

IN THIS ISSUE

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Cover

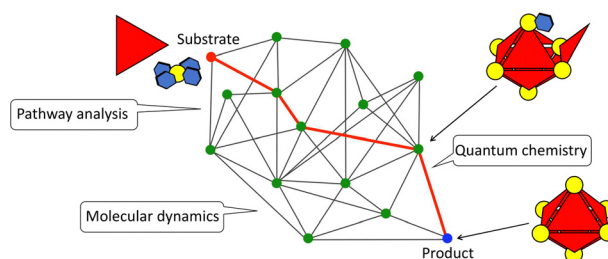
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PERSPECTIVES

14659

Theoretical and computational methodologies for understanding coordination self-assembly complexes

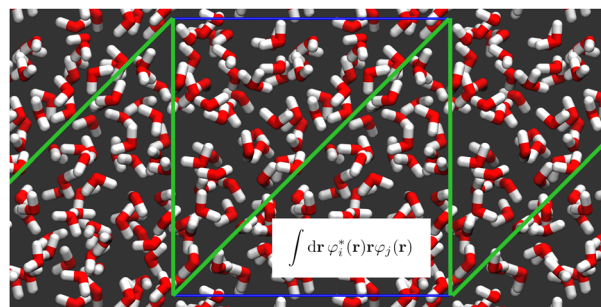
Satoshi Takahashi,* Satoru Iuchi, Shuichi Hiraoka and Hirofumi Sato*



14672

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

Edward Ditler, Johann Mattiat and Sandra Lubert*



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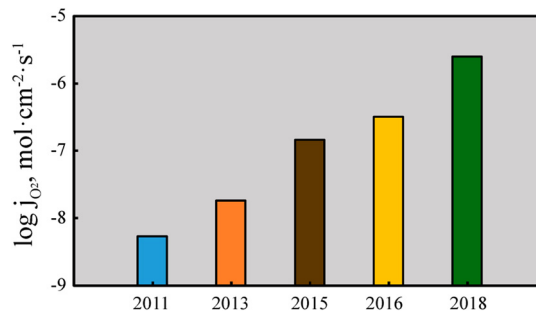


PERSPECTIVES

14686

Oxygen separation diffusion-bubbling membranes

Valery V. Belousov



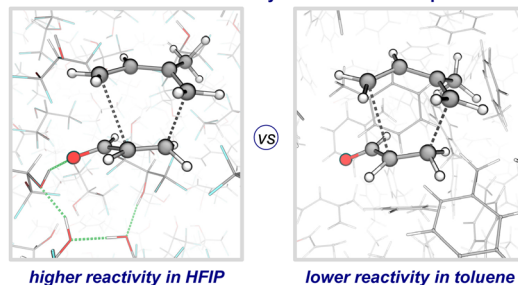
COMMUNICATION

14695

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

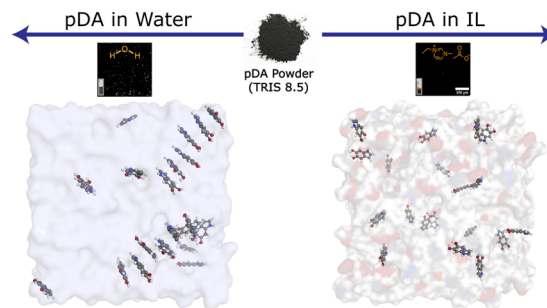


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14700

Structural elucidation of polydopamine facilitated by ionic liquid solvation

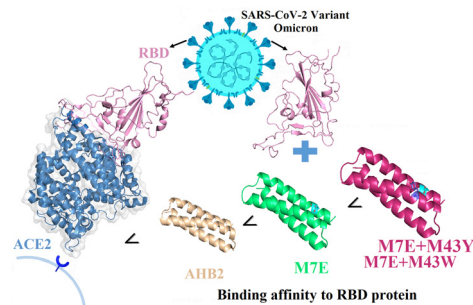
Abhishek Singh, Thomas G. Mason, Zhenzhen Lu, Anita J. Hill, Steven J. Pas, Boon Mia Teo, Benny D. Freeman and Ekaterina I. Izgorodina*



