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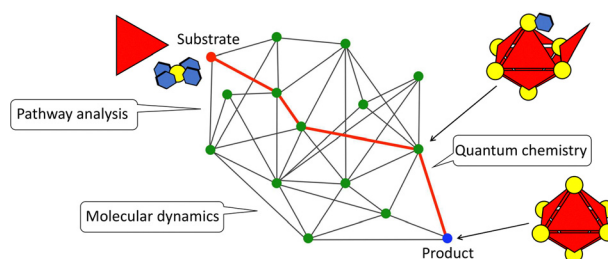
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Theoretical and computational methodologies for understanding coordination self-assembly complexes

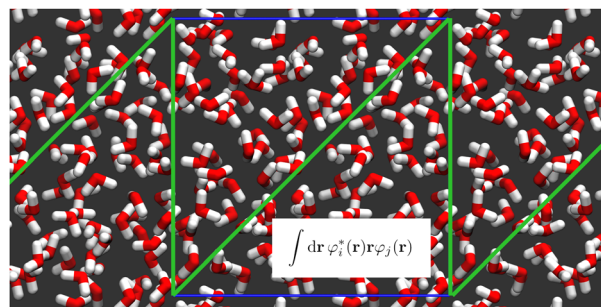
Satoshi Takahashi,* Satoru Iuchi, Shuichi Hiraoka and Hirofumi Sato*



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Edward Ditle, Johann Mattiat and Sandra Lubert*



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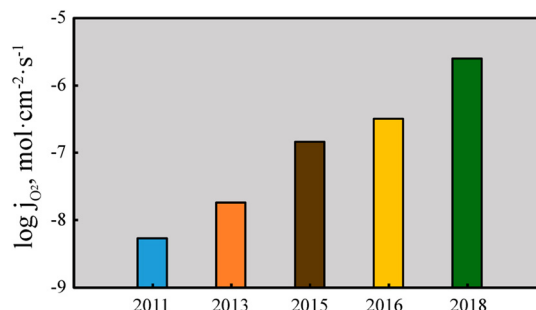


PERSPECTIVES

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Oxygen separation diffusion-bubbling membranes

Valery V. Belousov



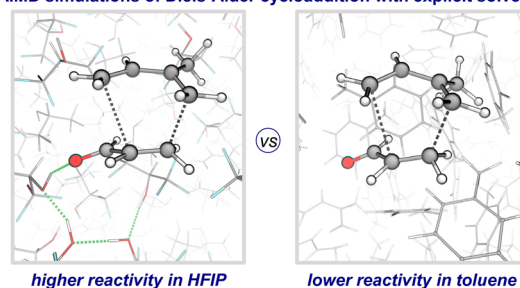
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How hexafluoroisopropanol solvent promotes Diels–Alder cycloadditions: *ab initio* metadynamics simulations

Xia Zhao, Xinmin Hu, Xiangying Lv, Yan-Bo Wu, Yuxiang Bu and Gang Lu*

AIMD simulations of Diels–Alder cycloaddition with explicit solvents

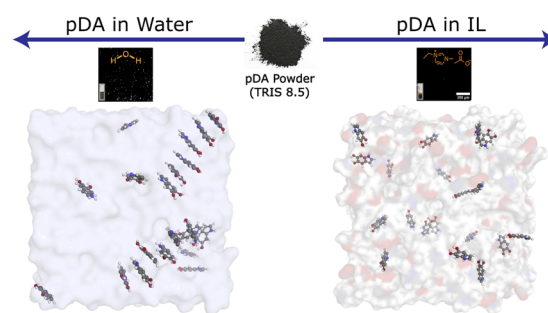


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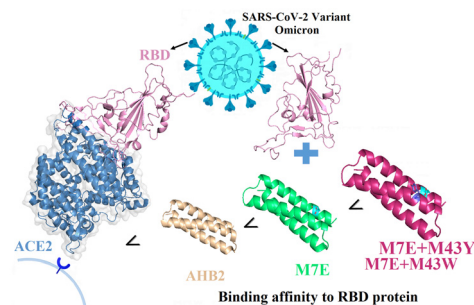
Abhishek Singh, Thomas G. Mason, Zhenzhen Lu, Anita J. Hill, Steven J. Pas, Boon Mia Teo, Benny D. Freeman and Ekaterina I. Izgorodina*



