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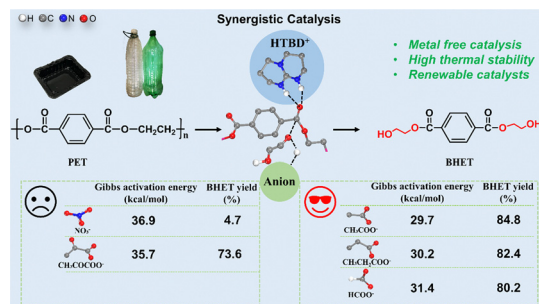


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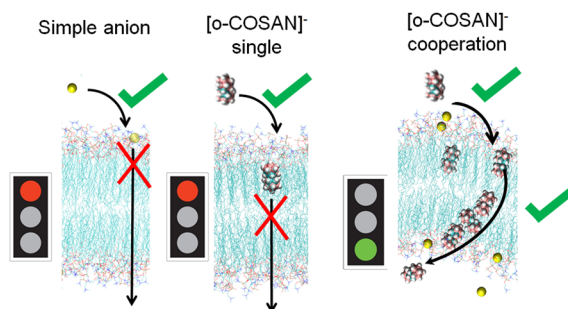
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How a few help all: cooperative crossing of lipid membranes by COSAN anions

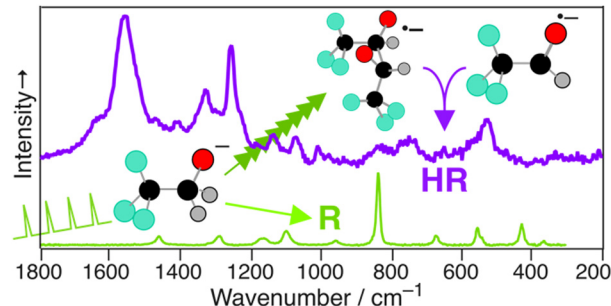
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Origin of unique hyper-Raman signals of trifluoroethanol

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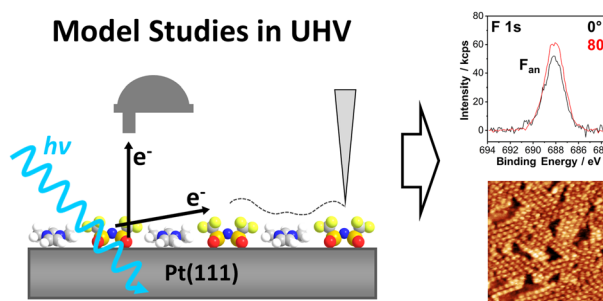


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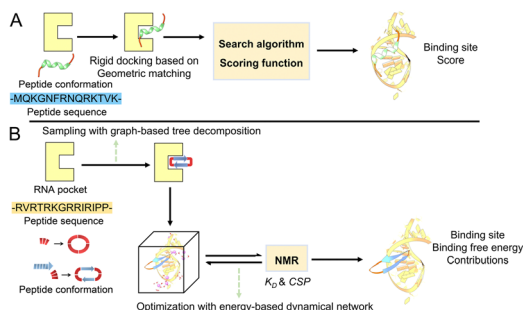
Adsorption and thermal evolution of [C₁C₁Im][Tf₂N] on Pt(111)

Stephen Massicot, Afra Gezmis, Timo Talwar, Manuel Meusel, Simon Jaekel, Rajan Adhikari, Leonhard Winter, Cynthia C. Fernández, Andreas Bayer, Florian Maier and Hans-Peter Steinrück*



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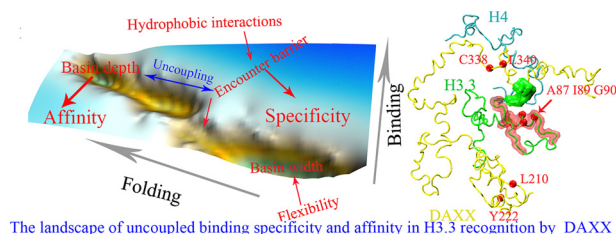
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Dynamic geometry design of cyclic peptide architectures for RNA structure

Shangbo Ning, Min Sun, Xu Dong, Anbang Li, Chen Zeng, Maili Liu, Zhou Gong* and Yunjie Zhao*

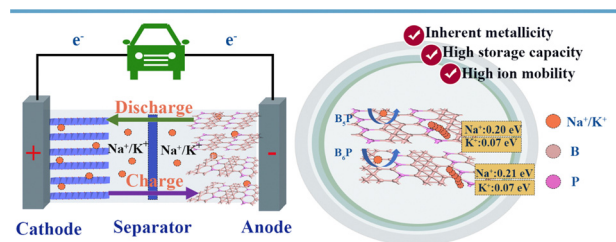
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Energy landscape quantifications of histone H3.3 recognition by chaperone DAXX reveal an uncoupled binding specificity and affinity

