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Inside cover
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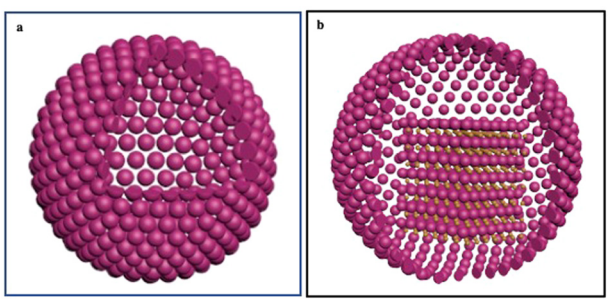
EDITORIAL

PERSPECTIVE



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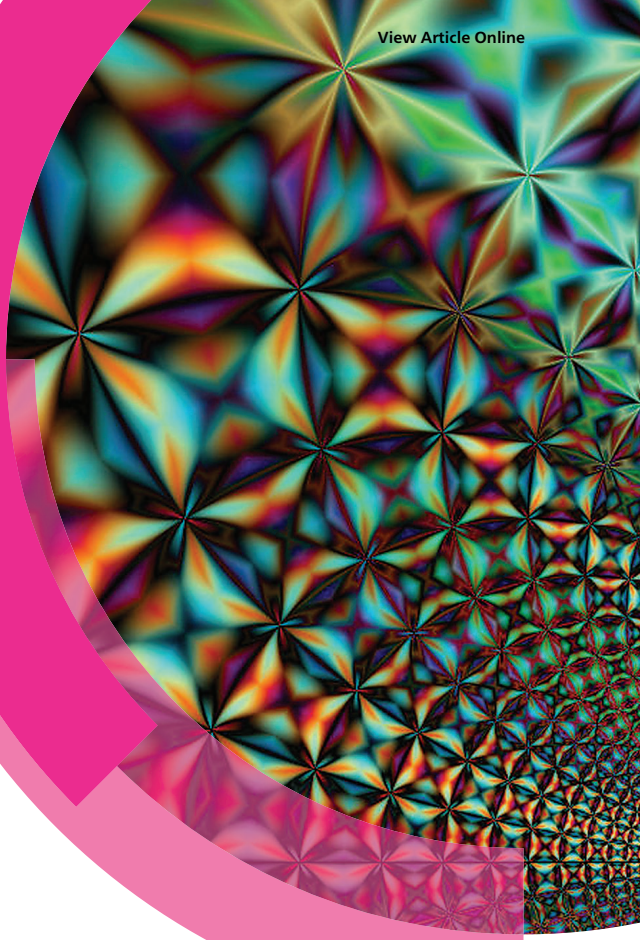

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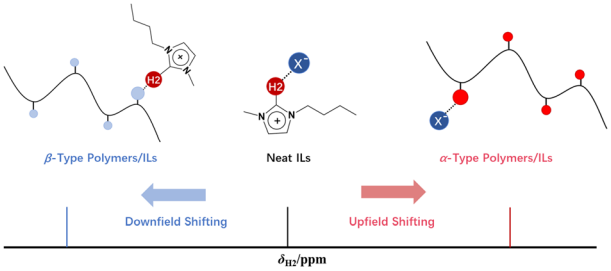

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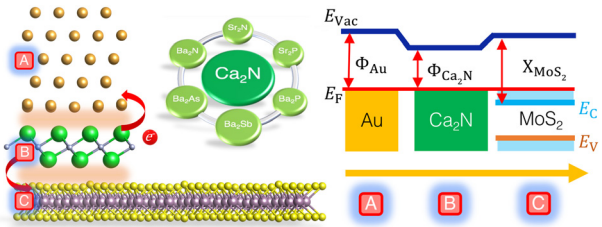

