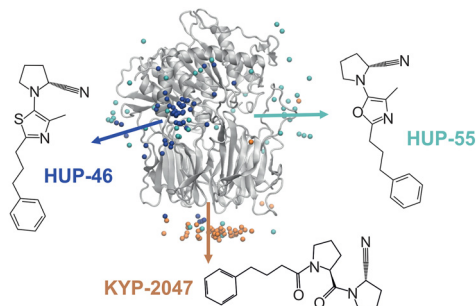
821



### Quantum chemical rovibrational spectroscopic data for possible observation of thiocarbonic acid (H<sub>2</sub>CS<sub>3</sub>) in interstellar environments

Megan McKissick and Ryan C. Fortenberry\*

829



### Decoding dissociation pathways of ligands in prolyl oligopeptidase

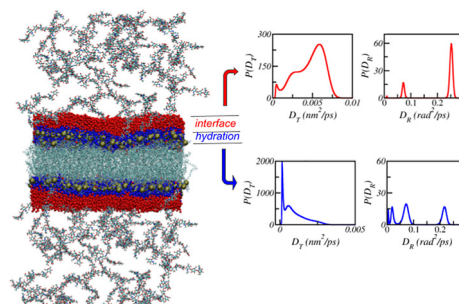
Katarzyna Walczewska-Szewc\* and Jakub Rydzewski



841

## Heterogeneous water dynamics in hyaluronan–DPPC interfaces

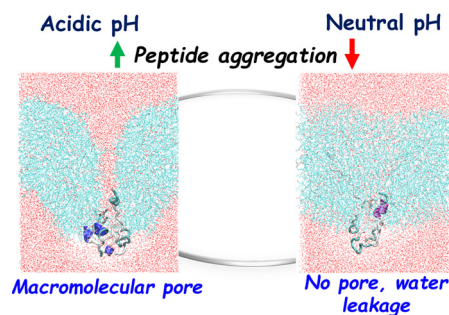
Anirban Paul\* and Jaydeb Chakrabarti\*



850

## pH-dependent peptide aggregation and translocation across octanol and hexane interfaces: insights from umbrella sampling simulations

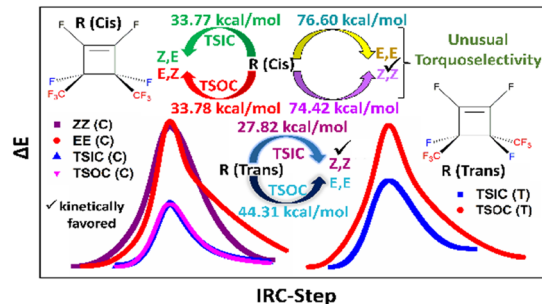
Anjana V. Mathath, Samrat Sarkar and Debashree Chakraborty\*



862

## Unraveling unusual torquoselectivity in ring-opening electrocyclic reactions: a DFT perspective

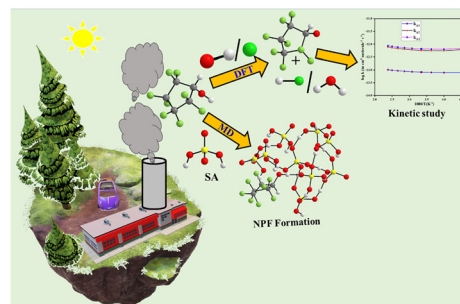
Arpita Poddar, Jesús Sánchez-Márquez, Alejandro Morales-Bayuelo\* and Pratim Kumar Chattaraj\*



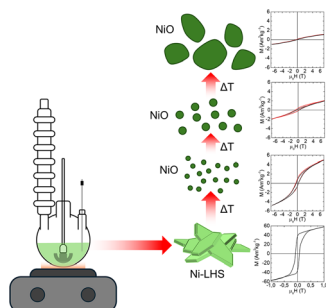
871

## A theoretical investigation on the mechanistic and kinetic study of 2,2,3,3,4,4,5,5-octafluorocyclopentanol with OH radicals and Cl atoms and its implications in new particle formation