Fei Liu, Jin Wang,* Rui-Ming Xu* and Na Yang*

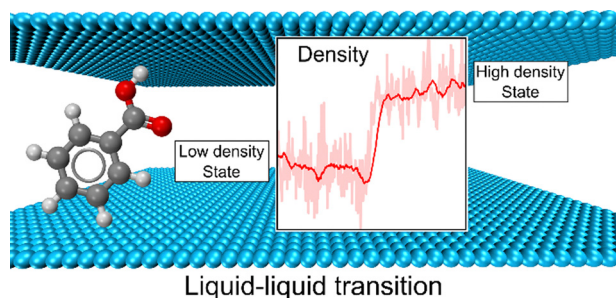
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Fang Liu, Xianfei Chen,* Yi Huang,* Chaozhu Shu, Na Li, Beibei Xiao and Lianli Wang

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Molecular dynamics investigation of benzoic acid in confined spaces

Luca Sironi, Giovanni Macetti and Leonardo Lo Presti*

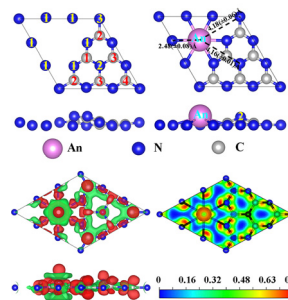


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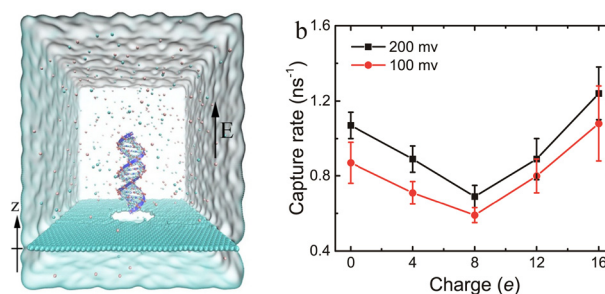
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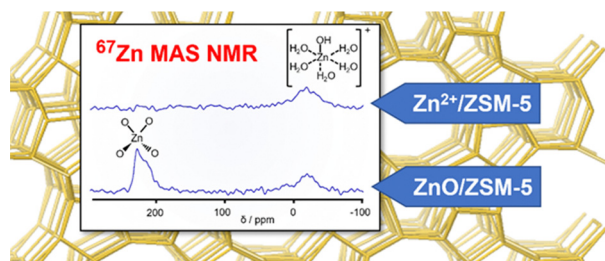
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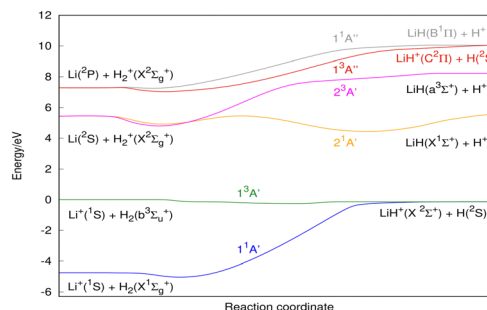
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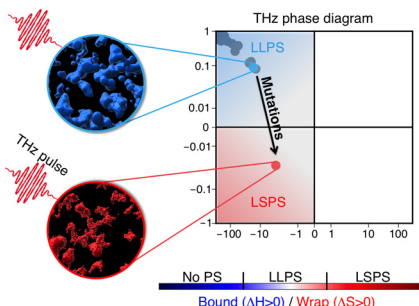
Potential energy surfaces for singlet and triplet states of the LiH₂⁺ system and quasi-classical trajectory cross sections for H + LiH⁺ and H⁺ + LiH

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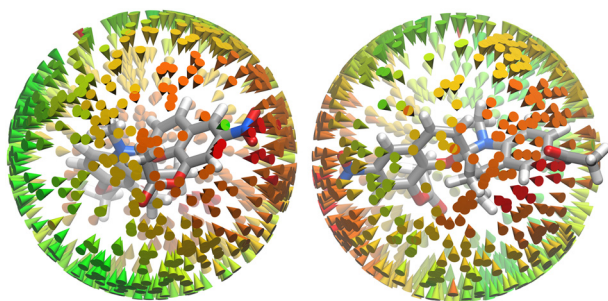
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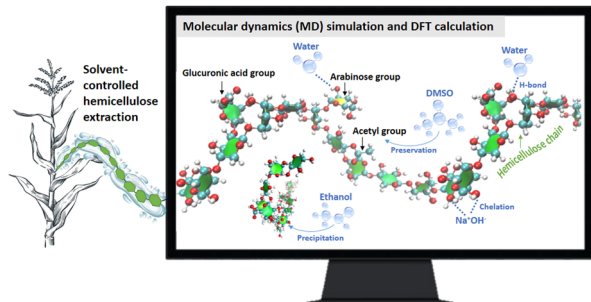
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Using oriented external electric fields to manipulate rupture forces of mechanophores

