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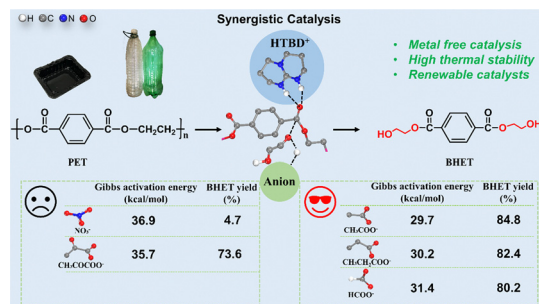


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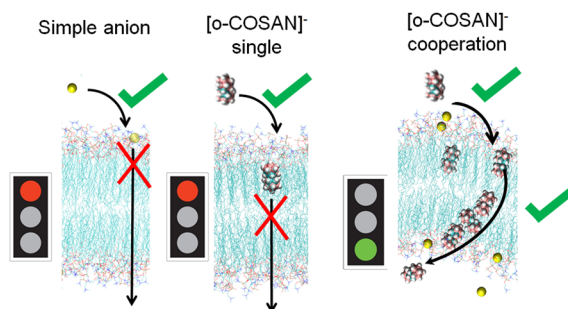
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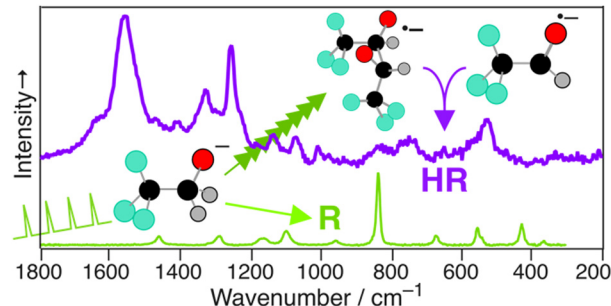
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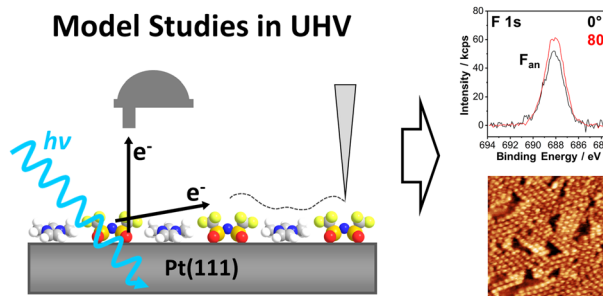


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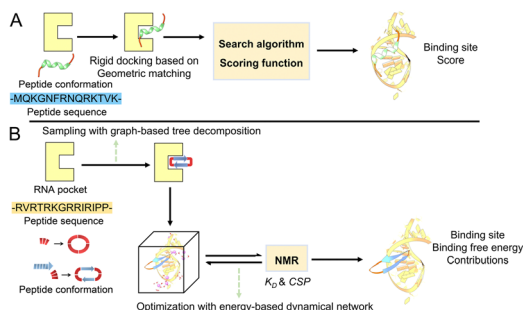
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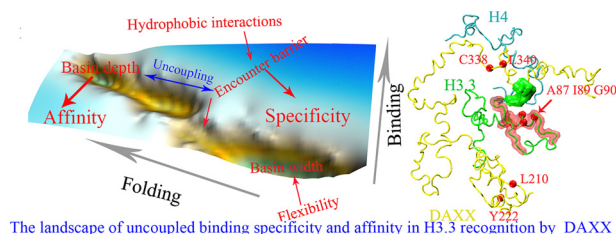
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Dynamic geometry design of cyclic peptide architectures for RNA structure

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

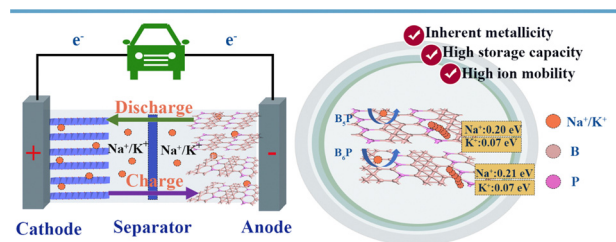
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Energy landscape quantifications of histone H3.3 recognition by chaperone DAXX reveal an uncoupled binding specificity and affinity