14711

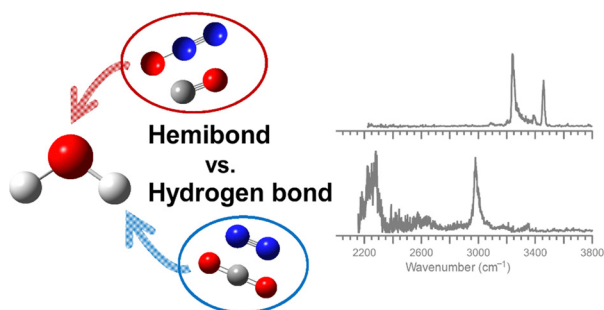
In silico design of miniprotein to inhibit SARS-CoV-2 variant Omicron spike protein

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



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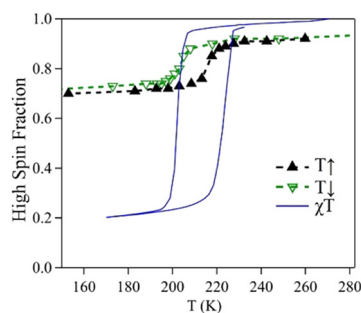
14726



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*

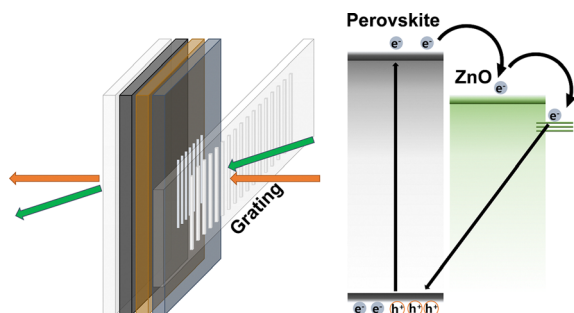
14736



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*

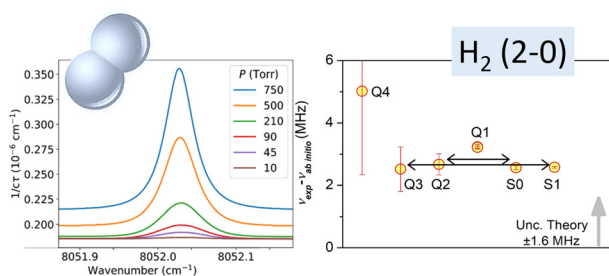
14742



A new strategy for monitoring the charge transfer from perovskite thin films to electron transport layers using a heterodyne transient grating technique

Young Hyun Kim and Woon Yong Sohn*

14749



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

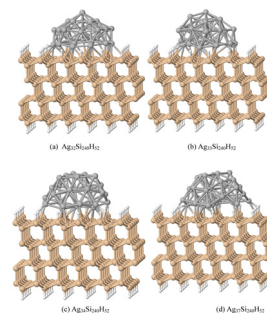
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14757

Photoabsorbance of supported metal clusters: *ab initio* density matrix and model studies of large Ag clusters on Si surfaces

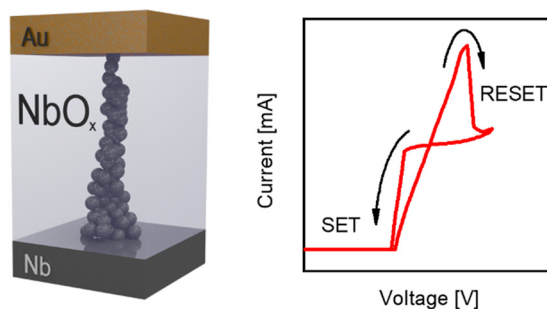
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14766

