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Cover

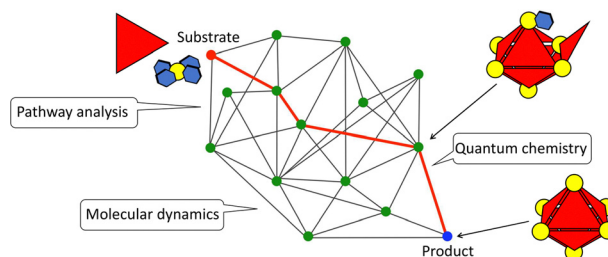
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PERSPECTIVES

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Theoretical and computational methodologies for understanding coordination self-assembly complexes

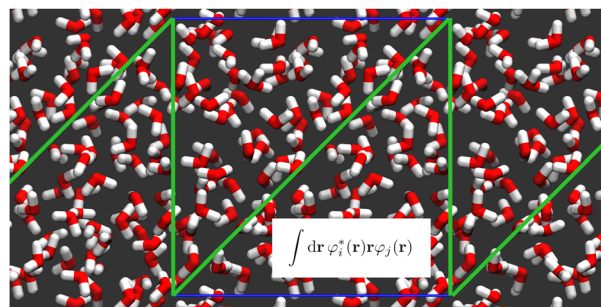
Satoshi Takahashi,* Satoru Iuchi, Shuichi Hiraoka and Hirofumi Sato*



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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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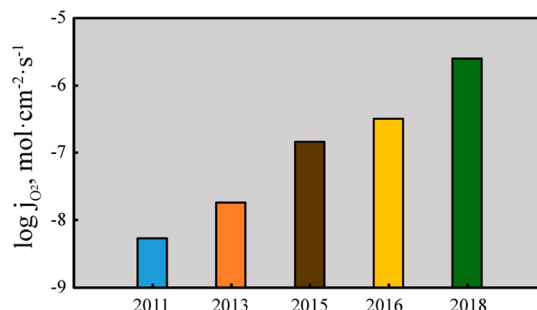


PERSPECTIVES

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Oxygen separation diffusion-bubbling membranes

Valery V. Belousov



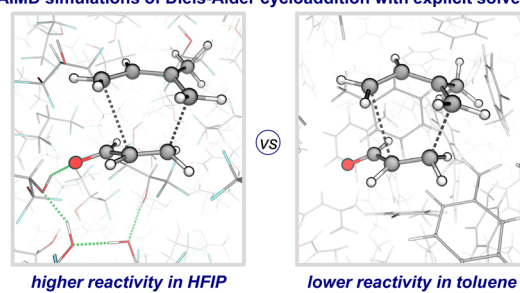
COMMUNICATION

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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

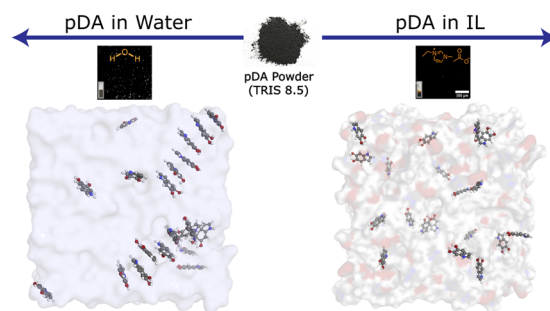


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14700

Structural elucidation of polydopamine facilitated by ionic liquid solvation

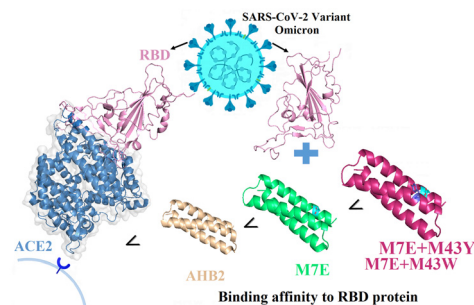
Abhishek Singh, Thomas G. Mason, Zhenzhen Lu, Anita J. Hill, Steven J. Pas, Boon Mia Teo, Benny D. Freeman and Ekaterina I. Izgorodina*