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

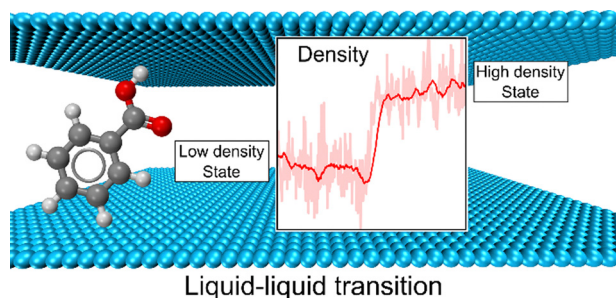
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Fang Liu, Xianfei Chen,* Yi Huang,* Chaozhu Shu, Na Li, Beibei Xiao and Lianli Wang

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Luca Sironi, Giovanni Macetti and Leonardo Lo Presti*

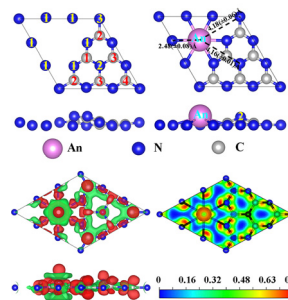


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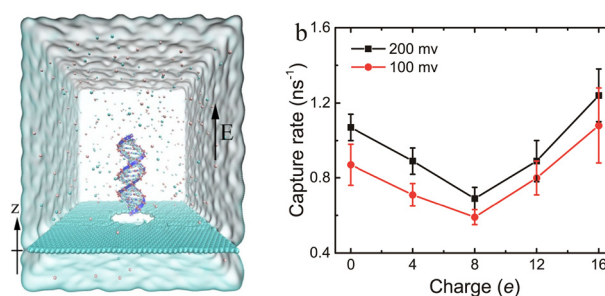
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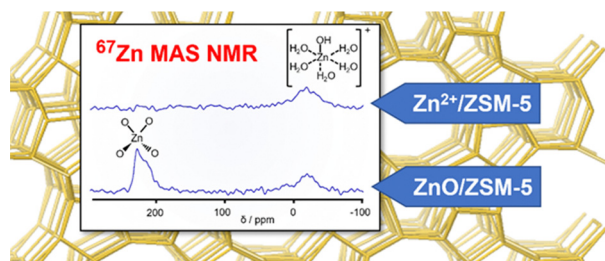
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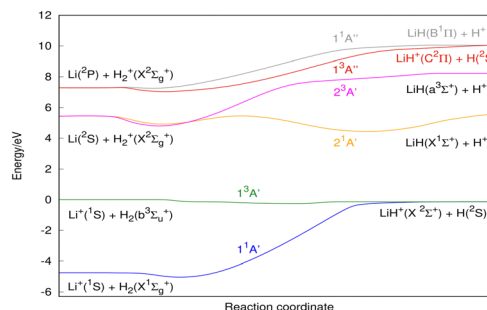
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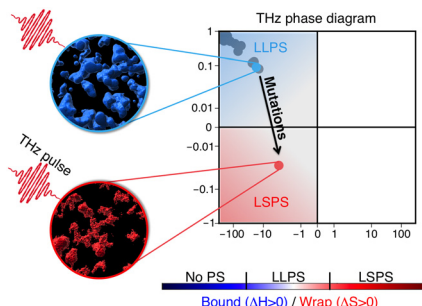
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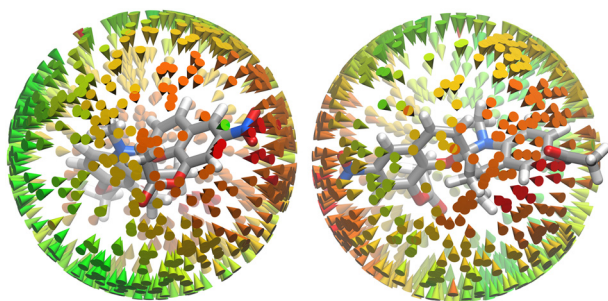
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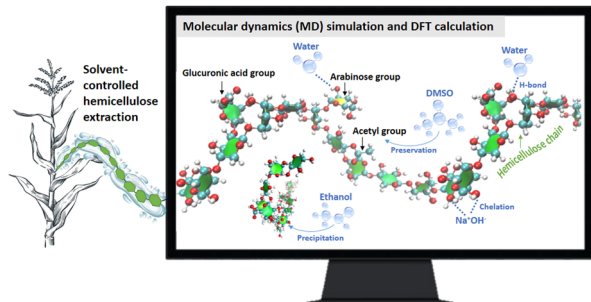
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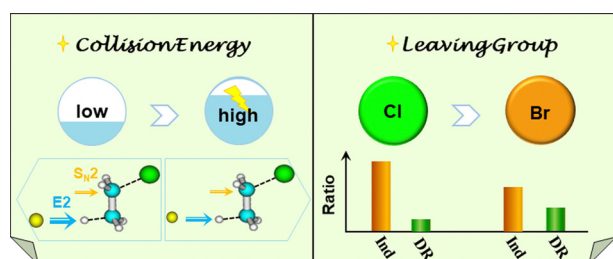
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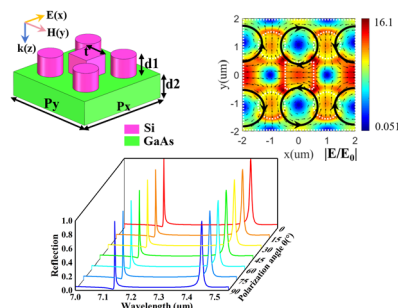