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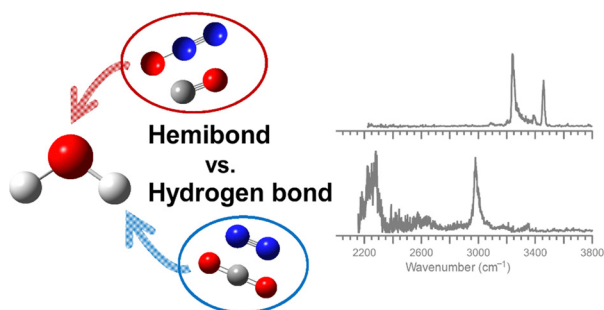
In silico design of miniprotein to inhibit SARS-CoV-2 variant Omicron spike protein

Jianhua Wu, Hong-Xing Zhang* and Jilong Zhang*



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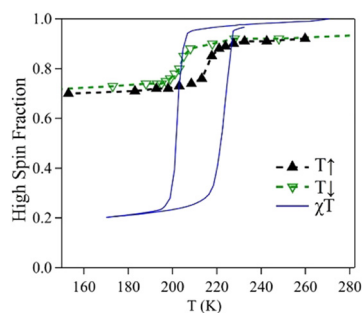
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Mizuhiro Kominato and Asuka Fujii*

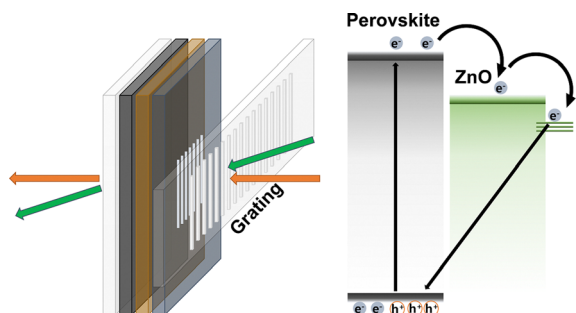
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Surface stabilisation of the high-spin state of Fe(II) spin-crossover complexes

Alejandro Martínez Serra, Archit Dhingra,*
 María Carmen Asensio, José Antonio Real and
 Juan Francisco Sánchez Royo*

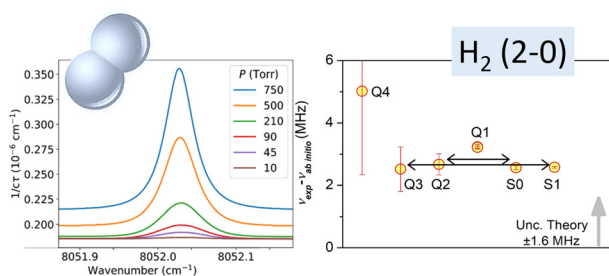
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Young Hyun Kim and Woon Yong Sohn*

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The high-accuracy spectroscopy of H_2 rovibrational transitions in the (2-0) band near $1.2 \mu\text{m}$

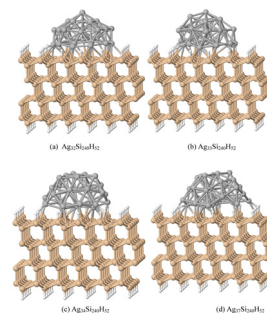
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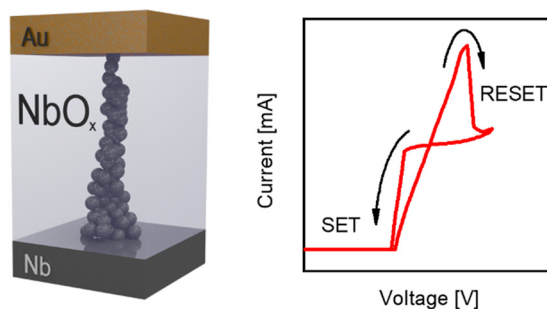
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Resistive switching and role of interfaces in memristive devices based on amorphous NbO_x grown by anodic oxidation