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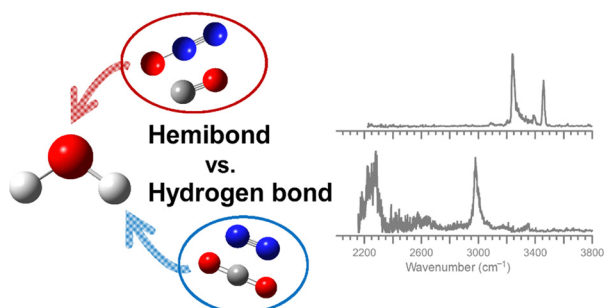
In silico design of miniprotein to inhibit SARS-CoV-2 variant Omicron spike protein

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



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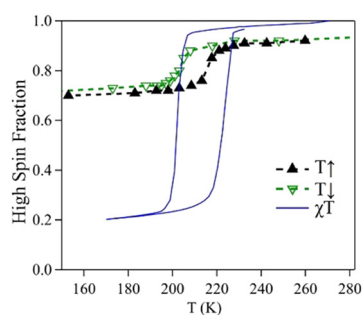
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Infrared spectroscopy of $[\text{H}_2\text{O}-\text{X}_n]^+$ ($n = 1-3$, $\text{X} = \text{N}_2, \text{CO}_2, \text{CO}$, and N_2O) radical cation clusters: competition between hydrogen bond and hemibond formation of the water radical cation

Mizuhiro Kominato and Asuka Fujii*

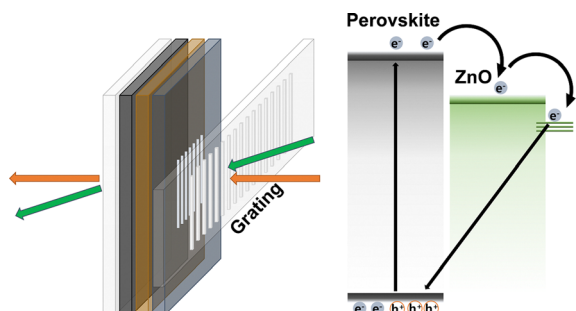
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Surface stabilisation of the high-spin state of Fe(II) spin-crossover complexes

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

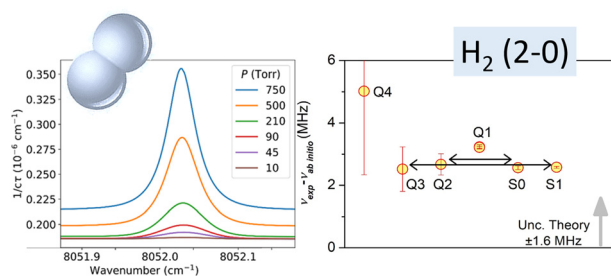
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A new strategy for monitoring the charge transfer from perovskite thin films to electron transport layers using a heterodyne transient grating technique

Young Hyun Kim and Woon Yong Sohn*

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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*

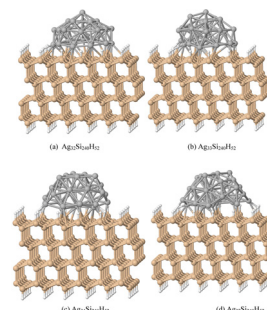


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Photoabsorbance of supported metal clusters: *ab initio* density matrix and model studies of large Ag clusters on Si surfaces

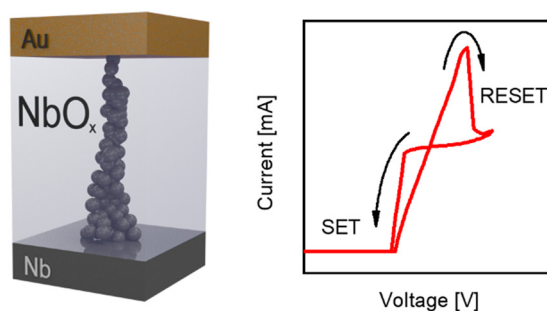
Tijo Vazhappilly, Dmitri S. Kilin and David A. Micha*



