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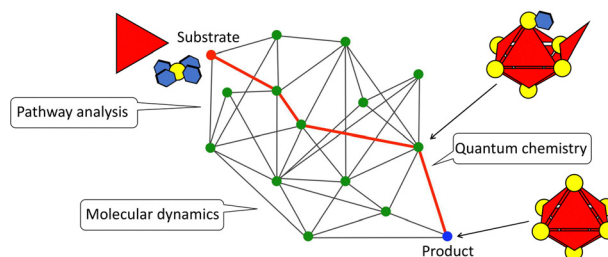
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Theoretical and computational methodologies for understanding coordination self-assembly complexes

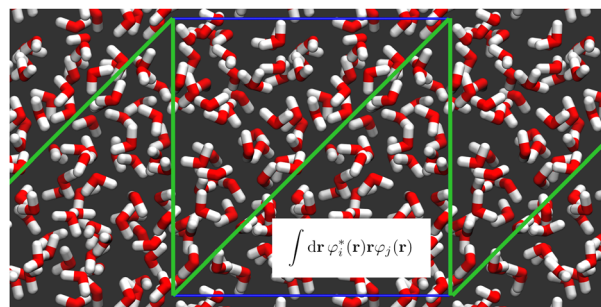
Satoshi Takahashi,* Satoru Iuchi, Shuichi Hiraoka and Hirofumi Sato*



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The position operator problem in periodic calculations with an emphasis on theoretical spectroscopy

Edward Ditle, Johann Mattiat and Sandra Lubert*



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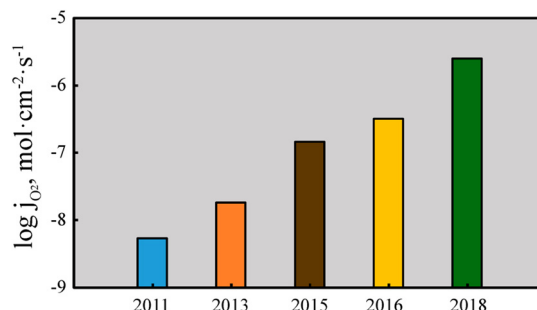


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Oxygen separation diffusion-bubbling membranes

Valery V. Belousov



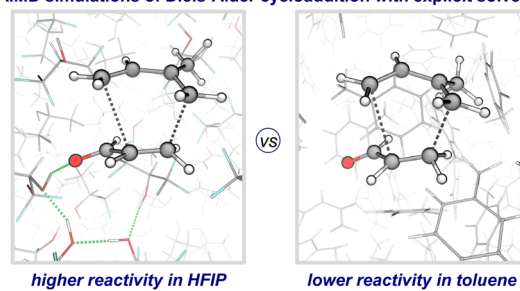
COMMUNICATION

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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

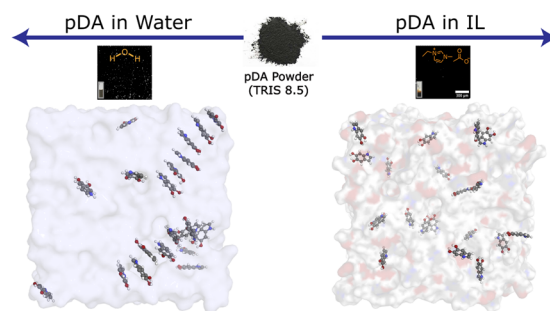


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Structural elucidation of polydopamine facilitated by ionic liquid solvation

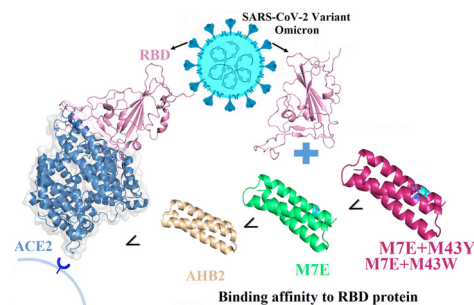
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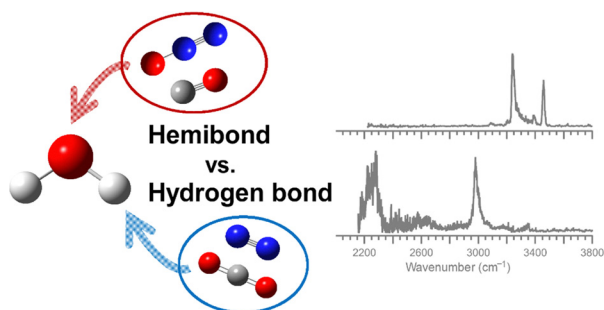
In silico design of miniprotein to inhibit SARS-CoV-2 variant Omicron spike protein