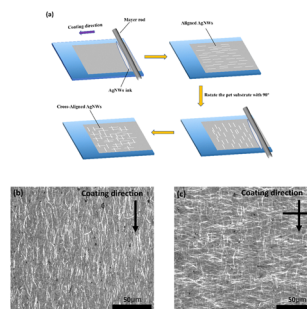
Giuseppe Leonetti, Matteo Fretto, Katarzyna Bejtka, Elena Sonia Olivetti, Fabrizio Candido Pirri, Natascia De Leo, Iliia Valov and Gianluca Milano*



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Multilayer directionally arranged silver nanowire networks for flexible transparent conductive films

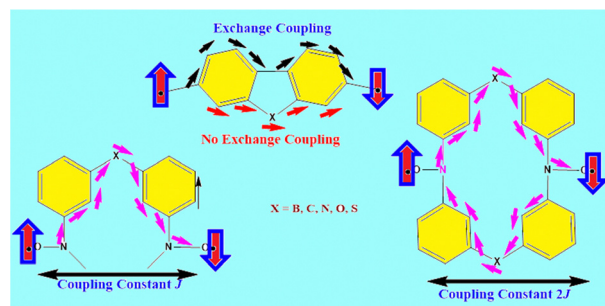
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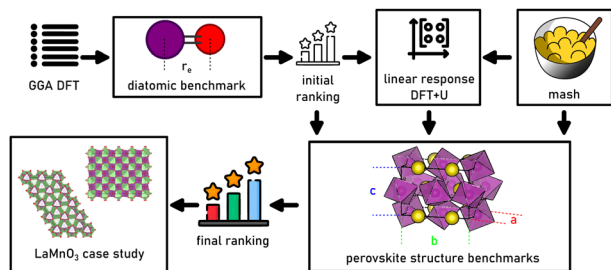
The effect of hetero-atoms on spin exchange coupling pathways (ECPs): a computational investigation

Suranjan Shil,* Debojit Bhattacharya, Anirban Misra, Yenni P. Ortiz and Douglas J. Klein



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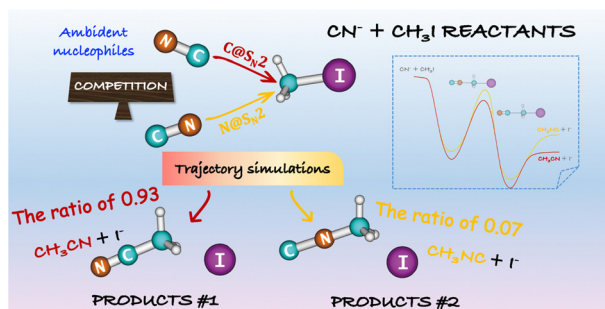
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Computational workflows for perovskites: case study for lanthanide manganites

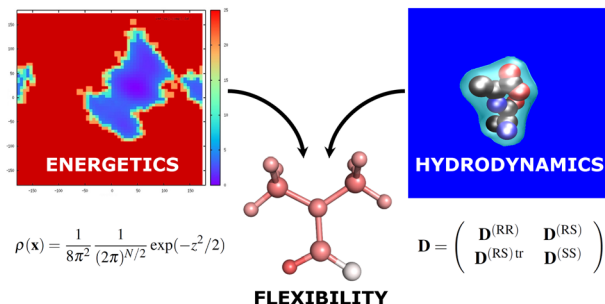
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Dynamics of nucleophilic substitution on ambident nucleophiles CN^- and iodomethane: insights into the competition mechanism with neutral isomeric products

Xu Liu, Shiqi Tian, Boxue Pang,* Hui Li and Yang Wu*

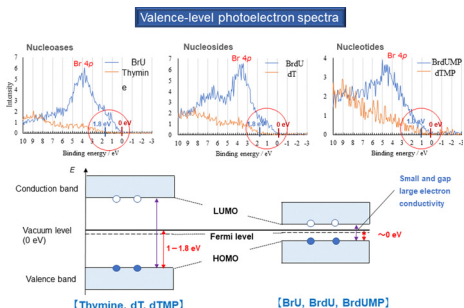
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The roto-conformational diffusion tensor as a tool to interpret molecular flexibility