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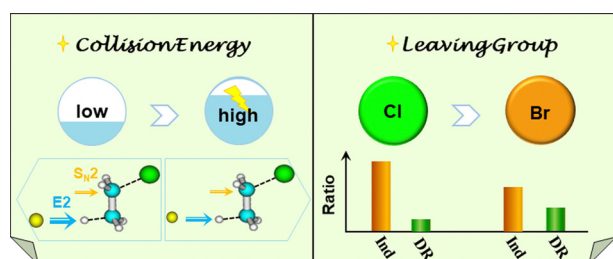
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Competitive dynamics of E2 and S_N2 reaction driven by collision energy and leaving group

Siwei Zhao, Gang Fu, Wenqing Zhen, Hongyi Wang, Li Yang* and Jiaxu Zhang*

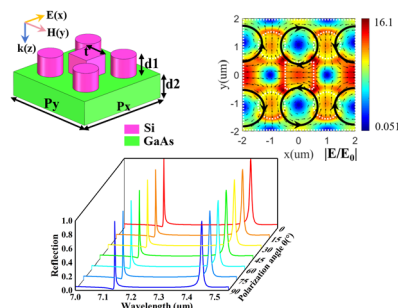


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An all-dielectric metasurface based on Fano resonance with tunable dual-peak insensitive polarization for high-performance refractive index sensing

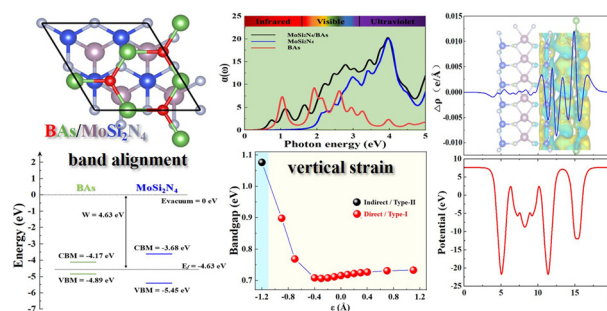
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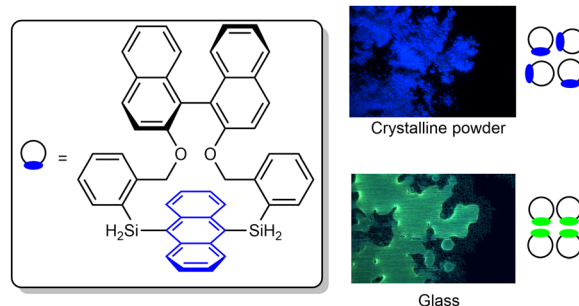
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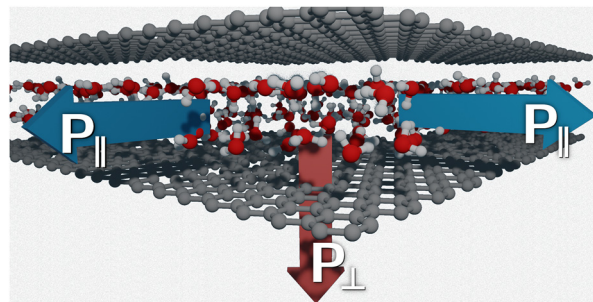
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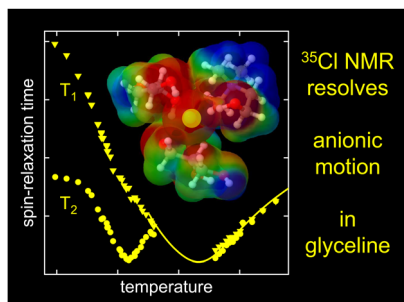
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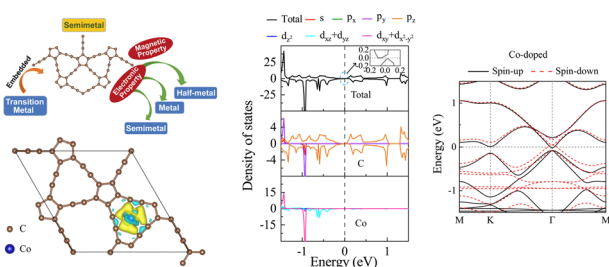
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Anion dynamics and motional decoupling in a glycerol–choline chloride deep eutectic solvent studied by one- and two-dimensional ^{35}Cl NMR

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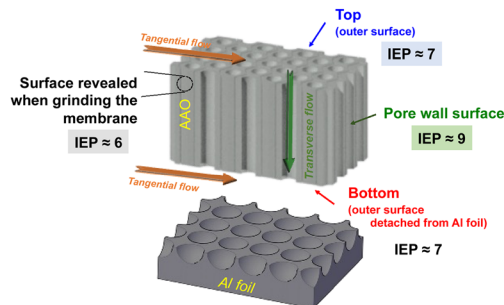
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Transition in electronic and magnetic properties of transition metal embedded semimetallic B-graphyne

