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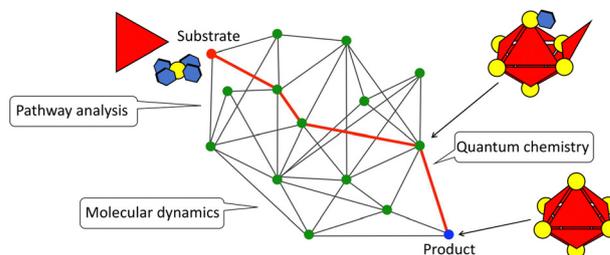
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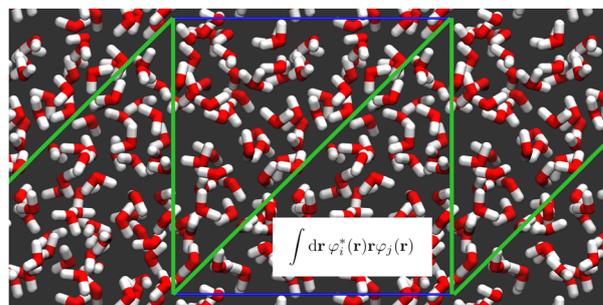
Satoshi Takahashi,\* Satoru Iuchi, Shuichi Hiraoka and Hirofumi Sato\*



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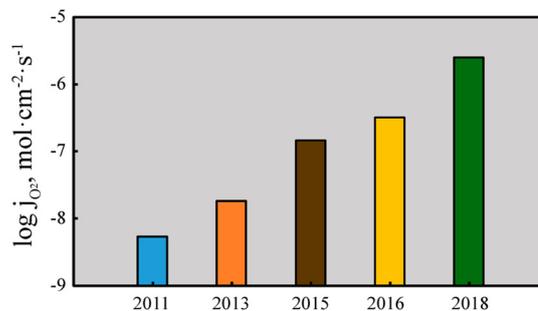


## PERSPECTIVES

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## Oxygen separation diffusion-bubbling membranes

Valery V. Belousov



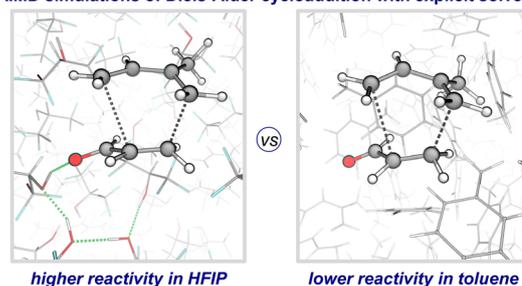
## COMMUNICATION

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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

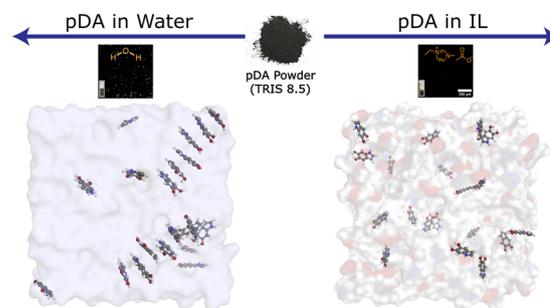


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## Structural elucidation of polydopamine facilitated by ionic liquid solvation

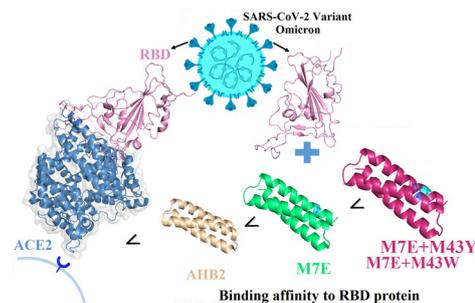
Abhishek Singh, Thomas G. Mason, Zhenzhen Lu, Anita J. Hill, Steven J. Pas, Boon Mia Teo, Benny D. Freeman and Ekaterina I. Izgorodina\*