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An all-dielectric metasurface based on Fano resonance with tunable dual-peak insensitive polarization for high-performance refractive index sensing

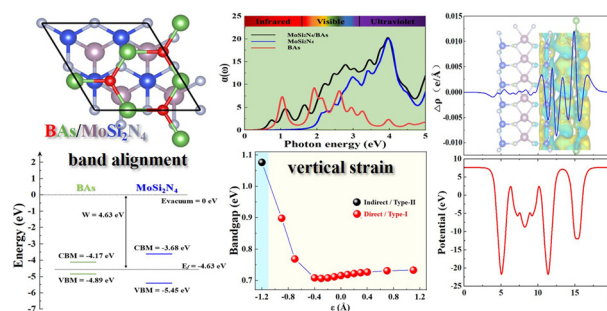
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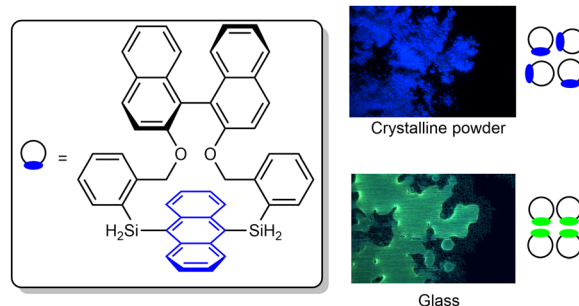
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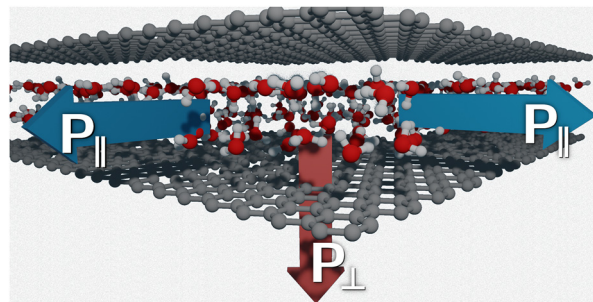
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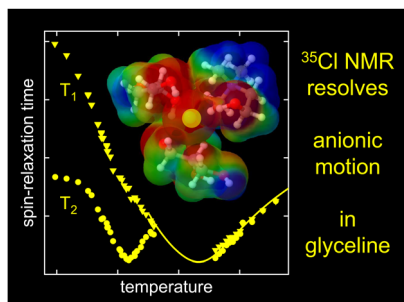
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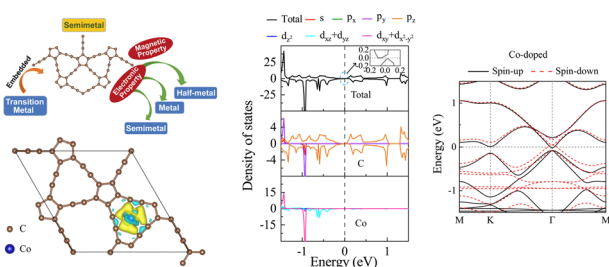
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Anion dynamics and motional decoupling in a glycerol–choline chloride deep eutectic solvent studied by one- and two-dimensional ^{35}Cl NMR