Han-Bing Li, Zhi-Gang Shao,* Cang-Long Wang* and Lei Yang

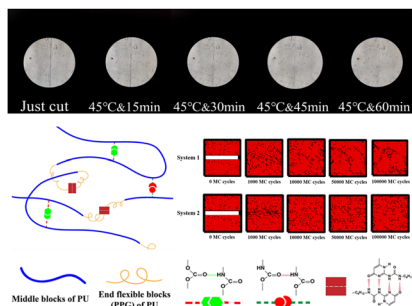
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Electrical surface properties of nanoporous alumina membranes: influence of nanochannels' curvature, roughness and composition studied via electrokinetic experiments

Ali Vakilinejad, Emmanuelle Dubois, Laurent Michot, Marie Jardat, Didier Lairez, Serge Durand-Vidal, Clément Guibert and Nicolas Jouault*

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Combing experimental methods and molecular simulations to study self-healing behaviors of polyurethane elastomers containing multiple hydrogen bond networks and flexible blocks

Jianlong Wen, Guangwei Xu, Zhaopeng Liang, Sumin Li, Yinmao Wang, Juan Yang and Yijing Nie*

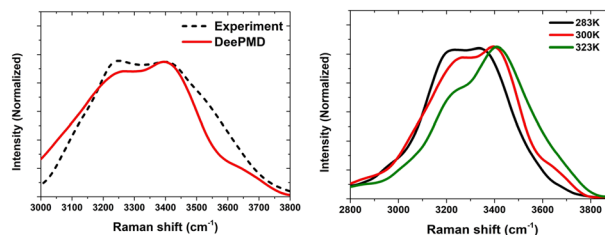


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Simulating the isotropic Raman spectra of O–H stretching mode in liquid H₂O based on a machine learning potential: the influence of vibrational couplings

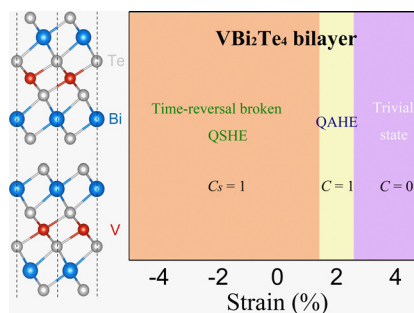
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Strain-tunable magnetism and topological states in layered VBi₂Te₄

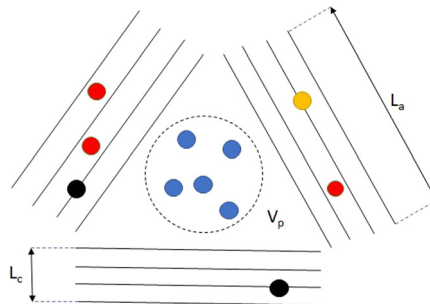
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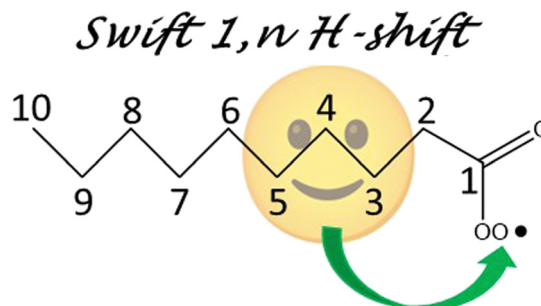
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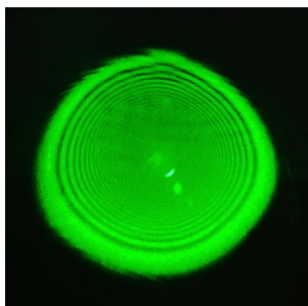
A systematic study on the kinetics of H-shift reactions in pristine acyl peroxy radicals

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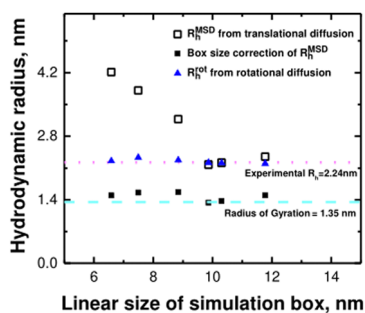
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Mechanism of optical limiting in metalloporphyrins under visible continuous radiation

Qian Zhang, Bishuai Lu, Shan Liu, Xiangfei Lü* and Xuemei Cheng*

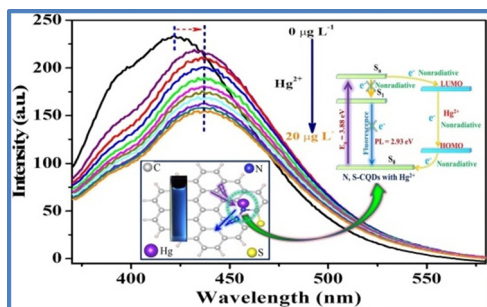
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Hydrodynamic radius of dendrimers in solvents