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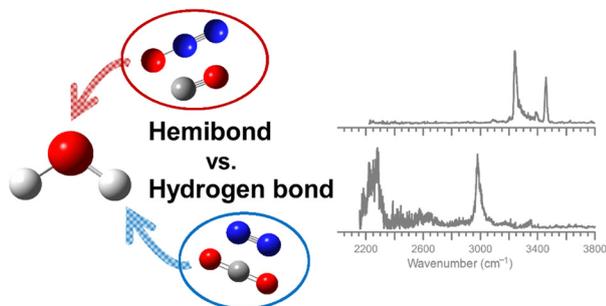
*In silico* design of miniprotein to inhibit SARS-CoV-2 variant Omicron spike protein

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



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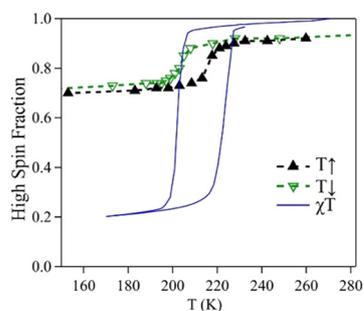
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**Infrared spectroscopy of  $[\text{H}_2\text{O}-\text{X}_n]^+$  ( $n = 1-3$ ,  $\text{X} = \text{N}_2, \text{CO}_2, \text{CO}$ , and  $\text{N}_2\text{O}$ ) radical cation clusters: competition between hydrogen bond and hemibond formation of the water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

Mizuhiro Kominato and Asuka Fujii\*

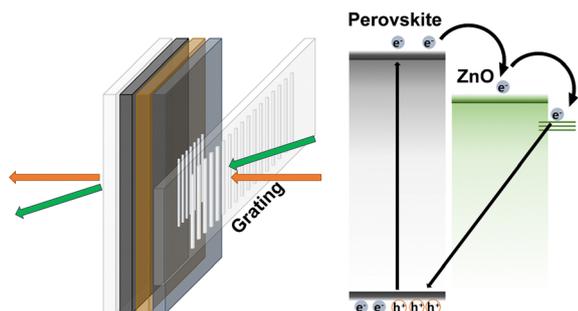
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**Surface stabilisation of the high-spin state of Fe(II) spin-crossover complexes**

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

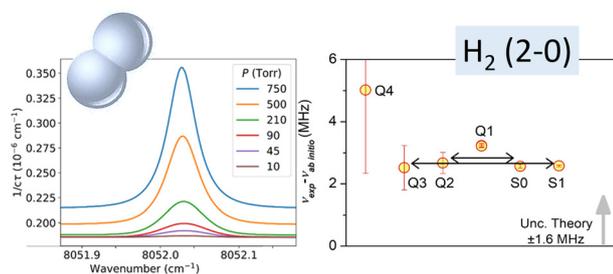
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Young Hyun Kim and Woon Yong Sohn\*

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**The high-accuracy spectroscopy of  $\text{H}_2$  rovibrational transitions in the (2-0) band near  $1.2 \mu\text{m}$**

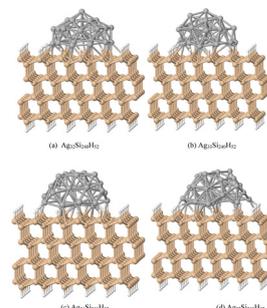
H. Fleurbaey, A. O. Koroleva, S. Kassi and A. Campargue\*



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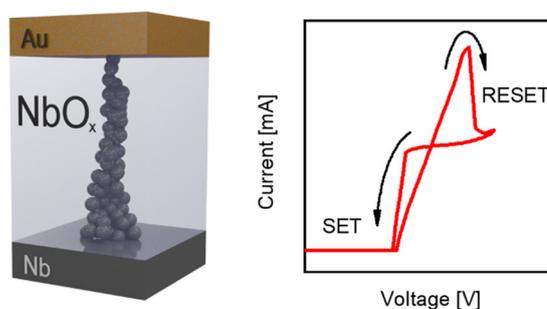
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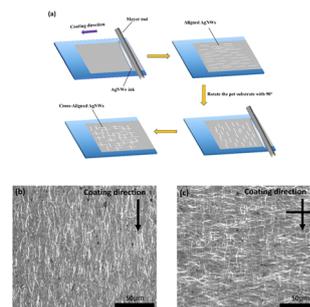
Giuseppe Leonetti, Matteo Fretto, Katarzyna Bejtka, Elena Sonia Olivetti, Fabrizio Candido Pirri, Natascia De Leo, Iliia Valov and Gianluca Milano\*