Sergio Rampino, Mirco Zerbetto* and Antonino Polimeno

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Incorporation of a bromine atom into DNA-related molecules changes their electronic properties

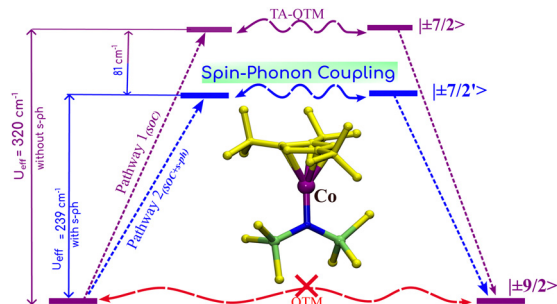
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The impact of spin-vibrational coupling on magnetic relaxation of a Co(II) single-molecule magnet

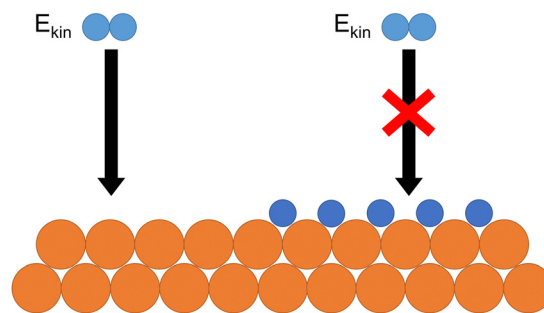
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Adsorption dynamics of O₂ on Cu(111): a supersonic molecular beam study

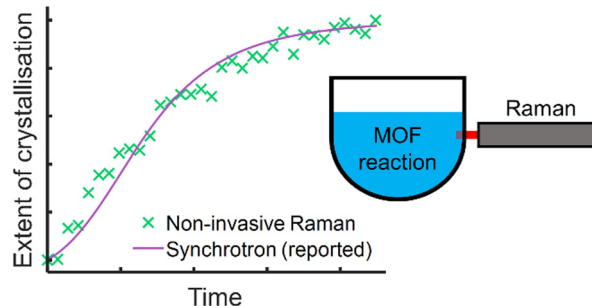
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Non-invasive monitoring of the growth of metal-organic frameworks (MOFs) via Raman spectroscopy

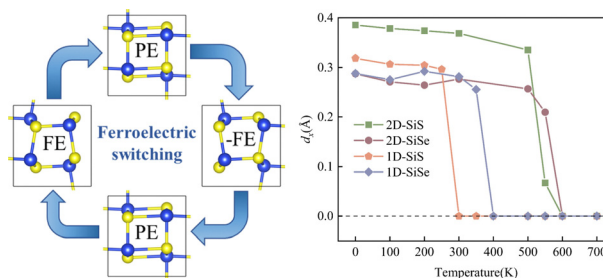
Magdalene W. S. Chong,* Andrew J. Parrott,* David J. Ashworth, Ashleigh J. Fletcher and Alison Nordon



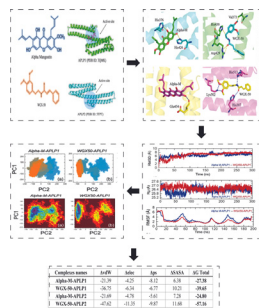
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Robust ferroelectricity in low-dimensional δ -SiX (X = S/Se): a first-principles study

Yuehua Dai, Xiaoteng Wang, Xiuquan Fang, Zihan Qu, Jishun Zhang, Zuheng Wu, Zuyu Xu, Fei Yang and Yunlai Zhu*



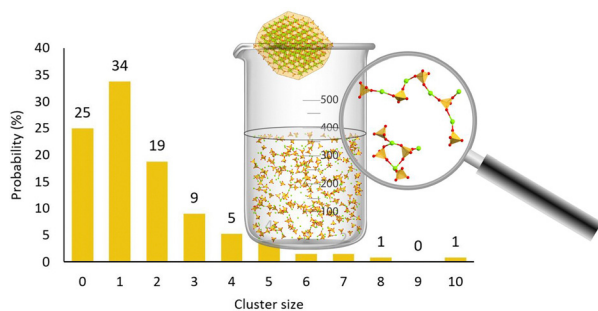
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Comparative binding analysis of WGX50 and Alpha-M with APP family proteins APLP1 and APLP2 using structural-dynamics and free energy calculation approaches