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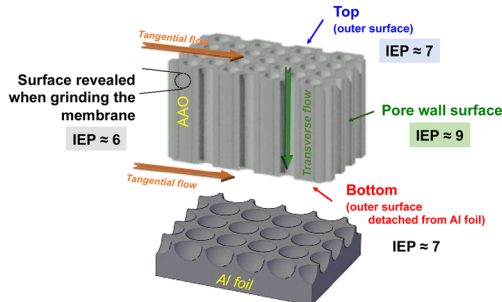
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Transition in electronic and magnetic properties of transition metal embedded semimetallic B-graphyne

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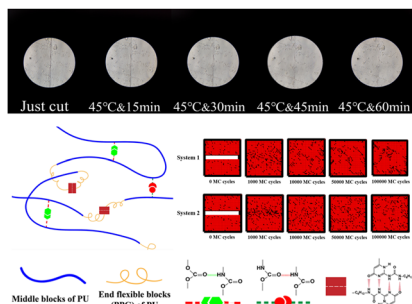
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Ali Vakilinejad, Emmanuelle Dubois, Laurent Michot, Marie Jardat, Didier Lairez, Serge Durand-Vidal, Clément Guibert and Nicolas Jouault*

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

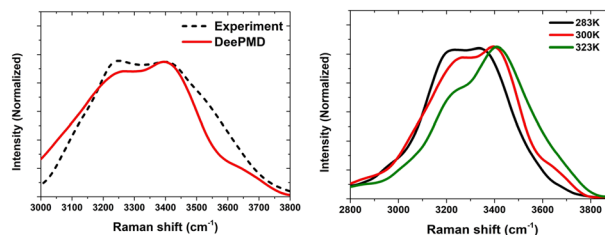


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Simulating the isotropic Raman spectra of O–H stretching mode in liquid H₂O based on a machine learning potential: the influence of vibrational couplings

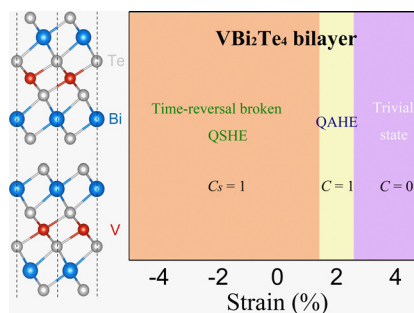
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Strain-tunable magnetism and topological states in layered VBi₂Te₄

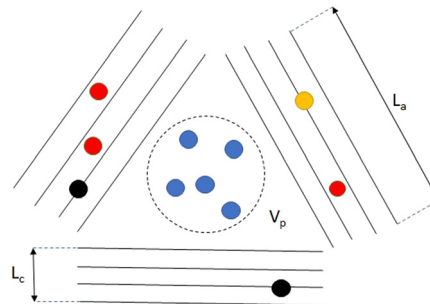
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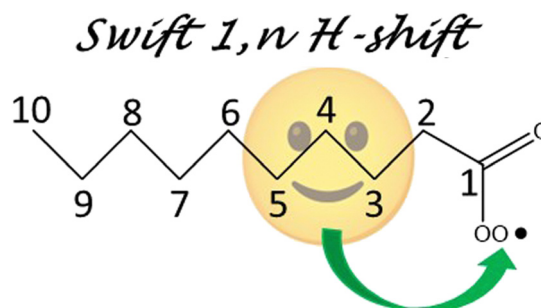
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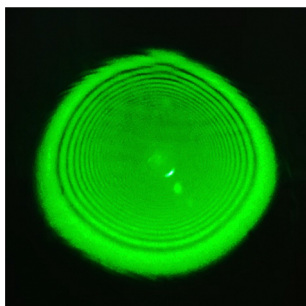
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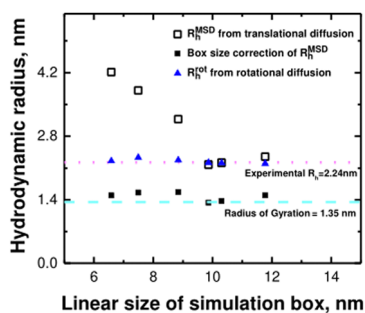
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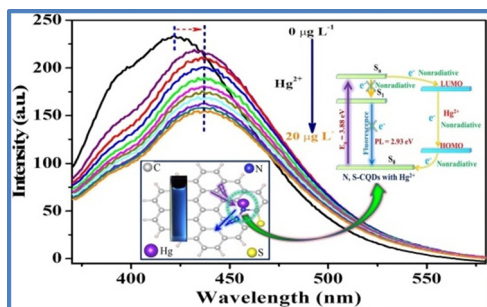
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Hydrodynamic radius of dendrimers in solvents