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

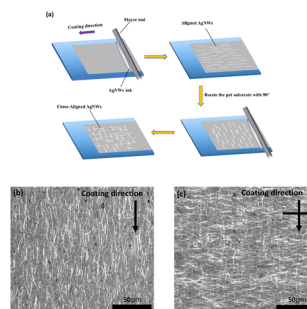
Giuseppe Leonetti, Matteo Fretto, Katarzyna Bejtka, Elena Sonia Olivetti, Fabrizio Candido Pirri, Natascia De Leo, Ilia Valov and Gianluca Milano*



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Multilayer directionally arranged silver nanowire networks for flexible transparent conductive films

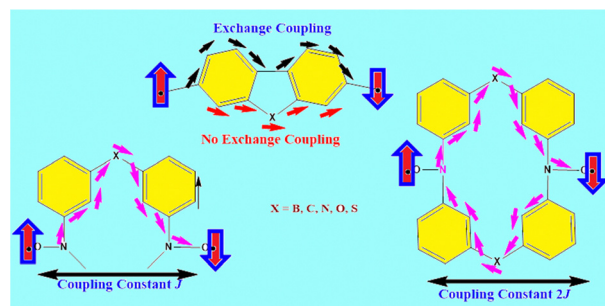
Zhijiang Guo, Xiaoli Li, Ning Li, Xuanji Liu, Haojie Li, Xuezhi Li, Yuxuan Wang, Jianguo Liang* and Zhanchun Chen*



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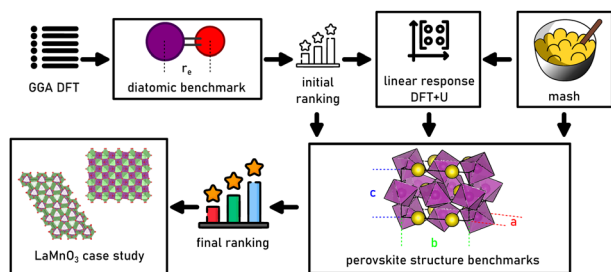
The effect of hetero-atoms on spin exchange coupling pathways (ECPs): a computational investigation

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



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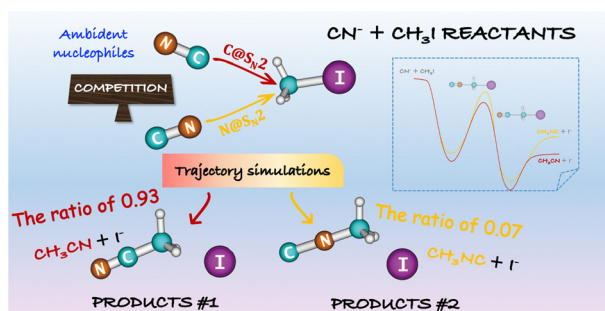
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Computational workflows for perovskites: case study for lanthanide manganites

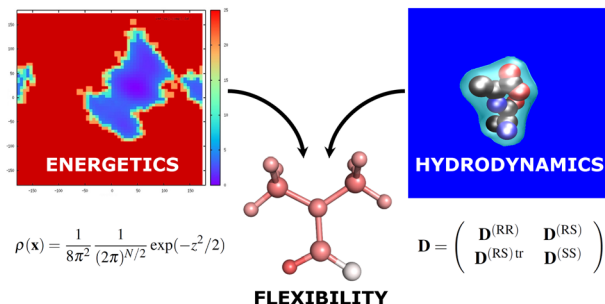
Peter Kraus,* Paolo Raiteri and Julian D. Gale

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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*

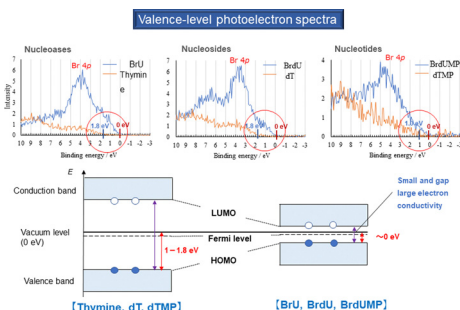
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The roto-conformational diffusion tensor as a tool to interpret molecular flexibility