Arif Ali, Adan Masood, Abdul Aziz Khan, Feng-Yun Zhu, Muhammad Arslan Rasheed Cheema, Abdus Samad, Abdul Wadood, Abbas Khan, Qiu Yu, Wang Heng,* Daixi Li and Dong-Qing Wei*

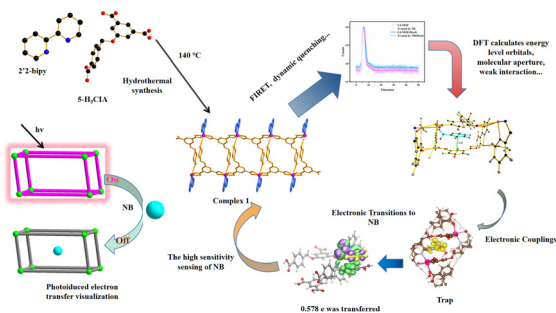
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A total scattering study of prenucleation structures in saturated aqueous magnesium sulfate – observation of extended clusters

Daniel J. M. Irving, Mark E. Light,* Matilda P. Rhodes, Terence Threlfall and Thomas F. Headen

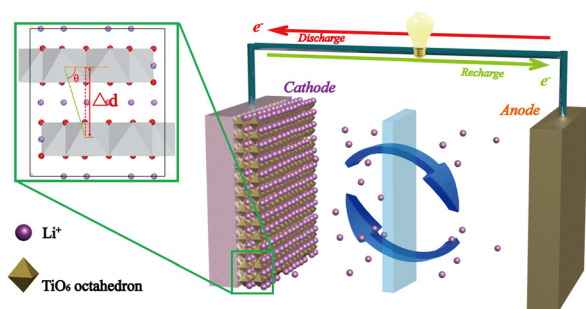
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The high fluorescence sensitivity property and quenching mechanism of one-dimensional Cd-HCIA-1 sensor for nitrobenzene

Xiaoming Song, Wenzhuo Dong, Xiufang Hou,* Qingxia Zhao, Zhuangzhuang Zhang and Yixia Ren*

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Pressure-induced phase transition toward high symmetry in zero-strain Li_2TiO_3

Wenming Qi, Hadiqa Abdugopur, Wei Xu, Min Gao,* Anwar Hushur* and Hongyan Zhang*

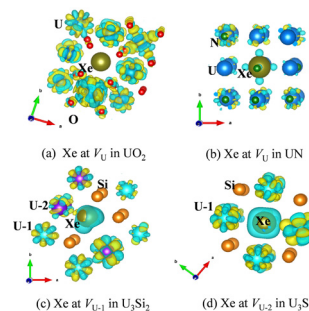


RESEARCH PAPERS

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Understanding xenon and vacancy behavior in UO_2 , UN and U_3Si_2 : a comparative DFT+ U study

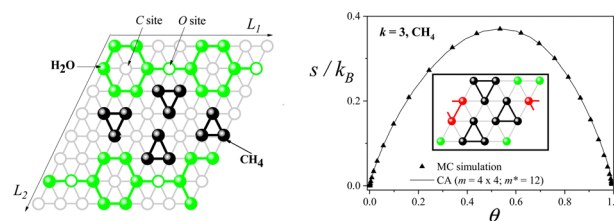
Jiajun Zhao, Dan Sun, Liu Xi, Ping Chen, Jijun Zhao and Yuanyuan Wang*



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Cluster approximation applied to multisite-occupancy adsorption: configurational entropy of the adsorbed phase for dimers and trimers on triangular lattices

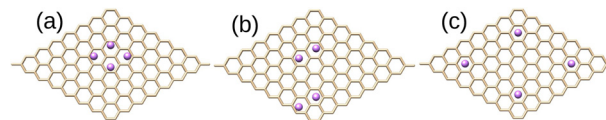
Noris M. De La Cruz Feliz, Pablo J. Longone, Fabricio O. Sanchez-Varretti, Fernando M. Bulnes and Antonio J. Ramirez-Pastor*