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



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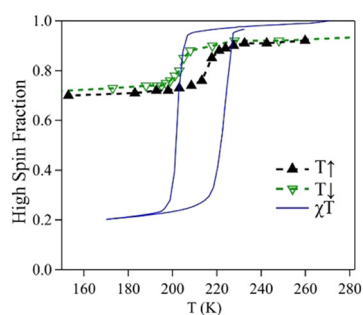
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Infrared spectroscopy of $[\text{H}_2\text{O}-\text{X}_n]^+$ ($n = 1-3$, $\text{X} = \text{N}_2, \text{CO}_2, \text{CO}$, and N_2O) radical cation clusters: competition between hydrogen bond and hemibond formation of the water radical cation

Mizuhiro Kominato and Asuka Fujii*

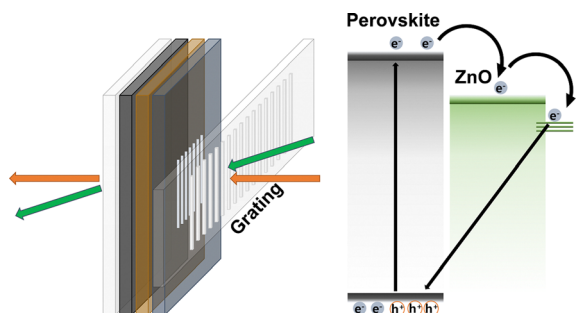
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Surface stabilisation of the high-spin state of Fe(II) spin-crossover complexes

Alejandro Martínez Serra, Archit Dhingra,*
 María Carmen Asensio, José Antonio Real and
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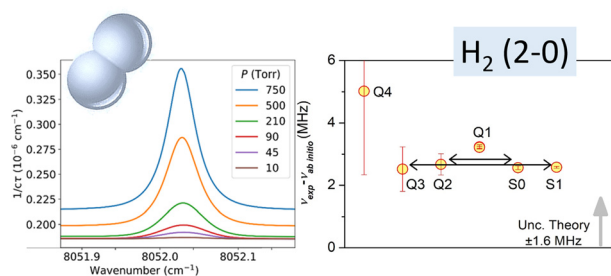
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Young Hyun Kim and Woon Yong Sohn*