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



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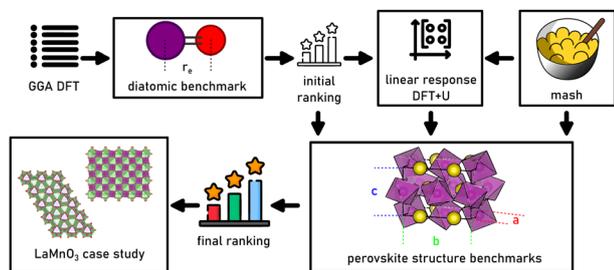
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Suranjan Shil,\* Debojit Bhattacharya, Anirban Misra, Yenni P. Ortiz and Douglas J. Klein



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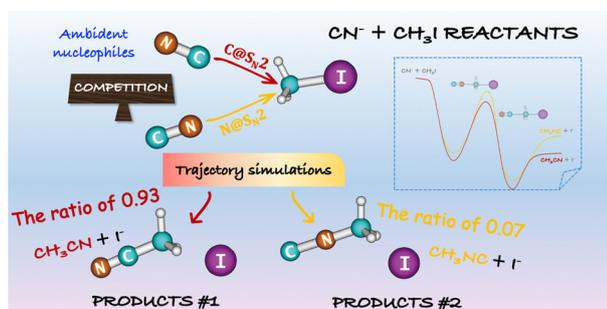
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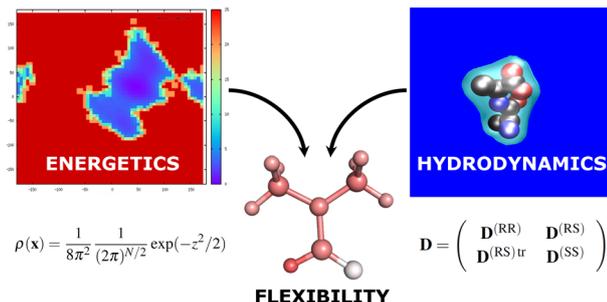
Peter Kraus,\* Paolo Raiteri and Julian D. Gale

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

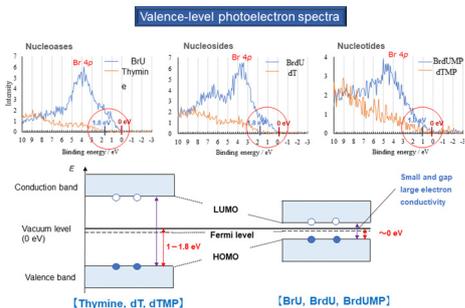
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Sergio Rampino, Mirco Zerbetto\* and Antonino Polimeno

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

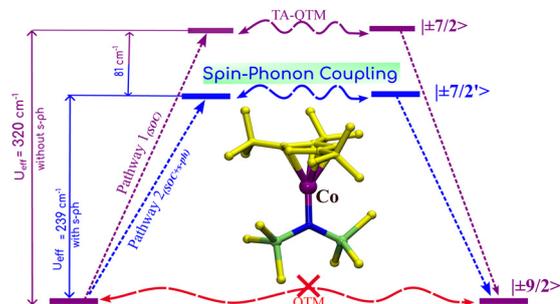


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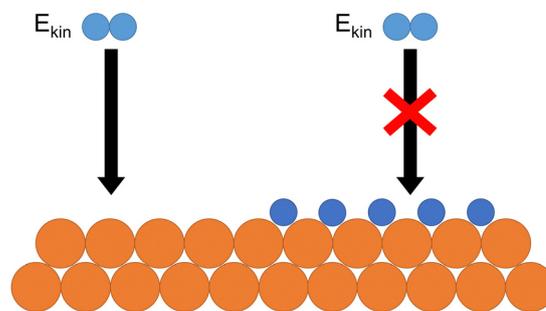
Sakshi Nain, Manish Kumar and Md. Ehesan Ali\*