Sergio Rampino, Mirco Zerbetto* and Antonino Polimeno

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

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

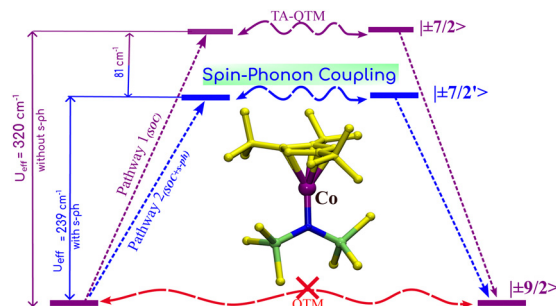


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The impact of spin-vibrational coupling on magnetic relaxation of a Co(II) single-molecule magnet

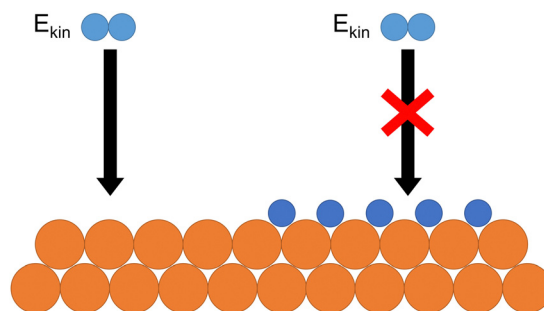
Sakshi Nain, Manish Kumar and Md. Ehesan Ali*



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

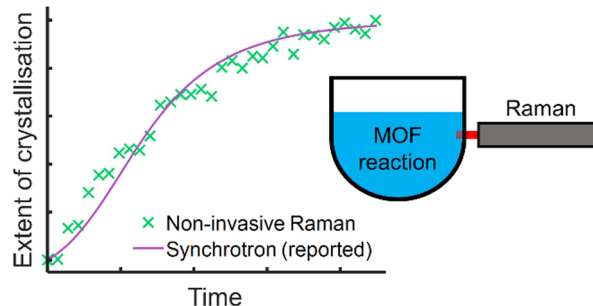
Diyu Zhang, Charlotte Jansen, Aart W. Kleyn and Ludo B. F. Juurlink*



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

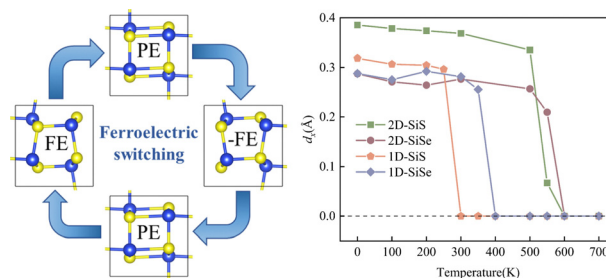
Magdalene W. S. Chong,* Andrew J. Parrott,* David J. Ashworth, Ashleigh J. Fletcher and Alison Nordon

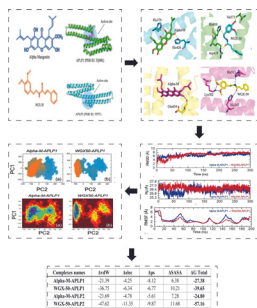


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Robust ferroelectricity in low-dimensional δ -SiX (X = S/Se): a first-principles study

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





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*

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*

Figure 1: Probability distribution of cluster sizes. The bar chart shows the probability (%) of clusters of size 0 to 10. The distribution is unimodal, peaking at size 1 (34%). An inset shows a 3D model of a cluster of size 10, with a magnified view of the molecular structure.

Cluster size	Probability (%)
0	25
1	34
2	19
3	9
4	5
5	3
6	2
7	1
8	1
9	0
10	1

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

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

2,2'-bipy

5-H₂C/TA

140 °C

Hydrothermal synthesis

$h\nu$

NB

OH⁻

Photoluminescence electron transfer visualization

Complex 1

The high sensitivity sensing of NB

0.578 eV was transferred

Trap

Electronic Transitions to NB

Electronic Coupling

DFT calculates energy level orbitals, molecular orbital, weak interaction...