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

H. Fleurbaey, A. O. Koroleva, S. Kassi and A. Campargue*

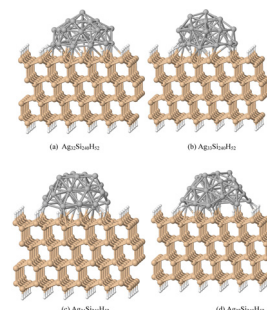


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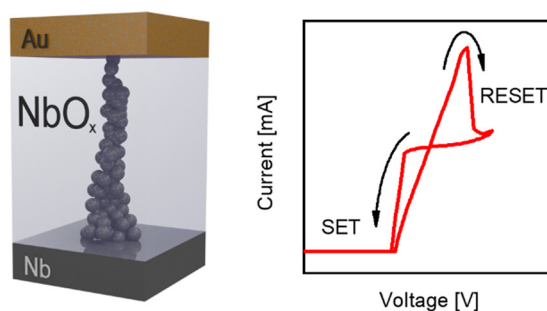
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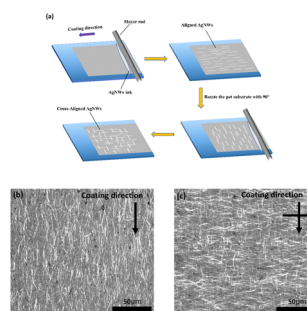
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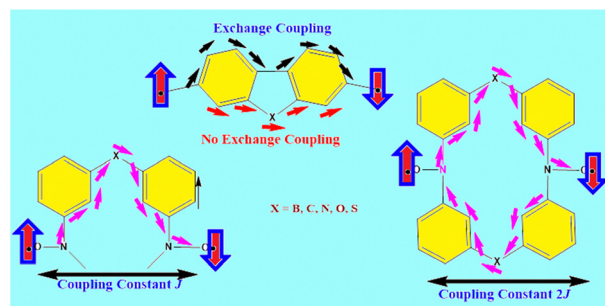
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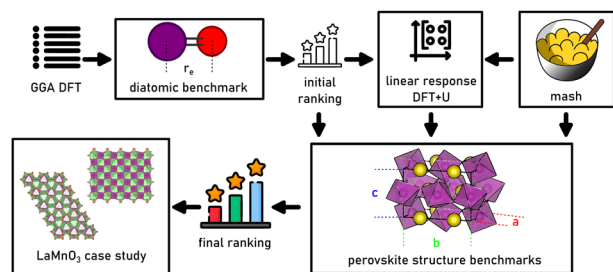
The effect of hetero-atoms on spin exchange coupling pathways (ECPs): a computational investigation

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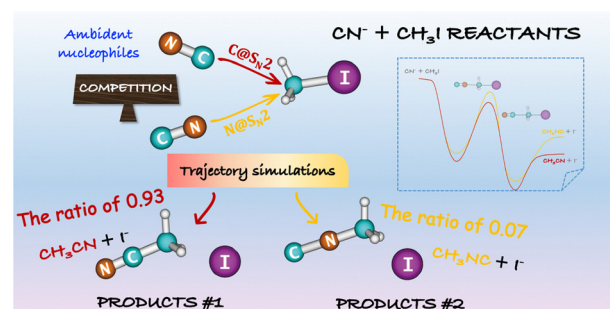
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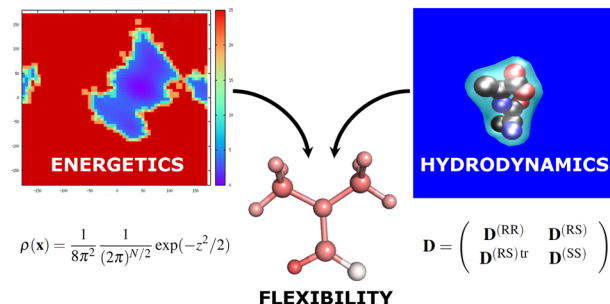
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Xu Liu, Shiqi Tian, Boxue Pang,* Hui Li and Yang Wu*

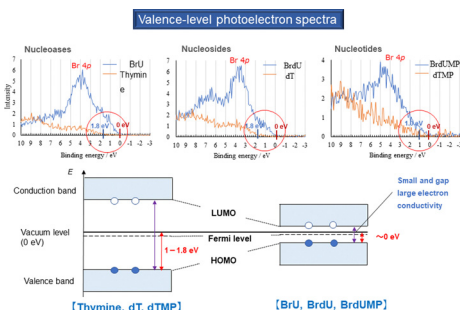
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The roto-conformational diffusion tensor as a tool to interpret molecular flexibility

Sergio Rampino, Mirco Zerbetto* and Antonino Polimeno

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

Misaki Hirato, Akinari Yokoya,* Yuji Baba, Seiji Mori, Kentaro Fujii, Shin-ichi Wada, Yudai Izumi and Yoshinori Haga