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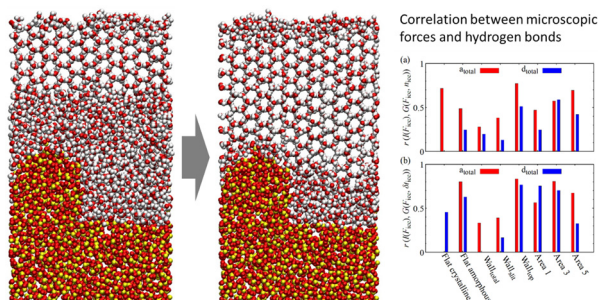
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N- and S-codoped carbon quantum dots for enhancing fluorescence sensing of trace Hg^{2+}

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

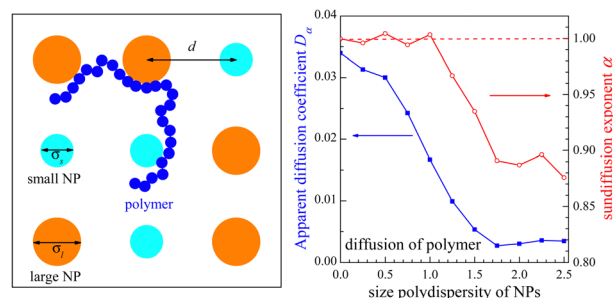


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Simulation study on the effect of polydisperse nanoparticles on polymer diffusion in crowded environments

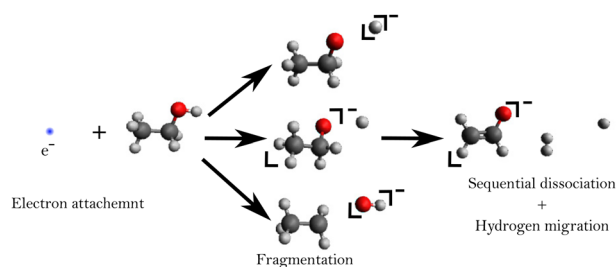
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Fragmentation dynamics and absolute dissociative electron attachment cross sections in the low energy electron collision with ethanol

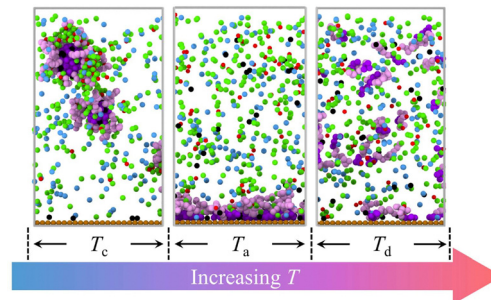
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Effects of temperature on microstructures of MSA-type electroplating solution: a coarse-grained molecular dynamics simulation

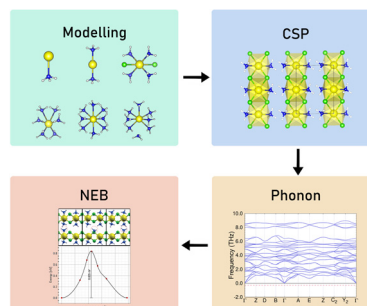
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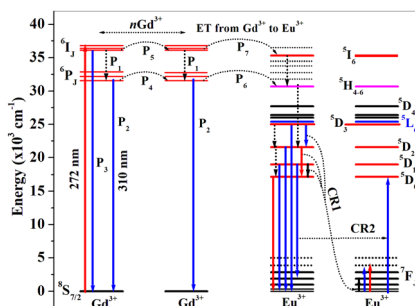