Suresh Tiwari and Ranga Subramanian\*



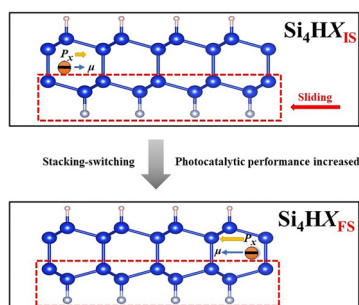
885



### Size-dependent magnetic properties of NiO nanoparticles synthesized *via* Ni-hydroxyacetate decomposition

Miran Baričić,\* Pierfrancesco Maltoni, Giulia Franceschin, Thomas Gaudisson, Sophie Nowak, Frederic Mazaleyrat, Davide Peddis and Souad Ammar\*

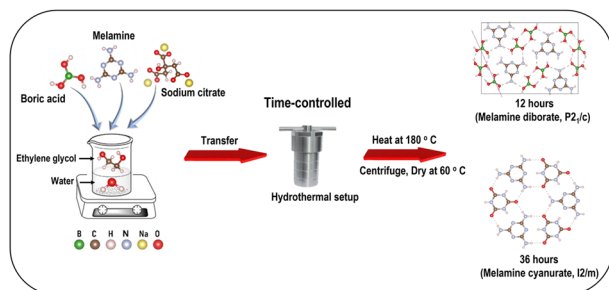
892



### Stacking-switching of silicon-based two-dimensional diamane structures to enhance photocatalytic water splitting performance

Min Tao, Chu-Chu Liu, Pan Ma, Xiao Shang, Hai-Bin Du, Xian-Yu Hu, Lu-Chao Du\* and Fu-Chun Liu\*

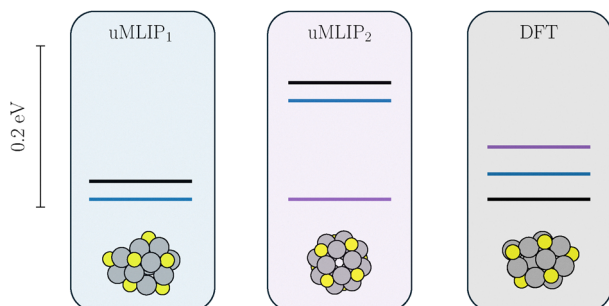
903



### Time-dependent solvothermal synthesis of melamine cyanurate and melamine diborate: experimental and theoretical insights

Atika, Zihan Zhang, Klaus Leifer, Jöns Hilborn, Dan Li, Jiefang Zhu, Rajeev Ahuja and Wei Luo\*

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### Active $\Delta$ -learning with universal potentials for global structure optimization

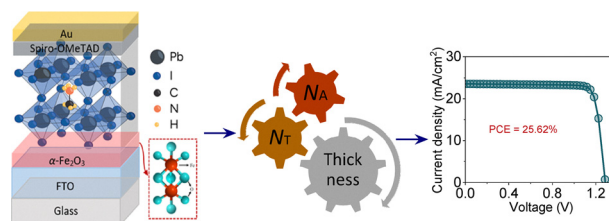
Joe Pitfield, Mads-Peter Verner Christiansen and Bjørk Hammer



927

### High-performance hematite-integrated perovskite solar cells

Mustafa Kareem,\* Ethar Yahya Salih, Malatesh Akkur, Satish Kumar Samal, Sridharan Sundharam and Sanjeev Kumar

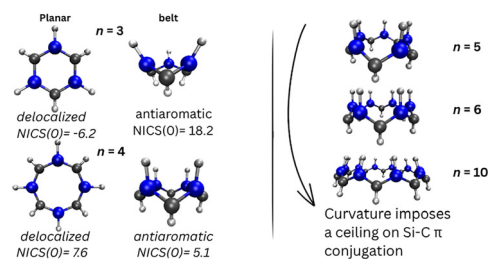


938

### Theoretical study of Si/C alternately substituted annulenes with a belt structure

Takako Kudo,\* Katherine N. Ferreras, Tajji Nakamura, Akira Imanishi, Ryuta Ikutomo and Mark S. Gordon\*