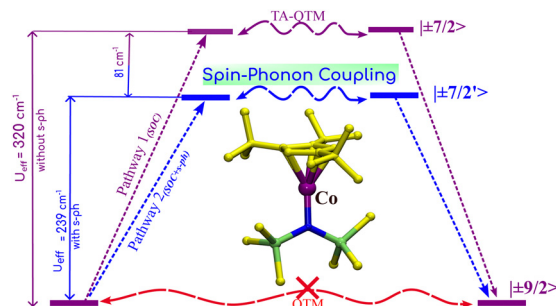


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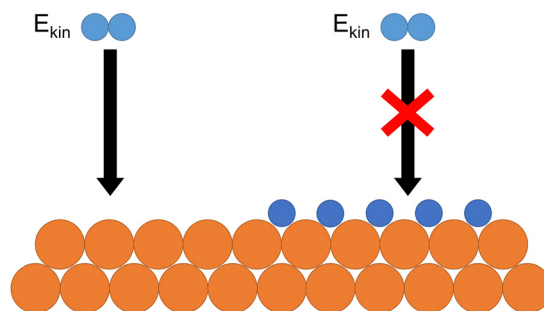
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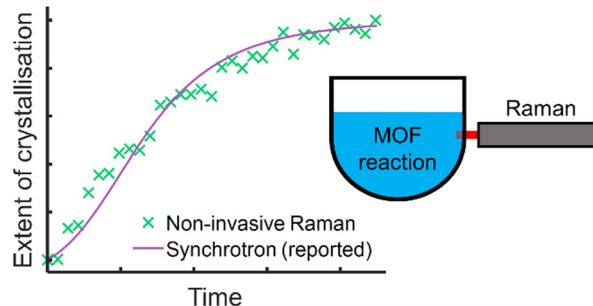
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Non-invasive monitoring of the growth of metal–organic frameworks (MOFs) via Raman spectroscopy

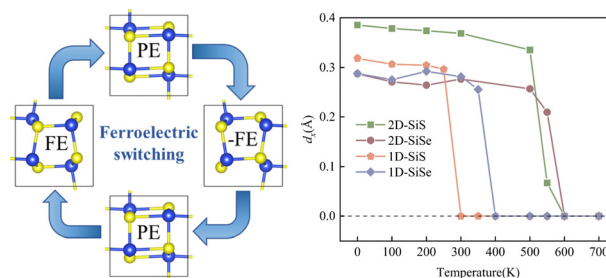
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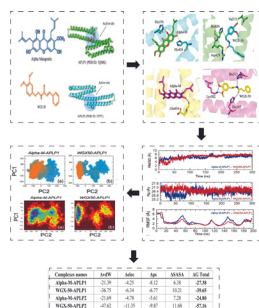
Robust ferroelectricity in low-dimensional δ -SiX (X = S/Se): a first-principles study

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



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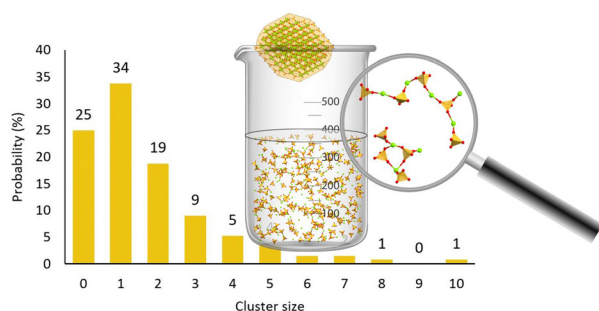
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Comparative binding analysis of WGX50 and Alpha-M with APP family proteins APLP1 and APLP2 using structural-dynamics and free energy calculation approaches

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*

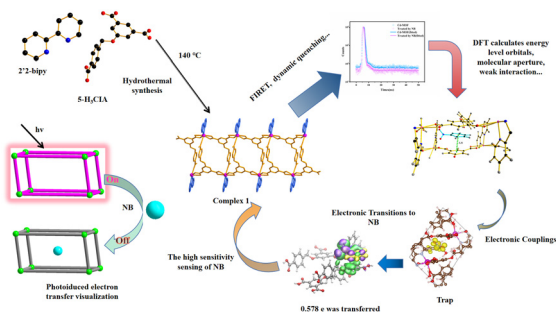
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A total scattering study of prenucleation structures in saturated aqueous magnesium sulfate – observation of extended clusters