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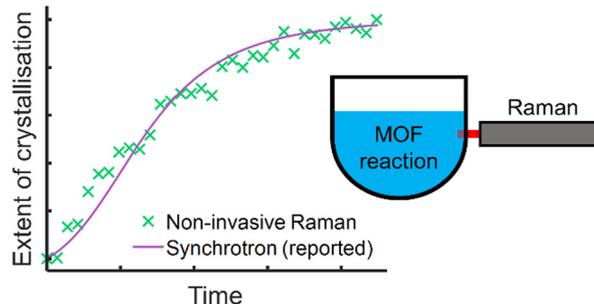
Diyu Zhang, Charlotte Jansen, Aart W. Kleyn and Ludo B. F. Juurlink\*



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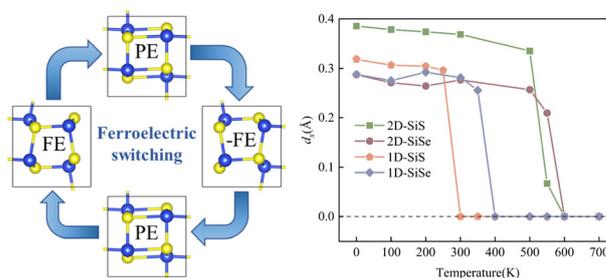
Magdalene W. S. Chong,\* Andrew J. Parrott,\* David J. Ashworth, Ashleigh J. Fletcher and Alison Nordon



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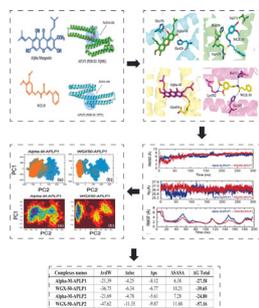
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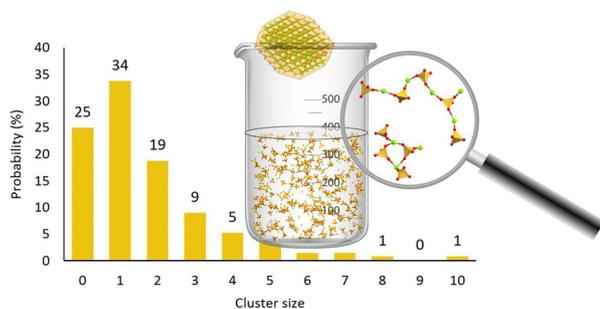
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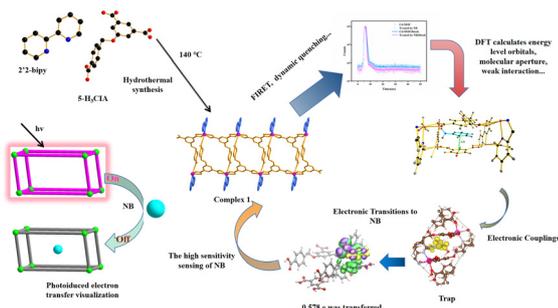
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### A total scattering study of prenucleation structures in saturated aqueous magnesium sulfate – observation of extended clusters

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

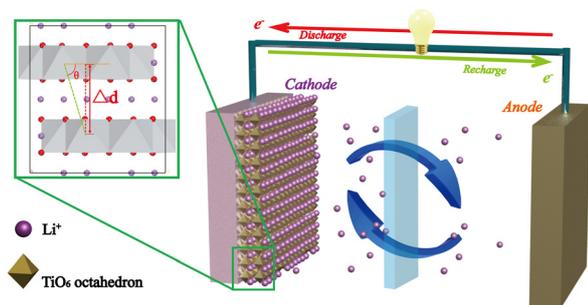
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Xiaoming Song, Wenzhuo Dong, Xiufang Hou,\* Qingxia Zhao, Zhuangzhuang Zhang and Yixia Ren\*