Naira R. Khusnutdinova and Denis A. Markelov*

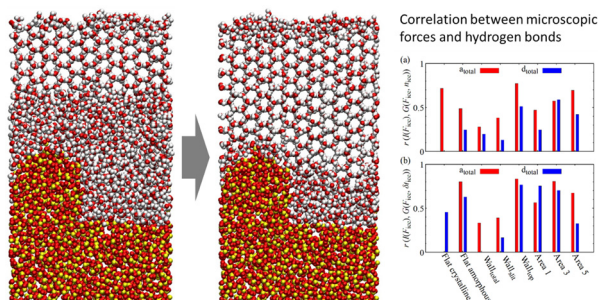
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N- and S-codoped carbon quantum dots for enhancing fluorescence sensing of trace Hg²⁺

Yujie Wang, Guoliang Xu,* Xinghe Zhang,* Xiaona Yang, Hongbo Hou, Wei Ai and Liju Zhao

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Microscopic properties of forces from ice solidification interface acting on silica surfaces based on molecular dynamics simulations

Shota Uchida,* Kunio Fujiwara and Masahiko Shibahara

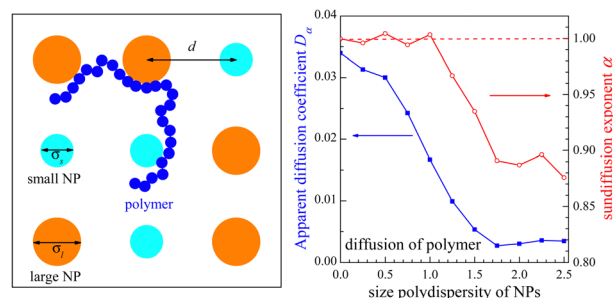


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Simulation study on the effect of polydisperse nanoparticles on polymer diffusion in crowded environments

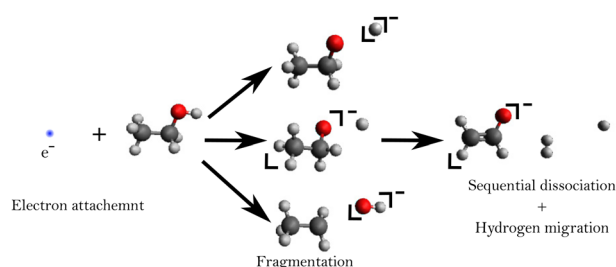
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Fragmentation dynamics and absolute dissociative electron attachment cross sections in the low energy electron collision with ethanol

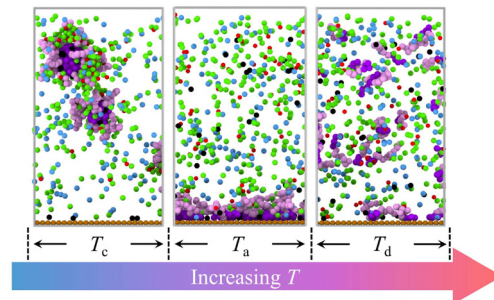
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Effects of temperature on microstructures of MSA-type electroplating solution: a coarse-grained molecular dynamics simulation

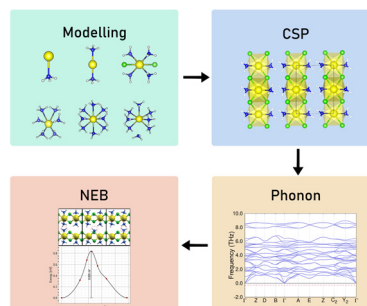
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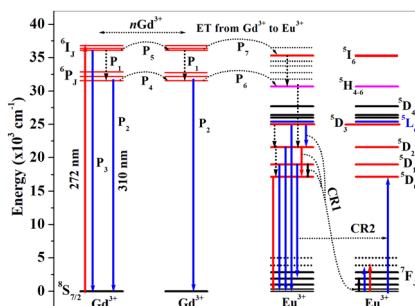
Stable and metastable crystal structures and ammonia dynamics in strontium chloride ammines

Samet Demir, Gözde İnış Demir, Mehmet Çankaya and Adem Tekin*



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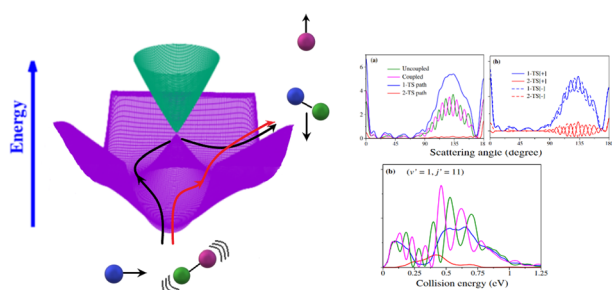
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NaGdF₄:Eu³⁺ nanocrystalline: an in-depth study of energy transfer processes and Judd–Ofelt analysis using the luminescence excitation spectrum