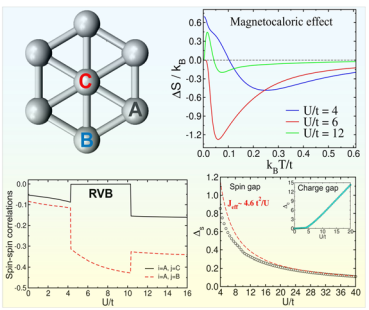

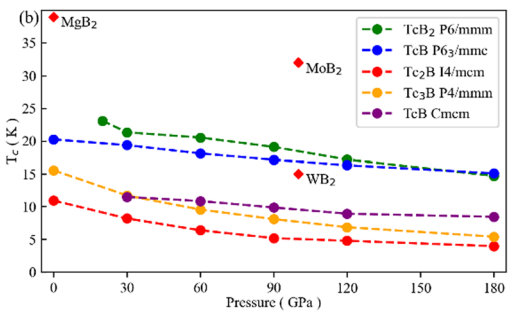

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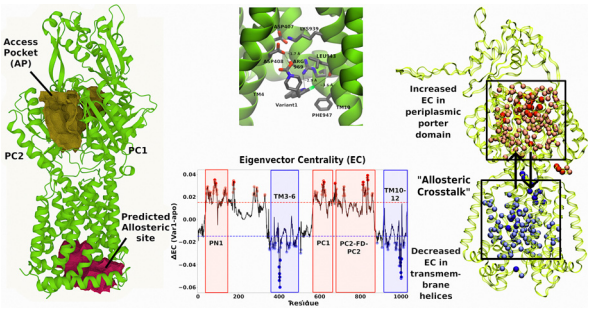

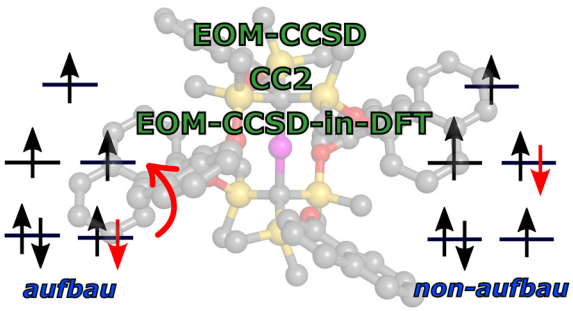

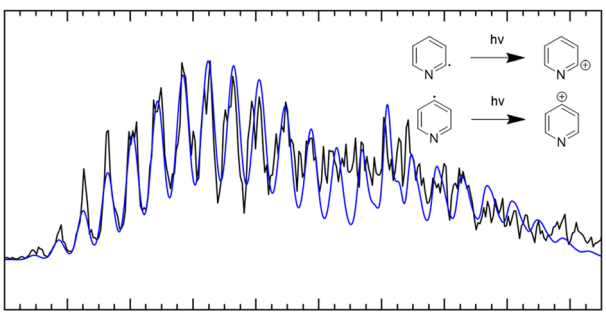

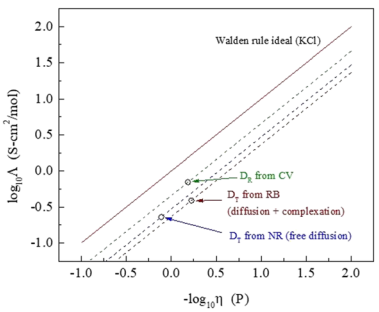

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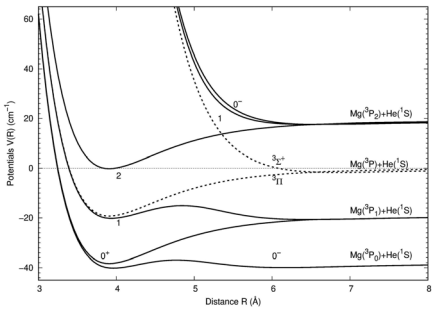

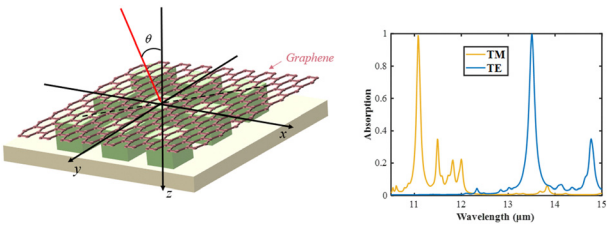

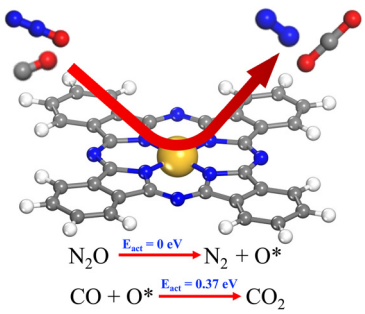

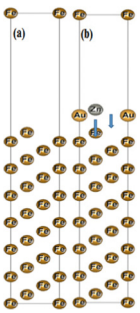

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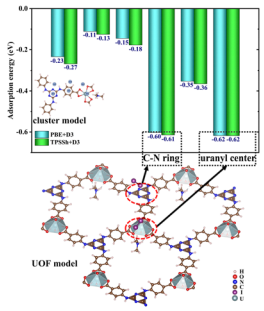