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

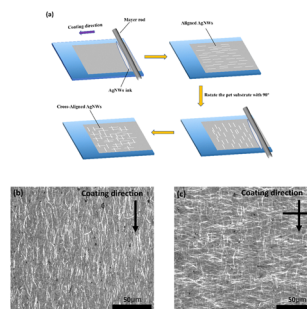
Giuseppe Leonetti, Matteo Fretto, Katarzyna Bejtka, Elena Sonia Olivetti, Fabrizio Candido Pirri, Natascia De Leo, Iliia Valov and Gianluca Milano*



14778

Multilayer directionally arranged silver nanowire networks for flexible transparent conductive films

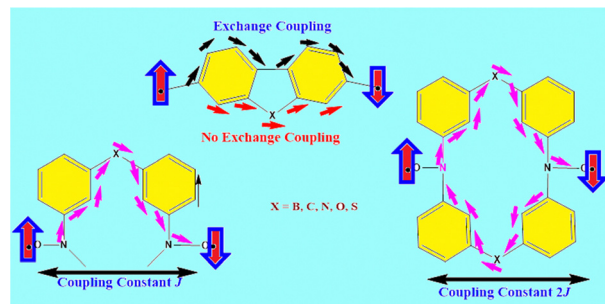
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14786

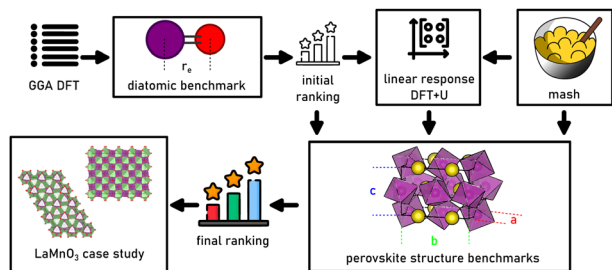
The effect of hetero-atoms on spin exchange coupling pathways (ECPs): a computational investigation

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



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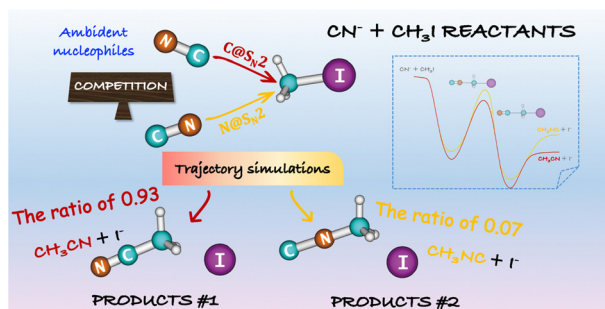
14799



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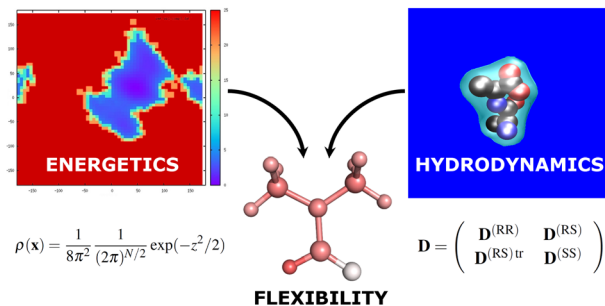
Peter Kraus,* Paolo Raiteri and Julian D. Gale