Phan Van Do,* Nguyen Xuan Ca, Luong Duy Thanh, Dang Dinh Quan, Nguyen Manh Hung, Pham Tien Du, Nguyen Thi Huong and Doan Tuan Anh

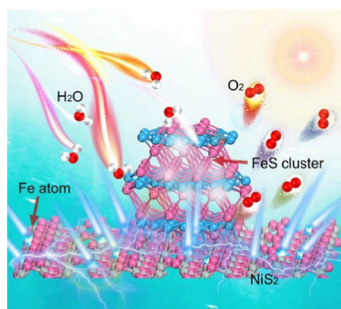
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Electronic nonadiabatic effects in the state-to-state dynamics of the H + H₂ → H₂ + H exchange reaction with a vibrationally excited reagent

Jayakrushna Sahoo and S. Mahapatra*

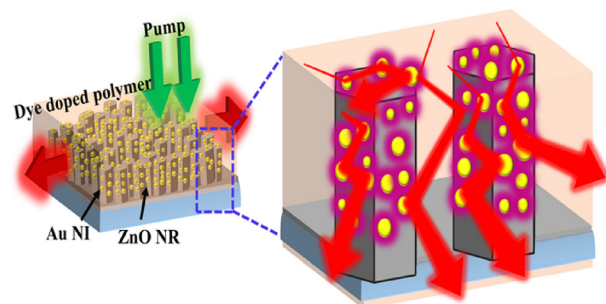
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Insight into the Fe atom–FeS cluster synergistic catalysis mechanism for the oxygen evolution reaction in NiS₂-based electrocatalysts

Changhong Zhang, Lulu Zhang, Kun Meng,* Yongqiang Yang,* Chengyi Hou, Sen Ming, Ju Rong, Wei Yan, Yannan Zhang and Xiaohua Yu

28336



Synergy between plasmonic nanocavities and random lasing modes: a tool to dequench plasmon quenched fluorophore emission

Renu Yadav, Sourabh Pal, Subhajit Jana, Shuvajit Roy, Kapil Debnath, Samit K. Ray, Maruthi M. Brundavanam and Shivakiran Bhaktha B. N.*

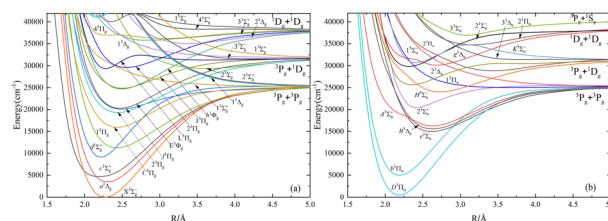


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28350

Theoretical study of the spectroscopy and radiative transition probabilities of Si₂ from visible to infrared

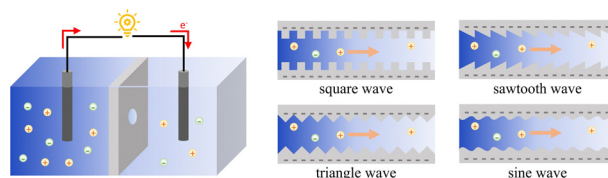
Lidan Xiao, Yun Yang, Xinyu Li, Boris F. Minaev* and Bing Yan*



28363

Enhancing the performance of a cylindrical nanopore in osmotic power generation through designing the waveform of its inner surface

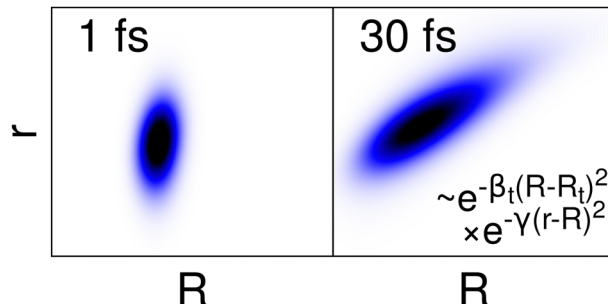
Chung-Wei Liu* and Jyh-Ping Hsu



28373

Differential Shannon entropies and correlation measures for Born–Oppenheimer electron–nuclear dynamics: numerical results and their analytical interpretation