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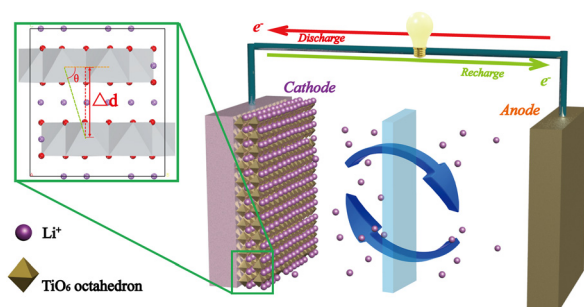
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The high fluorescence sensitivity property and quenching mechanism of one-dimensional Cd-HCIA-1 sensor for nitrobenzene

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 Li₂TiO₃

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

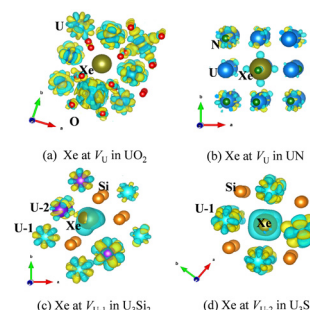


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Understanding xenon and vacancy behavior in UO_2 , UN and U_3Si_2 : a comparative DFT+ U study

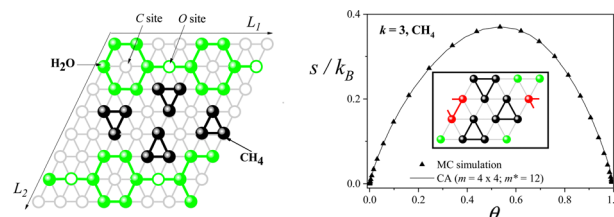
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Cluster approximation applied to multisite-occupancy adsorption: configurational entropy of the adsorbed phase for dimers and trimers on triangular lattices

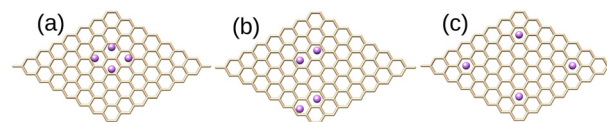
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Optical properties of Li-patterned graphene via a self-assembling molecular network

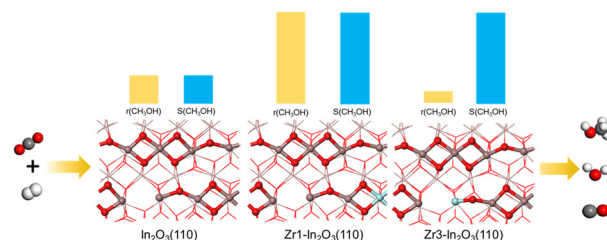
Hamed Abbasian



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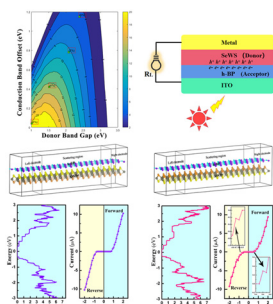
DFT-based microkinetic studies on methanol synthesis from CO_2 hydrogenation over In_2O_3 and Zr– In_2O_3 catalysts

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



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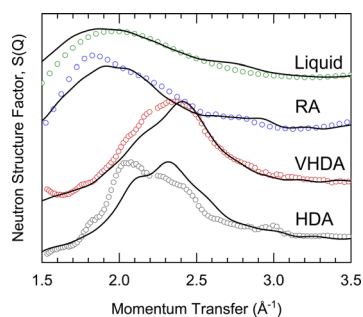
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Reconfigurable band alignment of SWSe/h-BP heterostructures for photoelectric applications

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

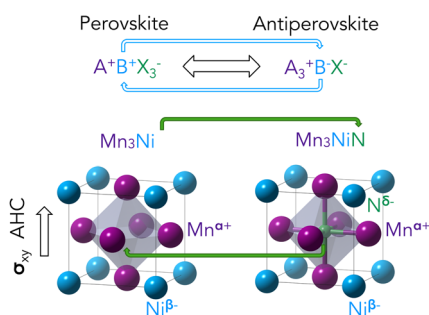
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Neutron scattering study of polyamorphic THF·17(H₂O) – toward a generalized picture of amorphous states and structures derived from clathrate hydrates