Iodine capture of a two-dimensional layered uranyl–organic framework: a combined DFT and AIMD study

Mingyang Shi, Kunyang Cheng, Xiujuan Cheng, Xuying Zhou, Gang Jiang and Jiguang Du*

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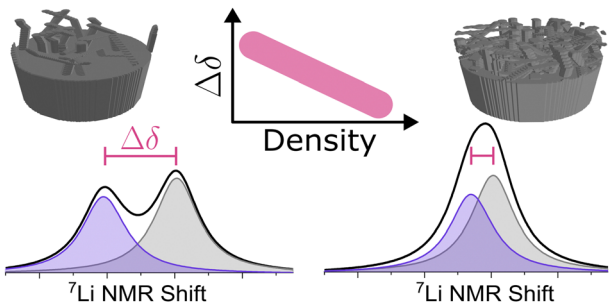

Morphology characterization of dendrites on lithium metal electrodes by NMR spectroscopy

Santiago Agustín Maldonado-Ochoa,* Muriel Zampieri, Manuel Otero and Fabián Vaca Chávez*

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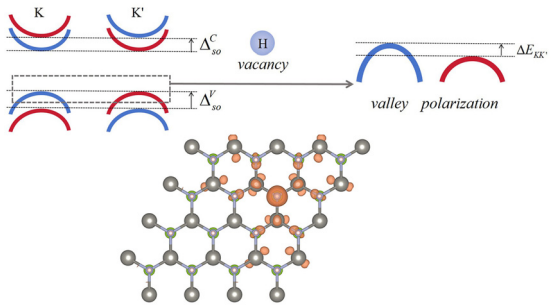

Large valley splitting and vacancy-induced valley polarization in two-dimensional WSeNH

Ziqi Wang, Xuening Han and Yan Liang*

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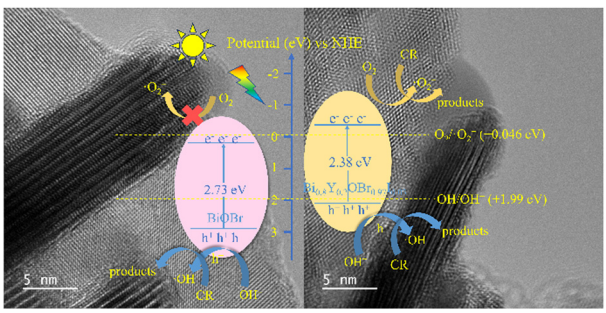

Enhancing the adsorption–photocatalytic efficiency of BiOBr for Congo red degradation by tuning the surface charge and bandgap *via* an Y^{3+}–I^{-} co-doping strategy

Dongsheng Chen, Keqian Gong, Xiangyang Xu,* Chenyu Huang and Pengtao Lei

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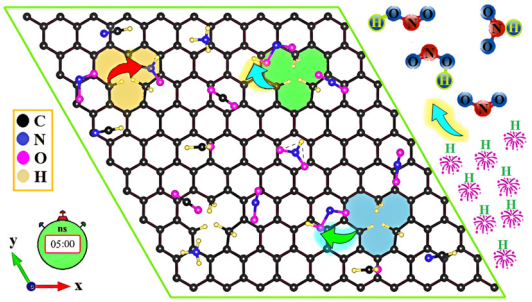