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

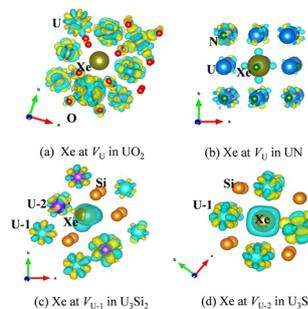


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Understanding xenon and vacancy behavior in  $\text{UO}_2$ ,  $\text{UN}$  and  $\text{U}_3\text{Si}_2$ : a comparative DFT+ $U$  study

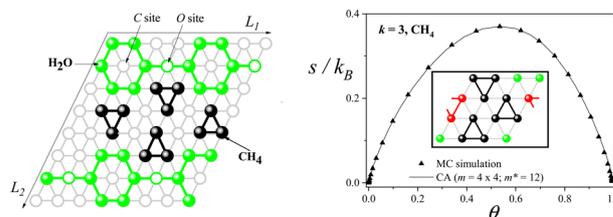
Jiajun Zhao, Dan Sun, Liu Xi, Ping Chen, Jijun Zhao and Yuanyuan Wang\*



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

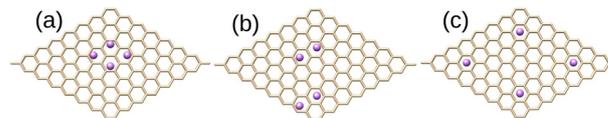
Noris M. De La Cruz Feliz, Pablo J. Longone, Fabricio O. Sanchez-Varretti, Fernando M. Bulnes and Antonio J. Ramirez-Pastor\*



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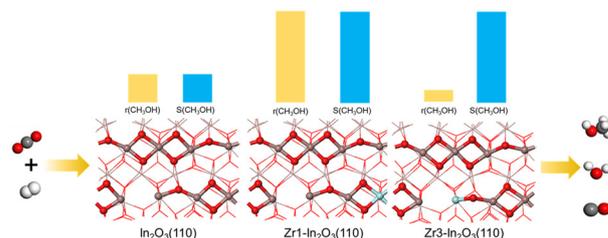
Hamed Abbasian



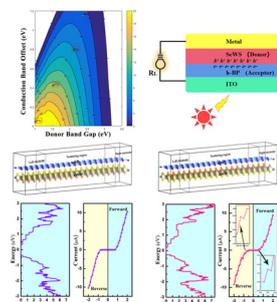
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DFT-based microkinetic studies on methanol synthesis from  $\text{CO}_2$  hydrogenation over  $\text{In}_2\text{O}_3$  and  $\text{Zr-In}_2\text{O}_3$  catalysts

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



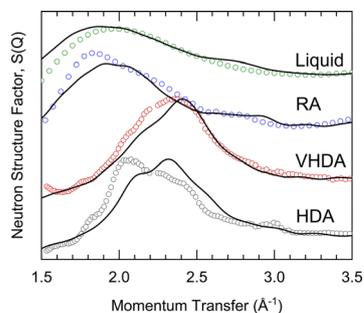
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### Reconfigurable band alignment of SWSe/h-BP heterostructures for photoelectric applications

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

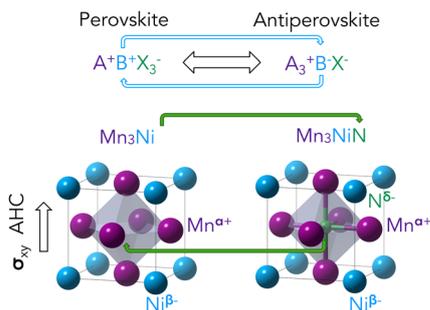
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### Neutron scattering study of polyamorphic THF·17(H<sub>2</sub>O) – toward a generalized picture of amorphous states and structures derived from clathrate hydrates