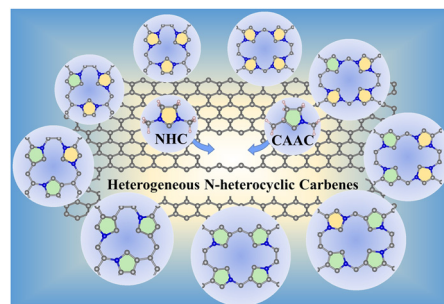
Peter Schürger and Volker Engel*



28382

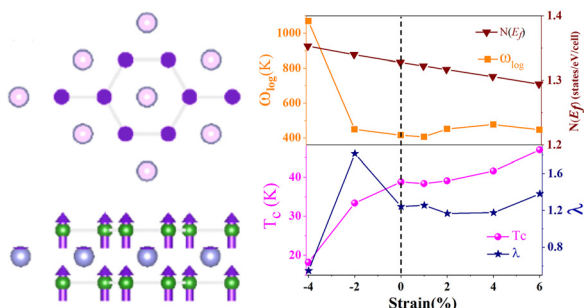
The effective regulation of heterogeneous N-heterocyclic carbenes: structures, electronic properties and transition metal adsorption

Wei Liu,* Jingchao Sun, Yunhao Xie, Liang Chen and Jing Xu*



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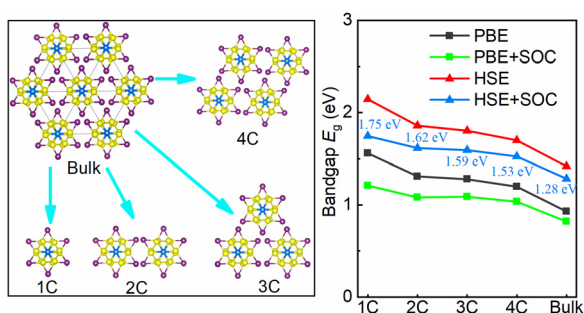
28393



Prediction of superconductivity in sandwich XB_4 ($\text{X} = \text{Li}, \text{Be}, \text{Zn}$ and Ga) films

Shuming Zeng,* Yinchang Zhao, Muhammad Zulfiqar* and Geng Li*

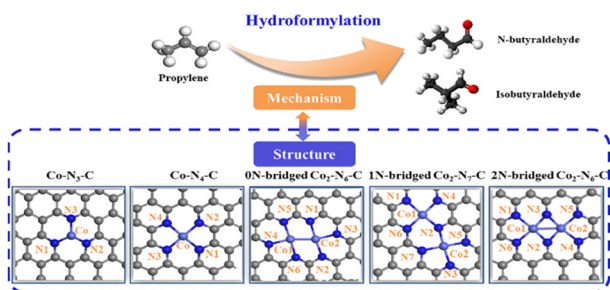
28402



Strong spin–orbital coupling induced tunable electronic structures and enhanced visible-light absorption in one-dimensional RhTe_6I_3 systems

Wenjiang Gao, Meiyang Yu, Bing Wang* and Huabing Yin*

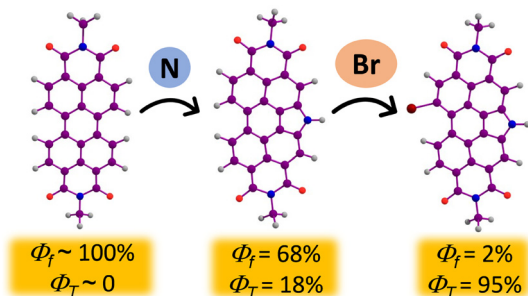
28412



Theoretical insights into the catalytic mechanism of propylene hydroformylation over Co–N–C materials

Yifei Chen, Yanan Zhu, Huaqiang Dou and Hao Gong*

28428



Unveiling the intersystem crossing dynamics in N-annulated perylene bisimides

Jeswin Sunny, Ebin Sebastian, Suvarna Sujilkumar, Frank Würthner, Bernd Engels* and Mahesh Hariharan*

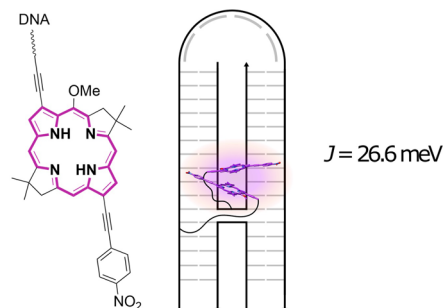


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28437

Exciton delocalization in a fully synthetic DNA-templated bacteriochlorin dimer

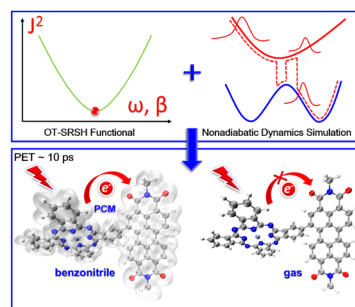
Olga A. Mass,* Devan R. Watt, Lance K. Patten, Ryan D. Pensack, Jeunghoon Lee, Daniel B. Turner, Bernard Yurke and William B. Knowlton



28452

Solvent effects on the photoinduced charge separation dynamics of directly linked zinc phthalocyanine-perylenediimide dyads: a nonadiabatic dynamics simulation with an optimally tuned screened range-separated hybrid functional