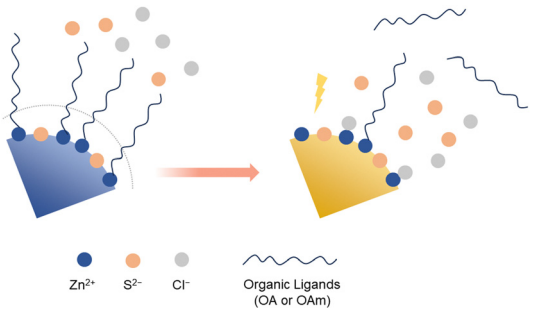

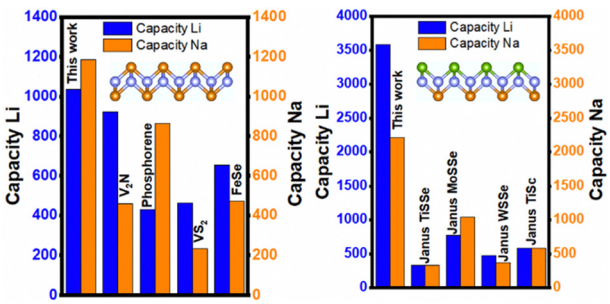

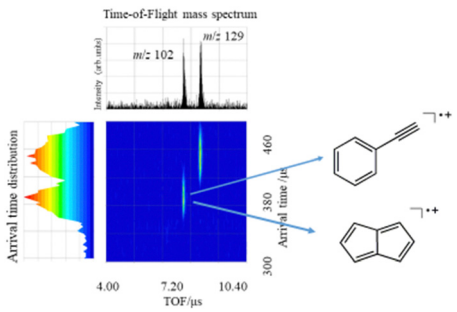

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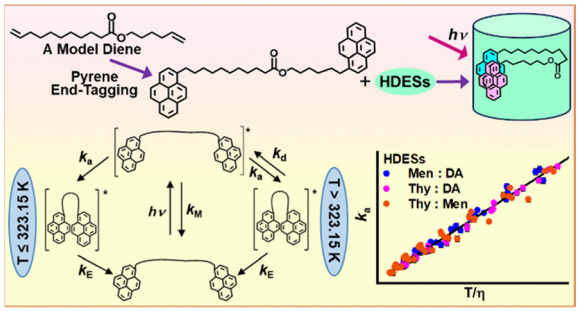
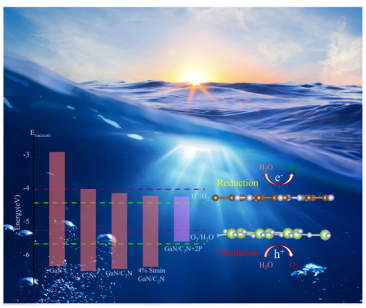


Assessing hydrophobic deep eutectic solvents for intramolecular excimer formation

Shreya Juneja and Siddharth Pandey*

17223



Doping and strain modulation of the electronic, optical and photocatalytic properties of the GaN/C_2N heterostructure

Fu Yin, Hui Wang,* Zhengqin Zhao, LiJia Luo, Yongliang Tang, Yanbo Zhang and Qiang Xue

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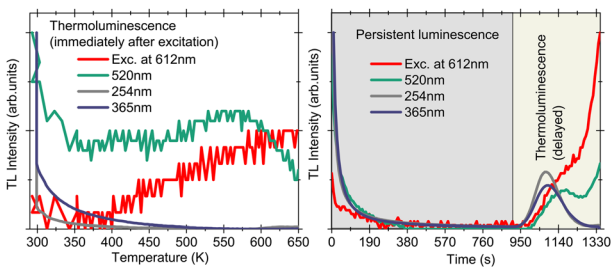

Delayed tunneling of charges to deep traps in a ZnO impurity containing Cr^{3+} doped Zn_2TiO_4 inverse spinel

Ankit Sharma and Suchinder K. Sharma*

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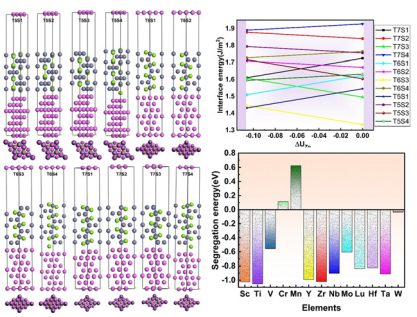

The first-principles study of interfacial bonding strength and segregation behavior of alloyed elements at the η($MgZn_2$)/Al interface

Qing Gao, Guoyu Qiao, Weibing Wang, Yuxiang Ge, Junqiang Ren, Wei Li, Ping Yang, Xuefeng Lu* and Jisen Qiao*

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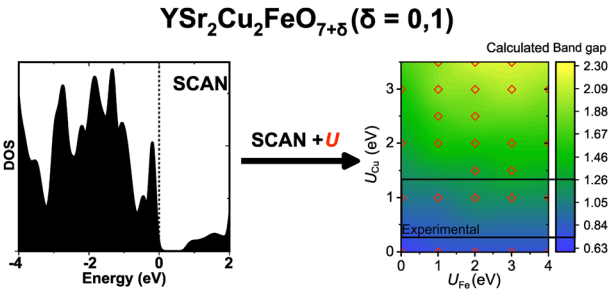
The SCAN+*U* method in the investigation of complex transition metal oxides: a case study on $YSr_2Cu_2FeO_{7+\delta}$ (δ = 0, 1)