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Optical properties of Li-patterned graphene via a self-assembling molecular network

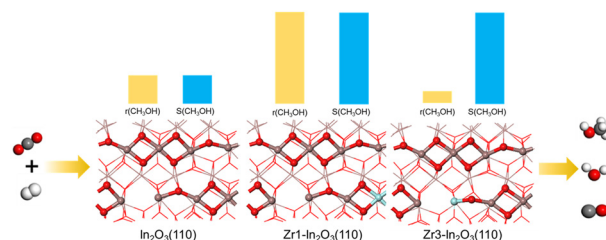
Hamed Abbasian



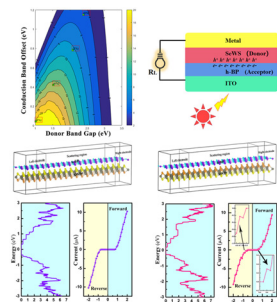
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DFT-based microkinetic studies on methanol synthesis from CO_2 hydrogenation over In_2O_3 and Zr– In_2O_3 catalysts

Kun Li, Zhangqian Wei, Qingyu Chang* and Shenggang Li*



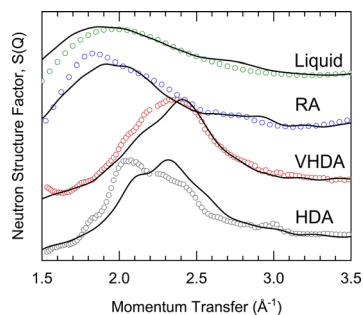
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Reconfigurable band alignment of SWSe/h-BP heterostructures for photoelectric applications

Dong Wei, Yi Li, Gaofu Guo, Heng Yu, Yaqiang Ma, Yanan Tang and Xianqi Dai*

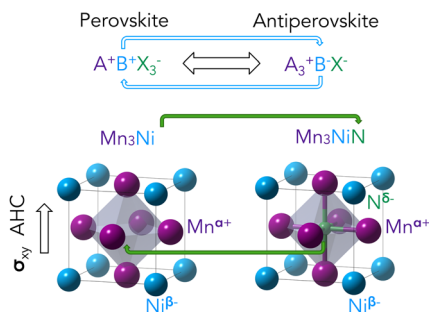
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Neutron scattering study of polyamorphic THF·17(H₂O) – toward a generalized picture of amorphous states and structures derived from clathrate hydrates

Paulo H. B. Brant Carvalho,* Mikhail Ivanov, Ove Andersson, Thomas Loerting, Marion Bauer, Chris A. Tulk, Bianca Haberl, Luke L. Daemen, Jamie J. Molaison, Katrin Amann-Winkel, Alexander P. Lyubartsev, Craig L. Bull, Nicholas P. Funnell and Ulrich Häussermann

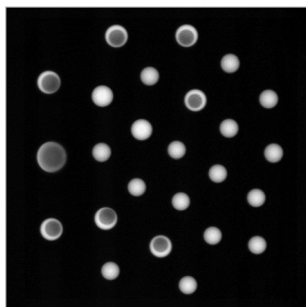
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Anionic nickel and nitrogen effects in the chiral antiferromagnetic antiperovskite Mn₃NiN

E. Triana-Ramírez, W. Ibarra-Hernandez and A. C. Garcia-Castro*

15000



Fluorescence profiles of water droplets in stable levitating droplet clusters

Alexander A. Fedorets, Eduard E. Kolmakov, Dmitry N. Medvedev, Michael Nosonovsky* and Leonid A. Dombrovsky

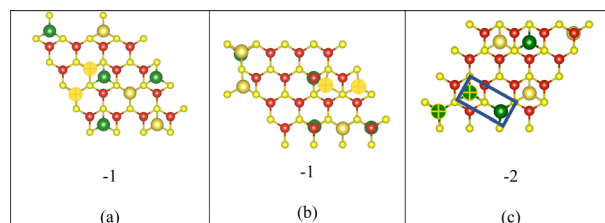


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Prediction of sodium binding energy on 2D VS₂ via machine learning: a robust accompanying method to *ab initio* random structure searching

