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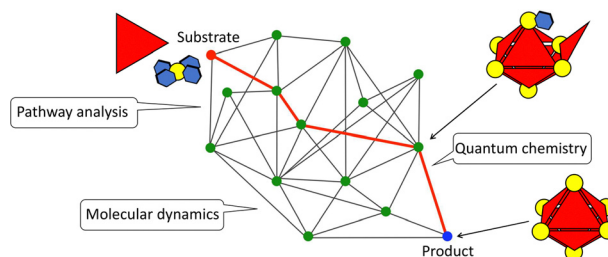
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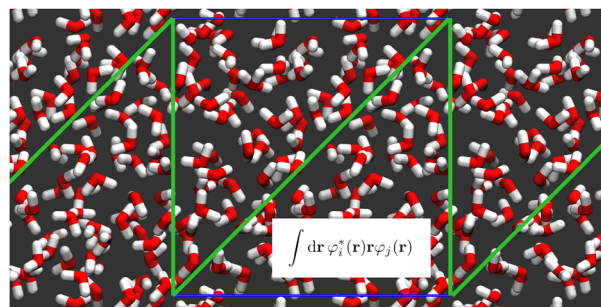
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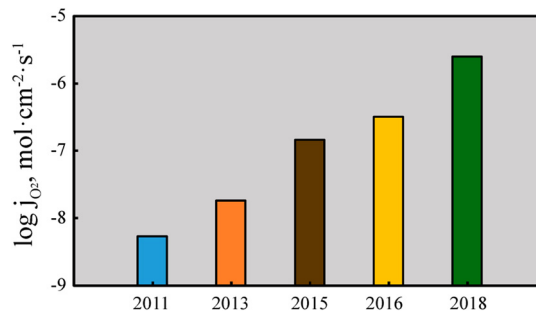


## PERSPECTIVES

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## Oxygen separation diffusion-bubbling membranes

Valery V. Belousov



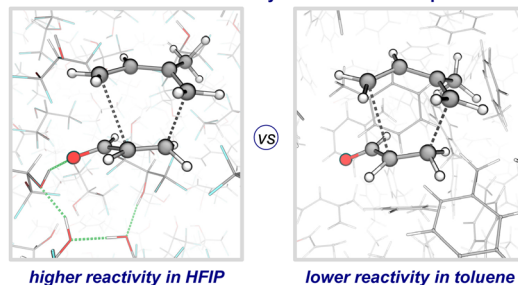
## COMMUNICATION

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

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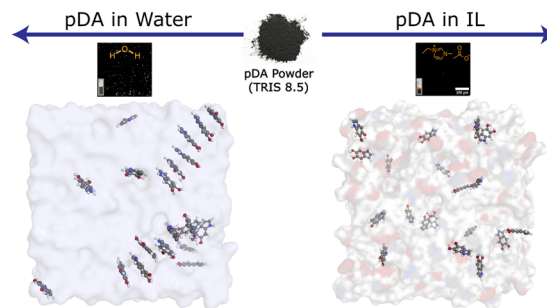


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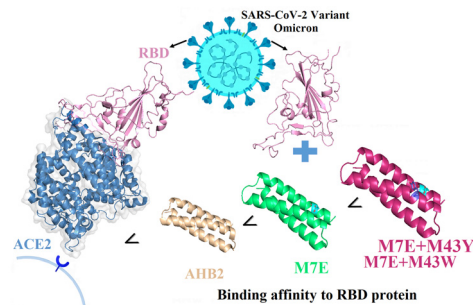
Abhishek Singh, Thomas G. Mason, Zhenzhen Lu, Anita J. Hill, Steven J. Pas, Boon Mia Teo, Benny D. Freeman and Ekaterina I. Izgorodina\*



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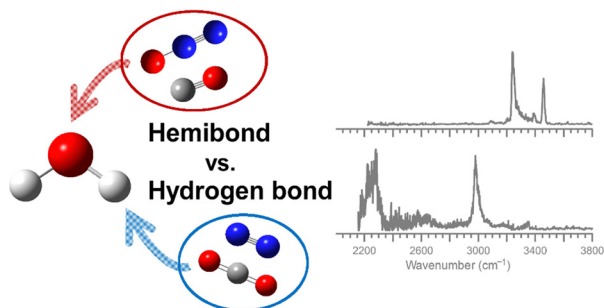
*In silico* design of miniprotein to inhibit SARS-CoV-2 variant Omicron spike protein

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



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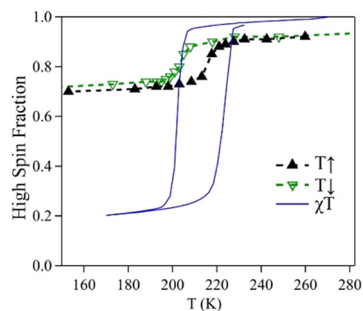
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**Infrared spectroscopy of  $[\text{H}_2\text{O}-\text{X}_n]^+$  ( $n = 1-3$ ,  $\text{X} = \text{N}_2, \text{CO}_2, \text{CO}$ , and  $\text{N}_2\text{O}$ ) radical cation clusters: competition between hydrogen bond and hemibond formation of the water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