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

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

Legend:

- Li^+ (purple circle)
- TiO_6 octahedron (brown diamond)

Diagram Labels:

- Cathode
- Anode
- Discharge
- Recharge
- e^-
- Δd
- θ

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

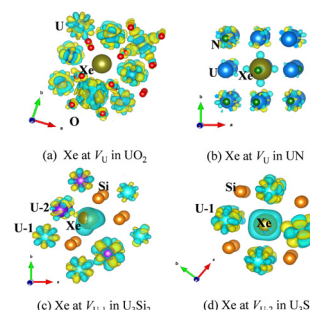
Wenming Qi, Hadiqa Abdugopur, Wei Xu, Min Gao,*
Anwar Hushur* and Hongyan Zhang*

RESEARCH PAPERS

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

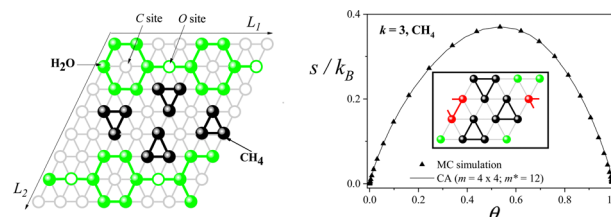
Jiajun Zhao, Dan Sun, Liu Xi, Ping Chen, Jijun Zhao and Yuanyuan Wang*



14942

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

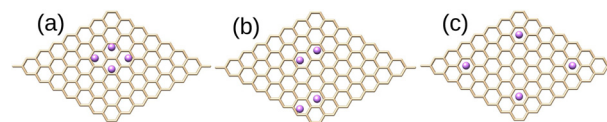
Noris M. De La Cruz Feliz, Pablo J. Longone, Fabricio O. Sanchez-Varretti, Fernando M. Bulnes and Antonio J. Ramirez-Pastor*



14955

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

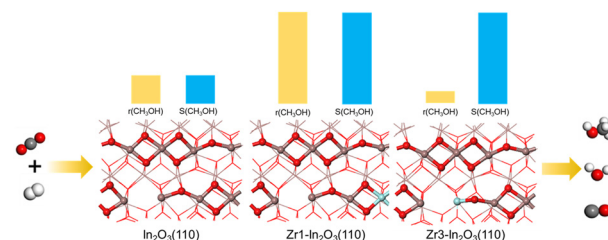
Hamed Abbasian



14961

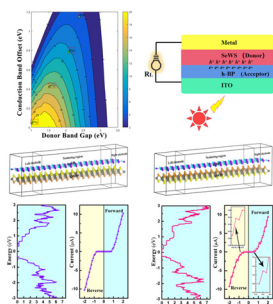
DFT-based microkinetic studies on methanol synthesis from CO_2 hydrogenation over In_2O_3 and Zr– In_2O_3 catalysts

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



RESEARCH PAPERS

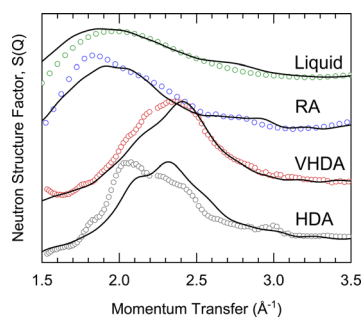
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Reconfigurable band alignment of SWSe/h-BP heterostructures for photoelectric applications

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

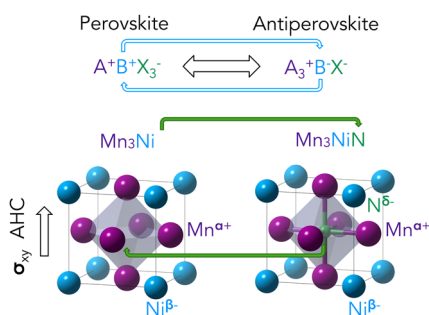
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Neutron scattering study of polyamorphic THF·17(H₂O) – toward a generalized picture of amorphous states and structures derived from clathrate hydrates