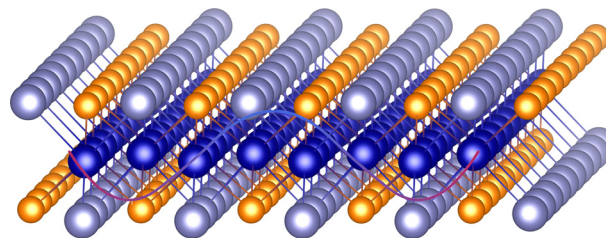
#### Curvature Driven $\pi$ Localization in Belt-Shaped Alternating Si/C Annulenes, $H_{2n}Si_nC_n$



953

### Strain-selected magnetic ordering in $1T'\alpha$ -CrXY (X, Y = S, Se, Te) monolayers

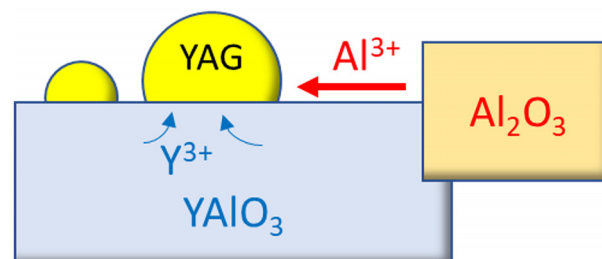
Deju Zhang and Yanning Zhang\*



960

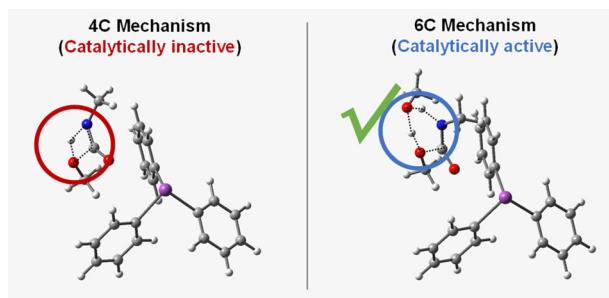
### A TMA and DSC study of the kinetics of the solid-state reaction in an $Al_2O_3$ - $Y_2O_3$ system

Nathan Kerkad, Loïck Bonnet, Loïc Favergeon, Alexandre Maître and Rémy Boulesteix\*



## RESEARCH PAPERS

969



### The catalytic role of triphenyl bismuth in curing reactions: a theoretical study

Bowen Zhang, Lu Gem Gao, Peng Guo, Ruiqing Lei, Pengchao Zhang, Xuefei Li\* and Xuefei Xu\*

## CORRECTIONS

977

### Correction: Electrolyte clusters as hydrogen sponges: diffusion Monte Carlo simulations

A. R. Zane and E. Curotto\*

978

### Correction: High-temperature and solid-state NMR investigation of the structural evolution and special phase transition in LiF–NaF–BeF<sub>2</sub> mixed salts

Jianchao Sun, Hailong Huang, Ling Han, Xiaobin Fu,\* Hongtao Liu\* and Yuan Qian\*

979

### Correction: Excited state dipole moments from $\Delta$ SCF: a benchmark

Lukas Paetow and Johannes Neugebauer\*



## CORRECTIONS

980

**Correction: Theoretical study of large-scale graphene on the Cu(111) surface using machine learning potential**

Jingli Han, Rubén Cabello, Jordi Bonet Ruiz, Alexandra Elena Plesu Popescu, Sergi Dosta Parras,\* Camila Barreneche and Yongpeng Yang\*

981

**Correction: Triggered release kinetics of living cells from composite microcapsules**

Shwan Abdullah Hamad, Simeon D. Stoyanov and Vesselin N. Paunov\*