Marianela Gómez-Toledo and Elena M. Arroyo-de Dompablo*



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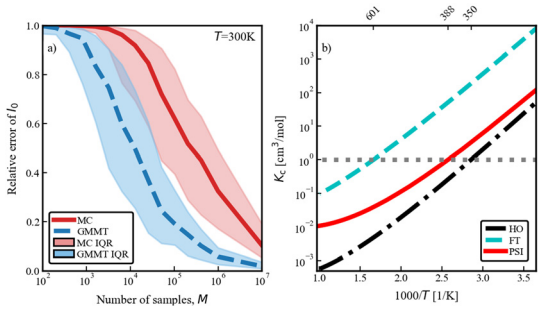
Importance sampling within configuration space integration for adsorbate thermophysical properties: a case study for CH_3/Ni(111)

Katrín Blöndal, Kirk Badger, Khachik Sargsyan, David H. Bross, Branko Ruscic and C. Franklin Goldsmith*



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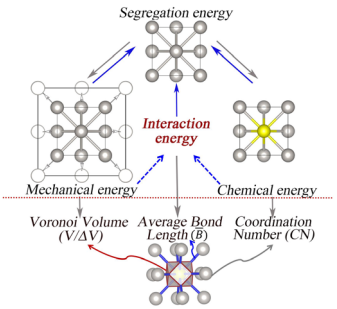
Preferential segregation of gold at the symmetrical tilt grain boundaries of platinum: an atomic-scale quantitative understanding

Xianxian Zhang, Jianfeng Tang,* Xingming Zhang, Liang Wang, Dingwang Yuan, Huiqiu Deng and Lei Deng*



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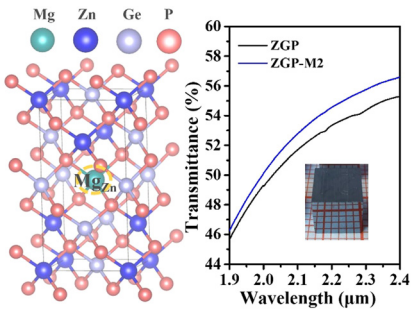
Enhanced near-infrared optical transmission in zinc germanium phosphide crystals *via* precise magnesium doping

Shichao Cheng, Xueyan Zhang, Xiangran Kong, Tao Liu, Jingdong Yan, Tetiana Prikhna, Yunfei Shang,* Zuotao Lei* and Chunhui Yang



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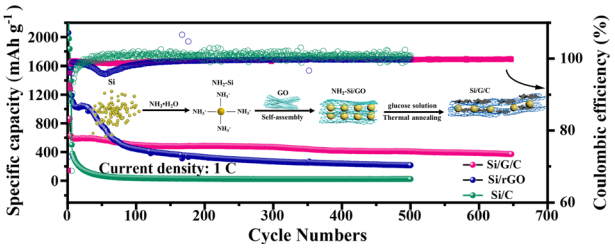

Carbon-coated silicon/graphite oxide composites as anode materials for highly stable lithium-ion batteries

Lujie Niu, Rui Zhang,* Qiang Zhang, Dong Wang, Yanlei Bi, Guangwu Wen and Lu-Chang Qin

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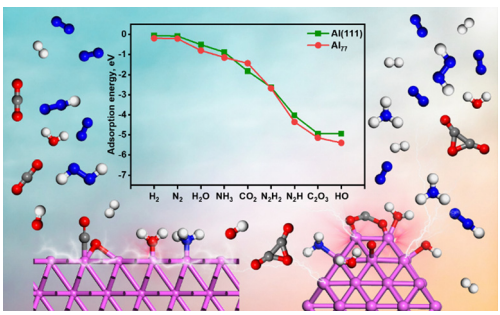

Adsorption mechanisms of decomposition species of CHON-containing explosives on aluminum surfaces

Kai Zhong and Chaoyang Zhang*

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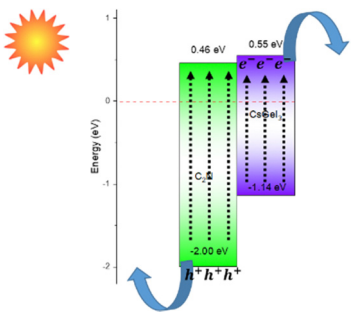

The lead-free perovskite-based heterojunction $C_2N/CsGeI_3$: an exploration for superior visible-light absorption

Junli Chang,* Yumeng Xie, Wenwu Shi, Jinguo Jiang, Hongyan Zhang and Guangzhao Wang*