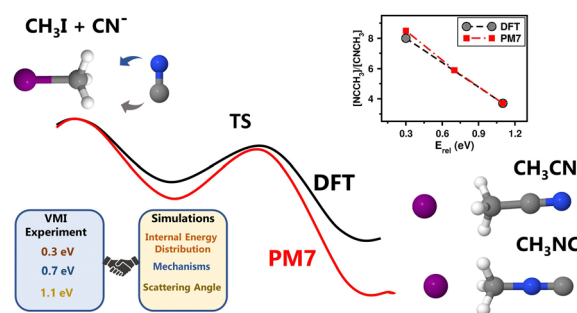
Darwin B. Putungan, Shaosen Su, Liang Gao, Ankit Goyal, Shi-Hsin Lin and Akhil Garg*



15015

Direct chemical dynamics simulations of CN⁻ + CH₃I bimolecular nucleophilic substitution reaction

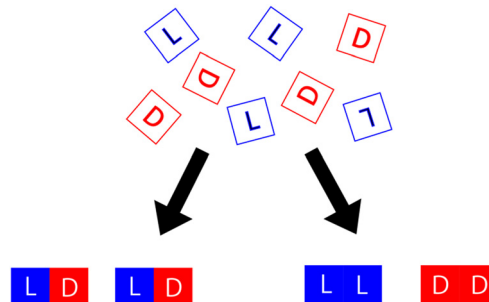
Akash Gutal and Manikandan Paranjothy*



15023

Enantioselective amino acid interactions in solution

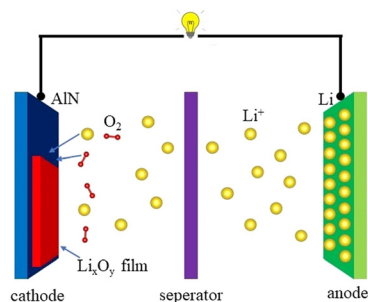
Natsuki Watanabe, Mitsuo Shoji,* Koichi Miyagawa, Yuta Hori, Mauro Boero, Masayuki Umemura and Yasuteru Shigeta



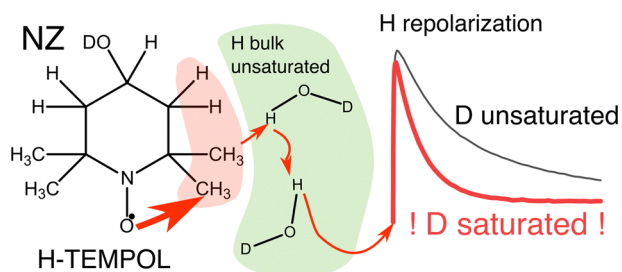
15030

Bilayer tetragonal AlN nanosheets as potential cathodes for Li-O₂ batteries

Jiaming Wang, Hao Wu, Min Pan,* Zhixiao Liu,* Lei Han, Zheng Huang and Huiqiu Deng



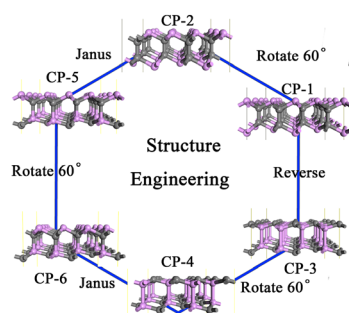
15040



Quantitative analysis of cross-talk in partly deuterated samples of nuclear spins hyperpolarized by dynamic nuclear polarization (DNP) in the thermal mixing regime

Bogdan A. Rodin,* Vineeth Thalakkottor, Mathieu Baudin, Nicolas Birilakis, Geoffrey Bodenhausen, Alexandra V. Yurkovskaya and Daniel Abergel*

15052



Structure-engineering the stability, electronic, optical and photocatalytic properties of hexagonal C₂P₂ monolayers

Jiahe Lin,* Bofeng Zhang,* Tian Zhang and Xiaowei Chen