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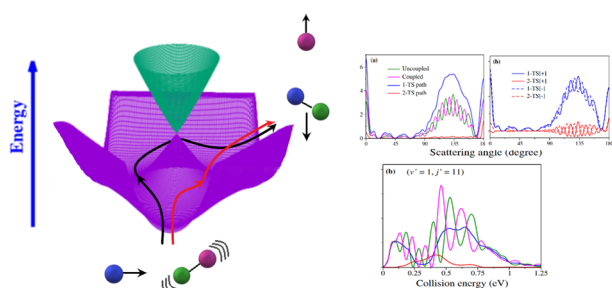
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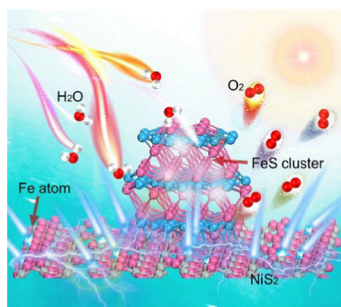
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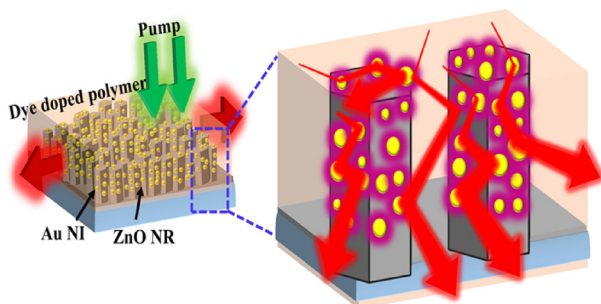
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Kapil Debnath, Samit K. Ray, Maruthi M. Brundavanam
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Theoretical study of the spectroscopy and radiative transition probabilities of Si₂ from visible to infrared

Figure 1 consists of two panels, (a) and (b), showing potential energy curves for the $D + D_2$ reaction. The y-axis represents Energy in cm^{-1} , ranging from 0 to 4000. The x-axis represents the internuclear distance $R/\text{\AA}$, ranging from 1.5 to 5.0. Panel (a) shows curves for $D_2 + D$ (black), $D + D_2$ (red), $D_2 + D$ (blue), and $D + D_2$ (green). Panel (b) shows curves for $D_2 + D$ (black), $D + D_2$ (red), $D_2 + D$ (blue), and $D + D_2$ (green). The curves show the energy levels of the reactants and products, with arrows indicating the reaction path.

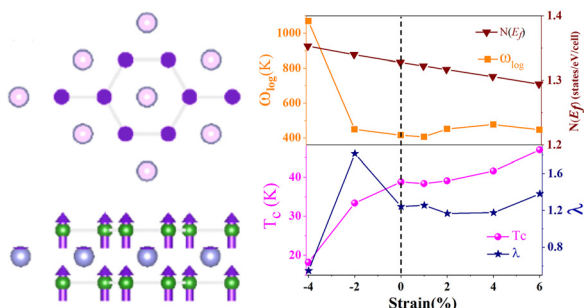
Enhancing the performance of a cylindrical nanopore in osmotic power generation through designing the waveform of its inner surface

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

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

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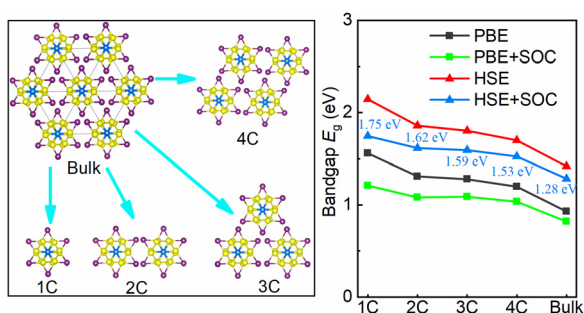
28393