14812

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*

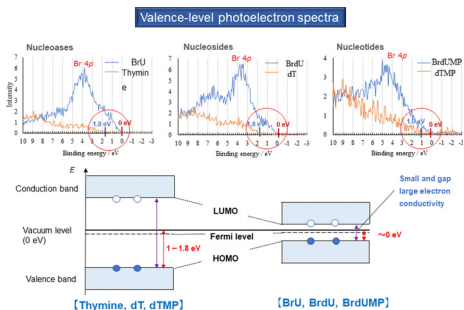
14822



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

Sergio Rampino, Mirco Zerbetto* and Antonino Polimeno

14836



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

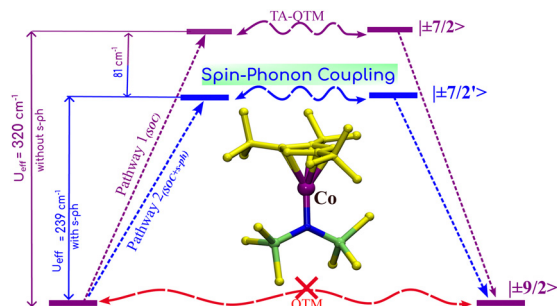


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14848

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

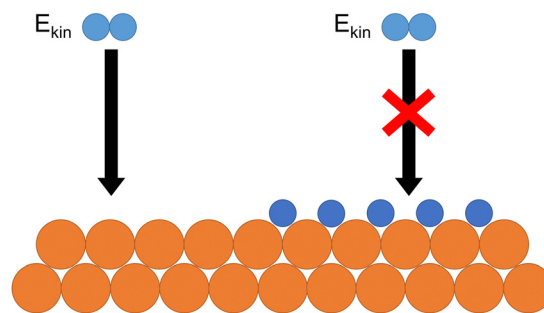
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14862

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

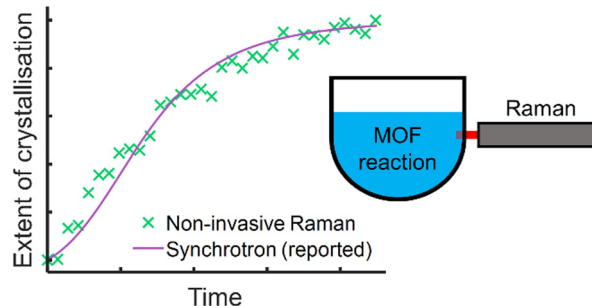
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14869

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

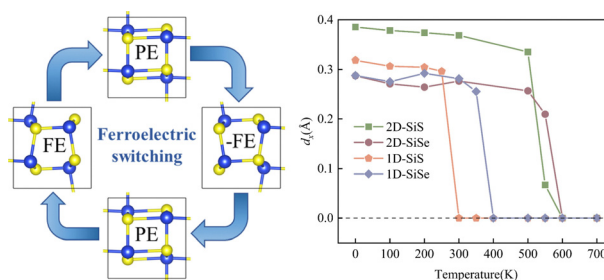
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14879

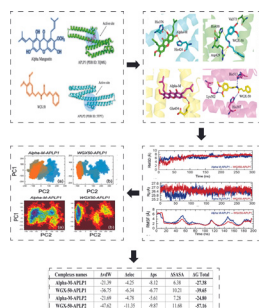
Robust ferroelectricity in low-dimensional δ-SiX (X = S/Se): a first-principles study

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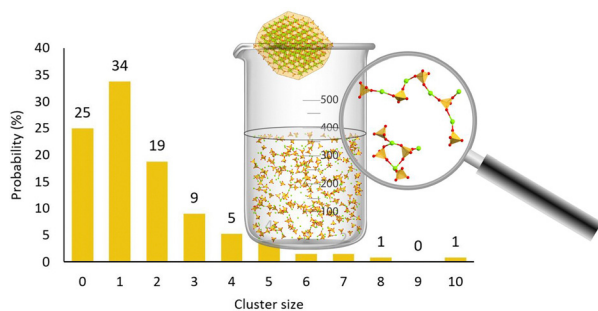
14887