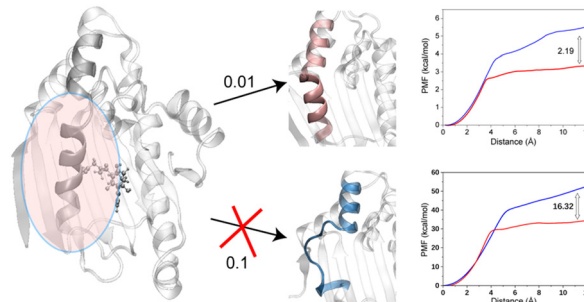
Shuai Liu, Sha-Sha Liu, Xiao-Mei Tang, Xiang-Yang Liu,* Jia-Jia Yang,* Ganglong Cui and Laicai Li*



28465

Simulation of the ligand-leaving process of the human heat shock protein

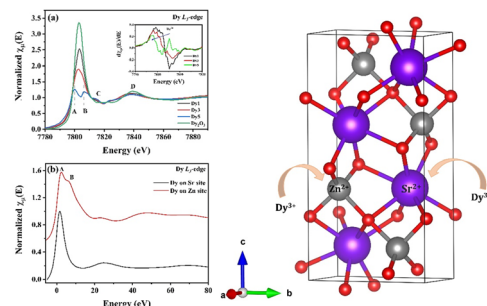
Yi-Xiao Hu, Jun-wen Fei, Li-Hua Bie* and Jun Gao*



28473

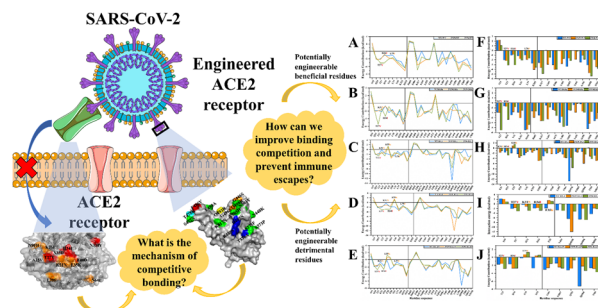
Dysprosium site occupancy in SrZnO₂ nanophosphors probed through XANES

Manju, Parasmani Rajput,* Ankush Vij and Anup Thakur*



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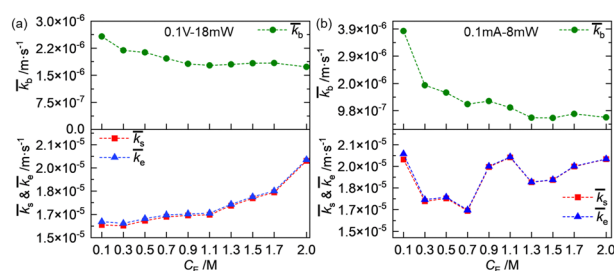
28479



Molecular insights and optimization strategies for the competitive binding of engineered ACE2 proteins: a multiple replica molecular dynamics study

Jiahao Sun, Xinguo Liu,* Shaolong Zhang, Meng Li, Qinggang Zhang and Jianzhong Chen*

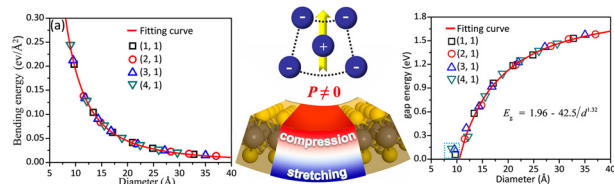
28497



Growth characteristics and the mass transfer mechanism of single bubble on a photoelectrode at different electrolyte concentrations

Mengsha Wang, Qiang Xu,* Tengfei Nie, Xinyi Luo, Yonglu She and Liejin Guo*

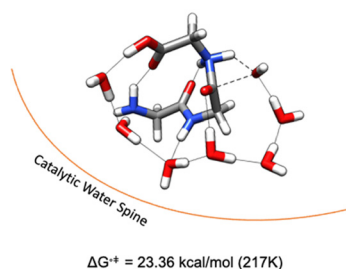
28510



Chirality dependent electromechanical properties of single-layer MoS₂ under out-of-plane deformation: a DFT study

Faling Ling,* Yi Ling, Xiaoqing Liu, Li Li, Xianju Zhou, Xiao Tang, Chuan Jing, Yongjie Wang, Sha Jiang and Yi Lu

28517



Prebiotic dimer and trimer peptide formation in gas-phase atmospheric nanoclusters of water

Shannon E. Harold, Skyler L. Warf and George C. Shields*



28533

Solar driven CO₂ hydrogenation to HCOOH on (TiO₂)_n (*n* = 1–6) atomic clusters

Jiaqi Tian, Lei Hou, Weizhi Xia, Zi Wang, Yusong Tu, Wei Pei,* Si Zhou and Jijun Zhao