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

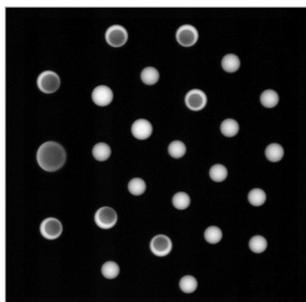
14992



### Anionic nickel and nitrogen effects in the chiral antiferromagnetic antiperovskite Mn<sub>3</sub>NiN

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

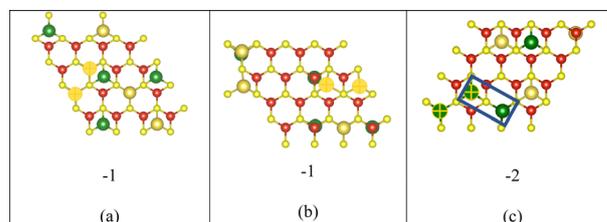


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15008

### Prediction of sodium binding energy on 2D VS<sub>2</sub> via machine learning: a robust accompanying method to *ab initio* random structure searching

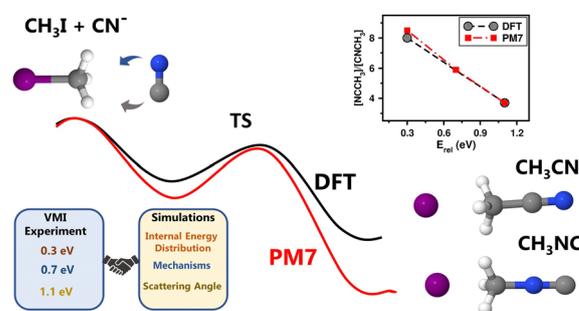
Darwin B. Putungan, Shaosen Su, Liang Gao, Ankit Goyal, Shi-Hsin Lin and Akhil Garg\*



15015

### Direct chemical dynamics simulations of CN<sup>-</sup> + CH<sub>3</sub>I bimolecular nucleophilic substitution reaction

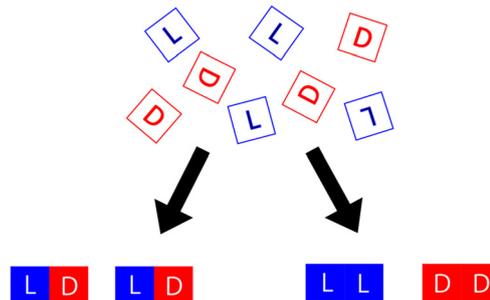
Akash Gutal and Manikandan Paranjothy\*



15023

### Enantioselective amino acid interactions in solution

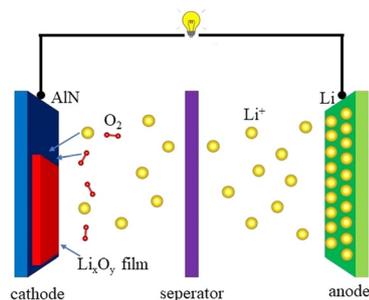
Natsuki Watanabe, Mitsuo Shoji,\* Koichi Miyagawa, Yuta Hori, Mauro Boero, Masayuki Umemura and Yasuteru Shigeta



15030

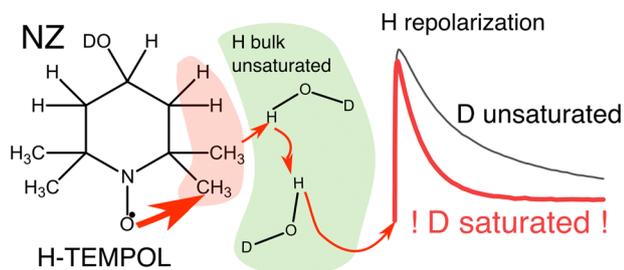
### Bilayer tetragonal AlN nanosheets as potential cathodes for Li-O<sub>2</sub> batteries

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



## RESEARCH PAPERS

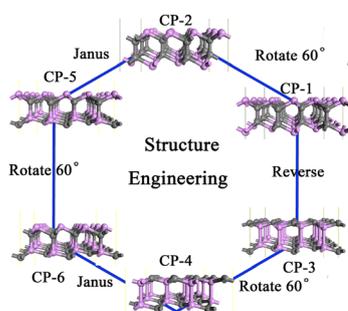
15040



### 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 Birlirakis, Geoffrey Bodenhausen, Alexandra V. Yurkovskaya and Daniel Abergel\*

15052



### Structure-engineering the stability, electronic, optical and photocatalytic properties of hexagonal C<sub>2</sub>P<sub>2</sub> monolayers

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