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

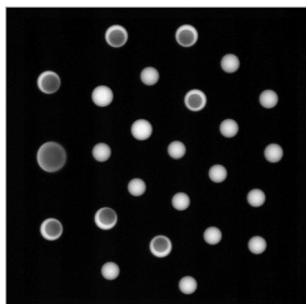
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Anionic nickel and nitrogen effects in the chiral antiferromagnetic antiperovskite Mn₃NiN

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

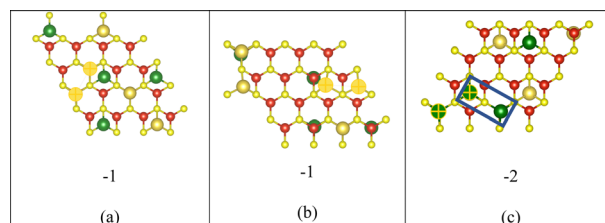


RESEARCH PAPERS

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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

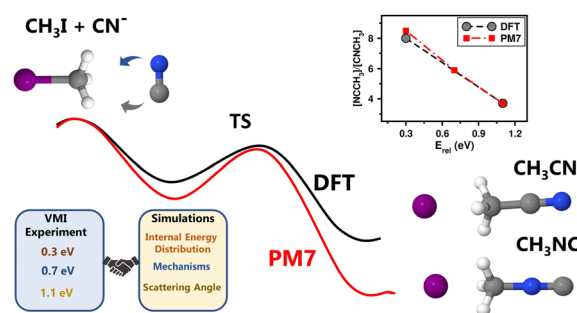
Darwin B. Putungan, Shaosen Su, Liang Gao, Ankit Goyal, Shi-Hsin Lin and Akhil Garg*



15015

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

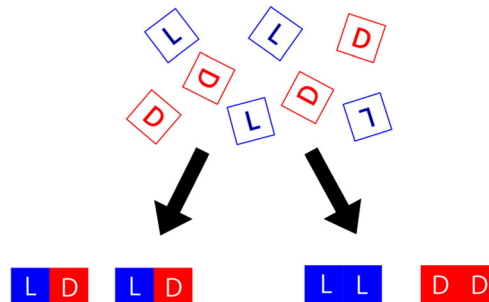
Akash Gutal and Manikandan Paranjothy*



15023

Enantioselective amino acid interactions in solution

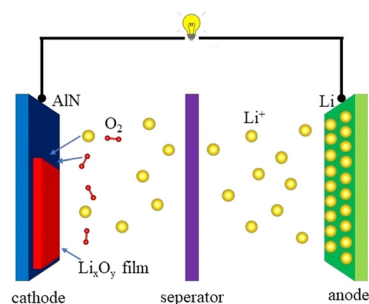
Natsuki Watanabe, Mitsuo Shoji,* Koichi Miyagawa, Yuta Hori, Mauro Boero, Masayuki Umemura and Yasuteru Shigeta



15030

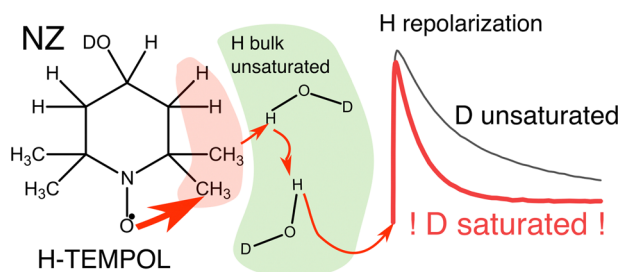
Bilayer tetragonal AlN nanosheets as potential cathodes for Li–O₂ batteries

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



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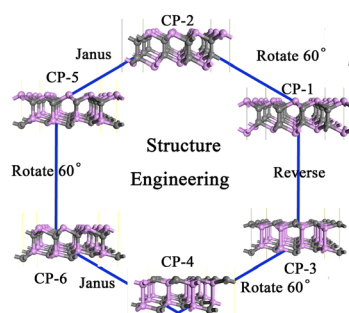
15040



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*

15052



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

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