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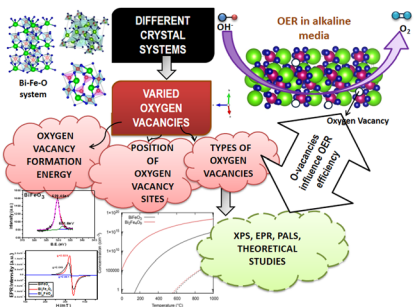

Electrocatalytic OER behavior of the Bi–Fe–O system: an understanding from the perspective of the presence of oxygen vacancies

Shaswati Jyoti, Aditi Vijay, Umberto Terranova, Santosh K Gupta, Kathi Sudarshan and Sonalika Vaidya*

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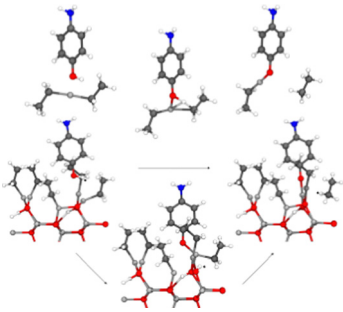

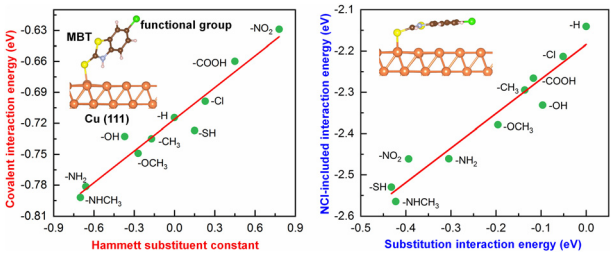

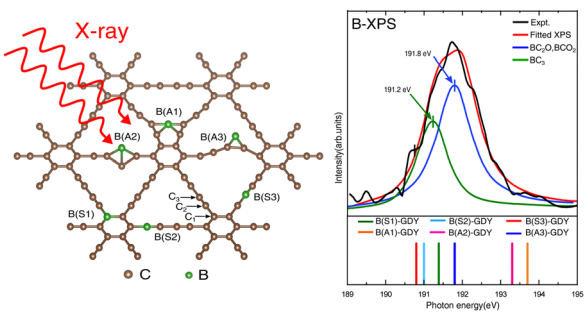

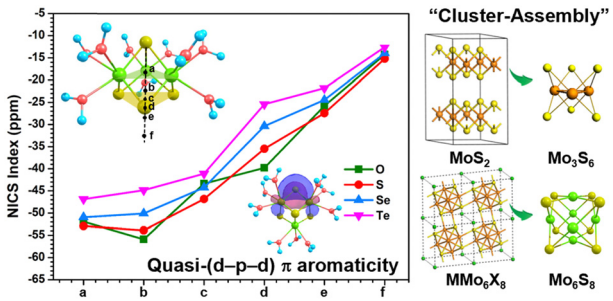

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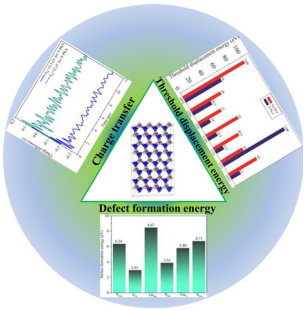
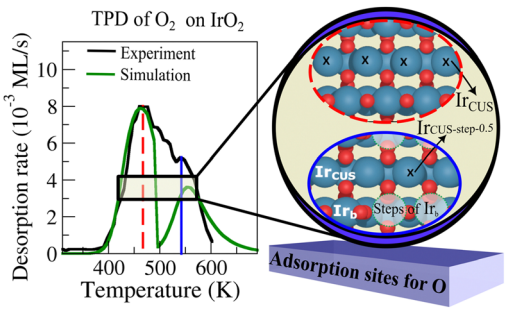


A combined AIMD and DFT study of the low-energy radiation responses of GaN

Ming Jiang,* Nuo Cheng, Xin-Yu Zhu, Xuan-Liang Hu, Zi-Han Wang, Ning Liu, Shuo Song, Sheng-Ze Wang, Xu-Sheng Liu* and Chandra Veer Singh*



Characterization of adsorption sites on IrO_2 *via* temperature programmed O_2 desorption simulations

Vivianne K. Ocampo-Restrepo, Sudarshan Vijay, G. T. Kasun Kalhara Gunasooriya and Jens K. Nørskov*