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*

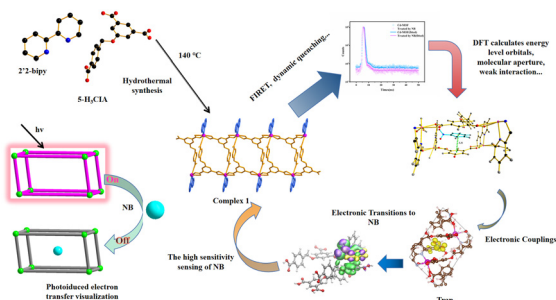
14898



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

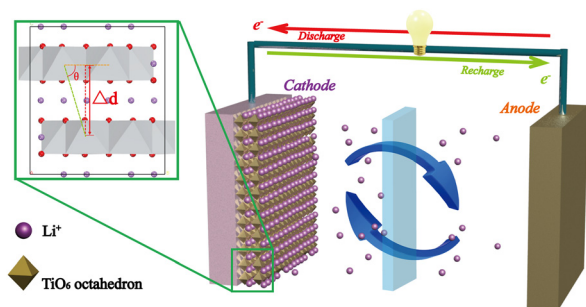
14907



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

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

14918



Pressure-induced phase transition toward high symmetry in zero-strain Li₂TiO₃

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

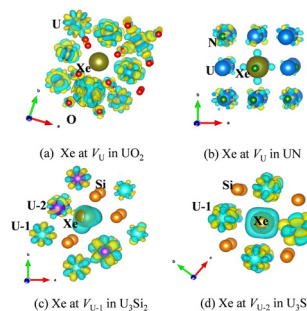


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14928

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

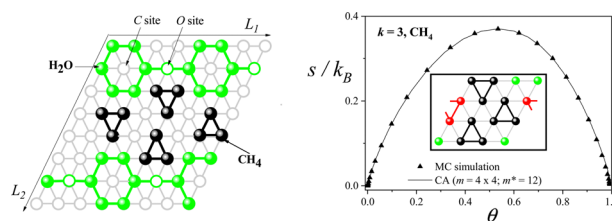
Jiajun Zhao, Dan Sun, Liu Xi, Ping Chen, Jijun Zhao and Yuanyuan Wang*



14942

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

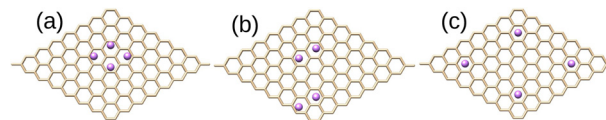
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14955

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

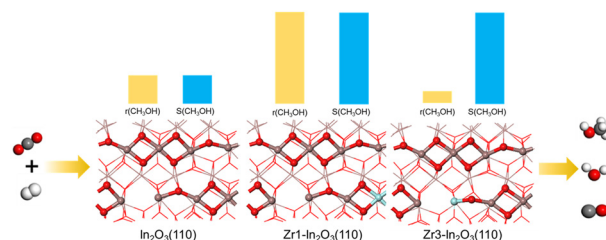
Hamed Abbasian



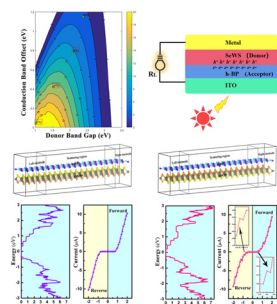
14961

DFT-based microkinetic studies on methanol synthesis from CO_2 hydrogenation over In_2O_3 and $\text{Zr-In}_2\text{O}_3$ catalysts