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

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

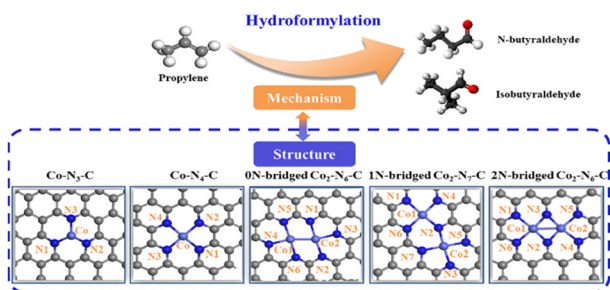
28402



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*

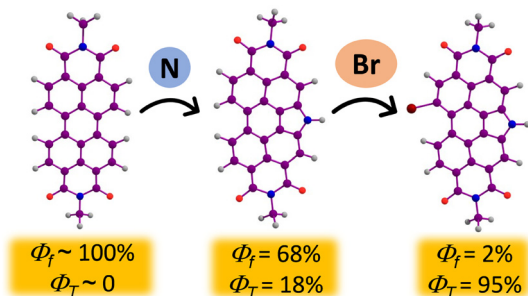
28412



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*

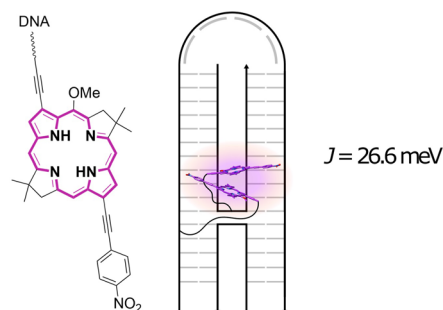


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28437

Exciton delocalization in a fully synthetic DNA-templated bacteriochlorin dimer

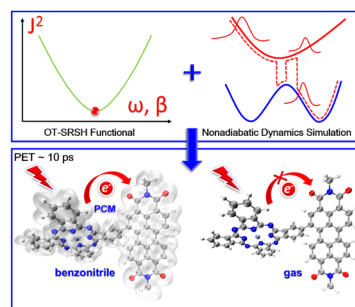
Olga A. Mass,* Devan R. Watt, Lance K. Patten, Ryan D. Pensack, Jeunghoon Lee, Daniel B. Turner, Bernard Yurke and William B. Knowlton



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

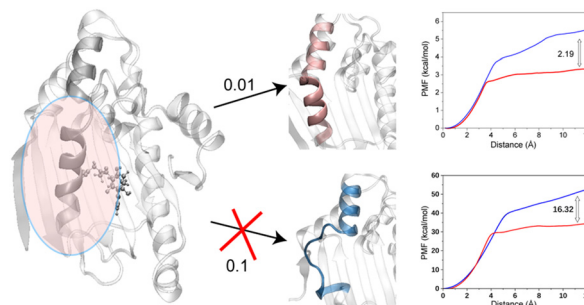
Shuai Liu, Sha-Sha Liu, Xiao-Mei Tang, Xiang-Yang Liu,* Jia-Jia Yang,* Ganglong Cui and Laicai Li*



28465

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

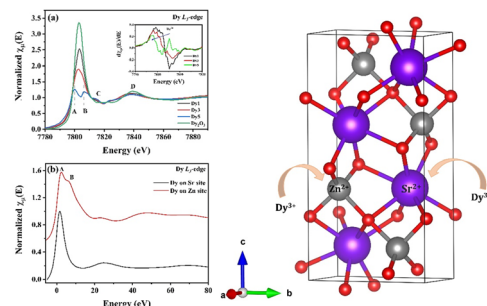
Yi-Xiao Hu, Jun-wen Fei, Li-Hua Bie* and Jun Gao*



28473

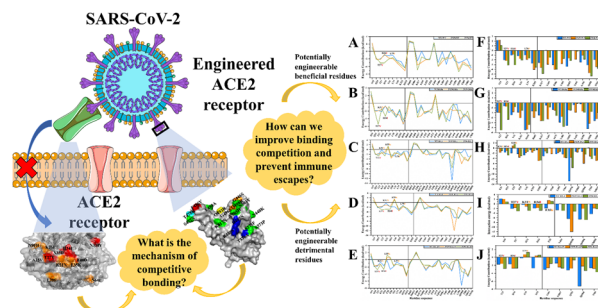
Dysprosium site occupancy in SrZnO₂ nanophosphors probed through XANES

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



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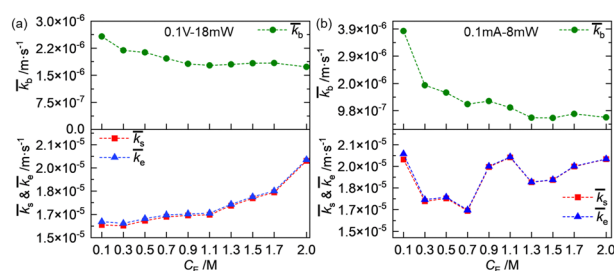
28479



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*

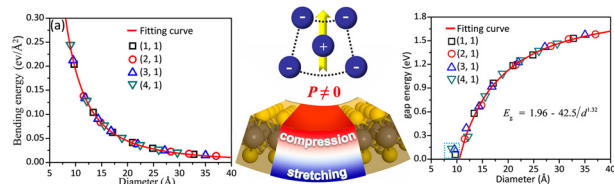
28497



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*

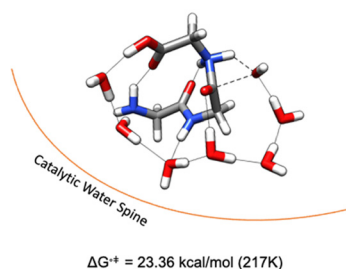
28510



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