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

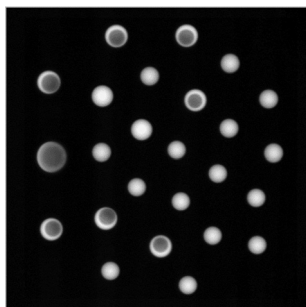
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Anionic nickel and nitrogen effects in the chiral antiferromagnetic antiperovskite Mn₃NiN

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

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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

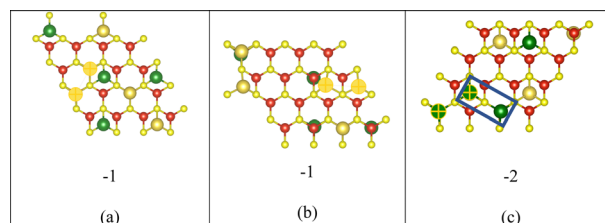


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Prediction of sodium binding energy on 2D VS₂ via machine learning: a robust accompanying method to *ab initio* random structure searching

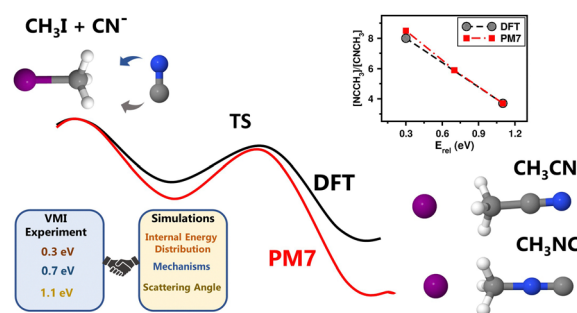
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Direct chemical dynamics simulations of CN[−] + CH₃I bimolecular nucleophilic substitution reaction

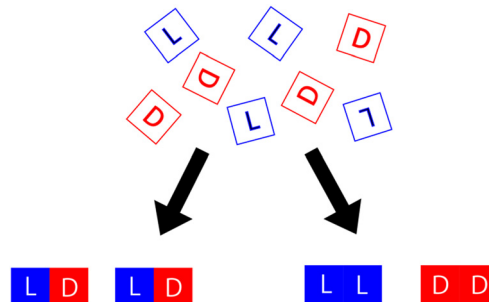
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15023

Enantioselective amino acid interactions in solution

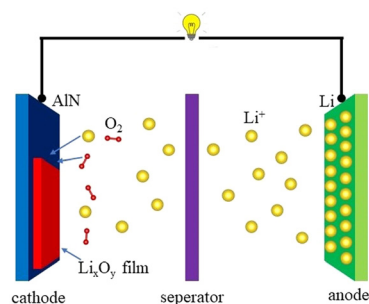
Natsuki Watanabe, Mitsuo Shoji,* Koichi Miyagawa, Yuta Hori, Mauro Boero, Masayuki Umemura and Yasuteru Shigeta



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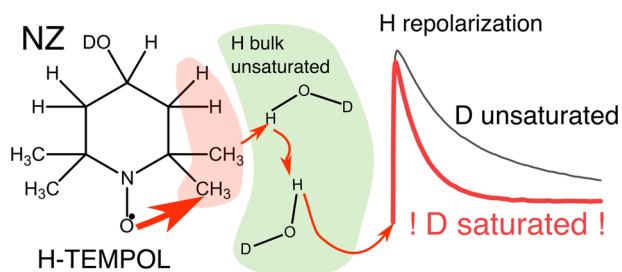
Bilayer tetragonal AlN nanosheets as potential cathodes for Li–O₂ batteries

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



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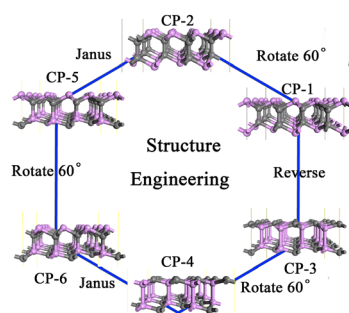
15040



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*

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

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