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



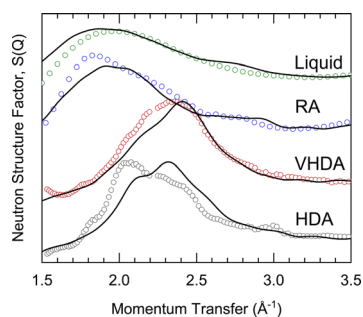
14969



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*

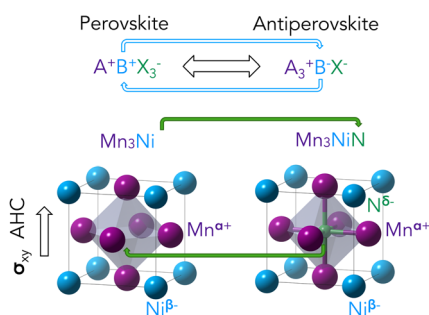
14981



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

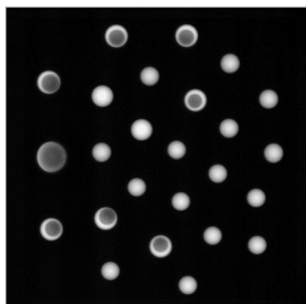
14992



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

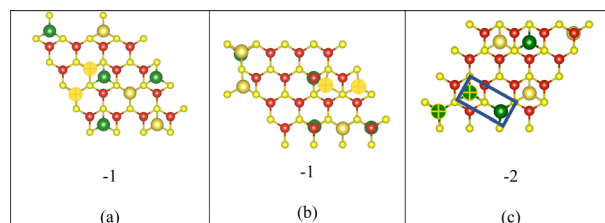


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15008

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

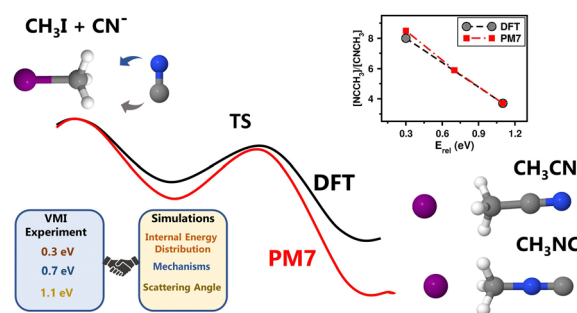
Darwin B. Putungan, Shaosen Su, Liang Gao, Ankit Goyal, Shi-Hsin Lin and Akhil Garg*



15015

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

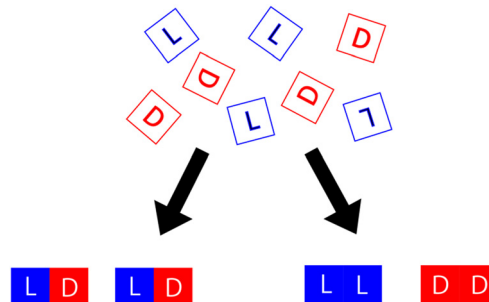
Akash Gutal and Manikandan Paranjothy*



15023

Enantioselective amino acid interactions in solution

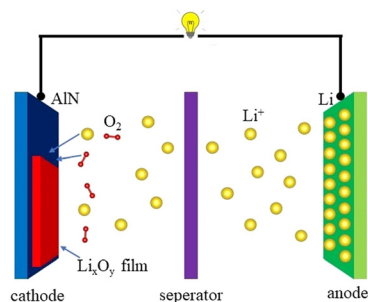
Natsuki Watanabe, Mitsuo Shoji,* Koichi Miyagawa, Yuta Hori, Mauro Boero, Masayuki Umemura and Yasuteru Shigeta



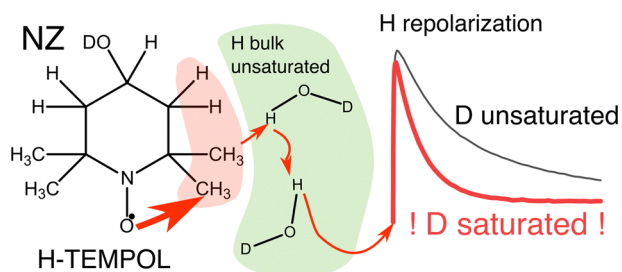
15030

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



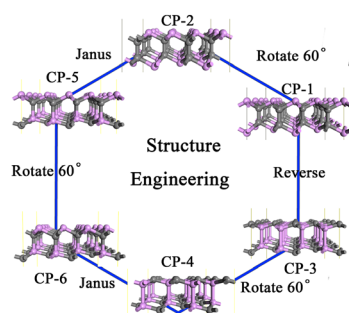
15040



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