Mizuhiro Kominato and Asuka Fujii\*

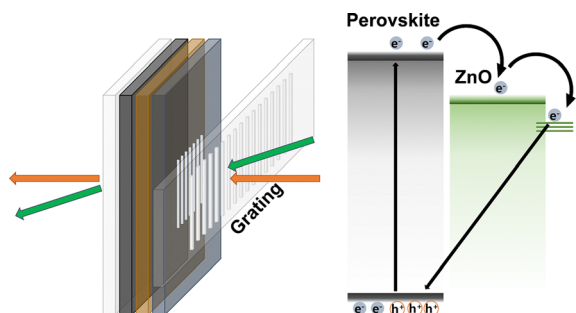
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**Surface stabilisation of the high-spin state of Fe(II) spin-crossover complexes**

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

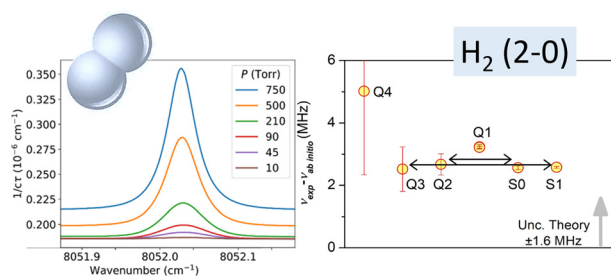
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Young Hyun Kim and Woon Yong Sohn\*

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

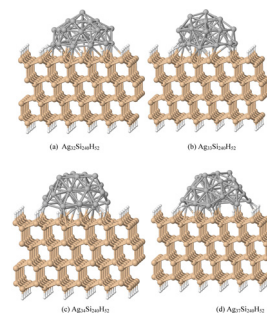


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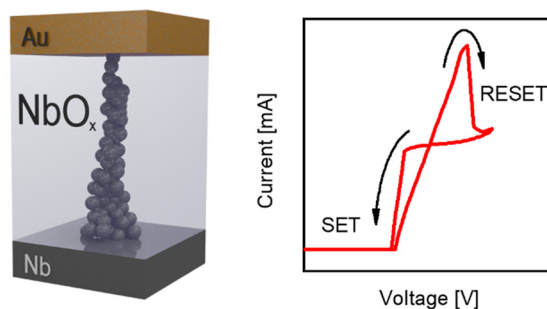
Tijo Vazhappilly, Dmitri S. Kilin and David A. Micha\*



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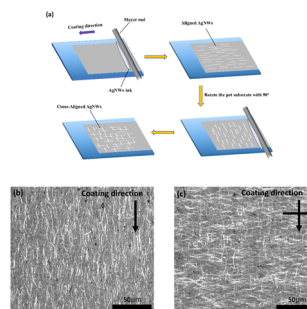
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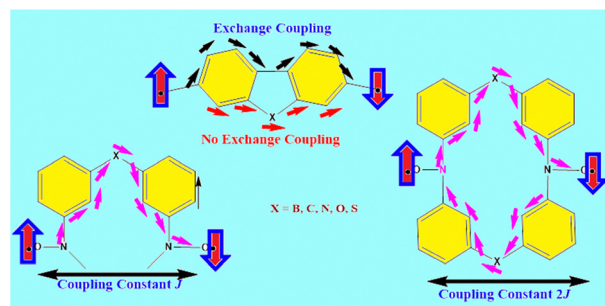
Zhijiang Guo, Xiaoli Li, Ning Li, Xuanji Liu, Haojie Li, Xuezhi Li, Yuxuan Wang, Jianguo Liang\* and Zhanchun Chen\*



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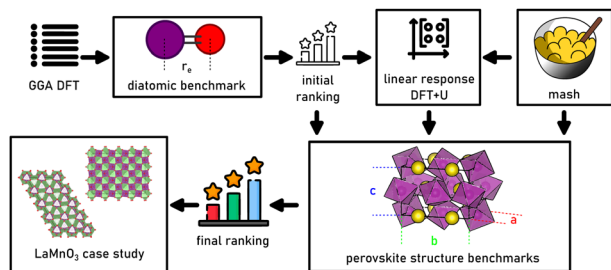
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Suranjan Shil,\* Debojit Bhattacharya, Anirban Misra, Yenni P. Ortiz and Douglas J. Klein



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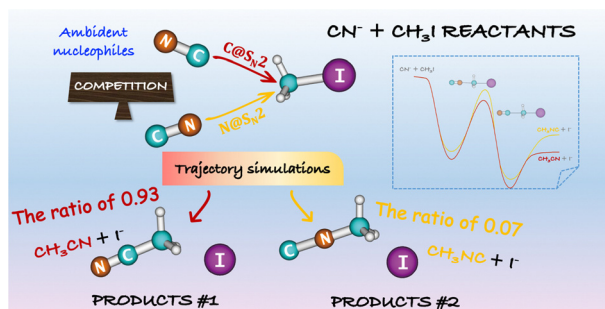
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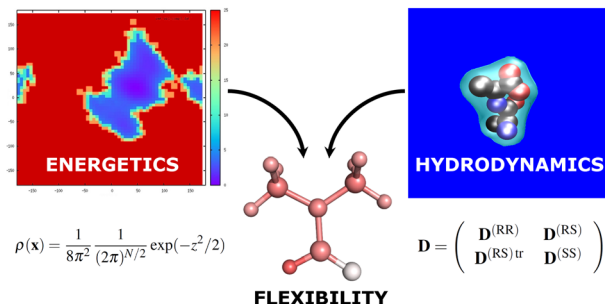
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Xu Liu, Shiqi Tian, Boxue Pang,\* Hui Li and Yang Wu\*

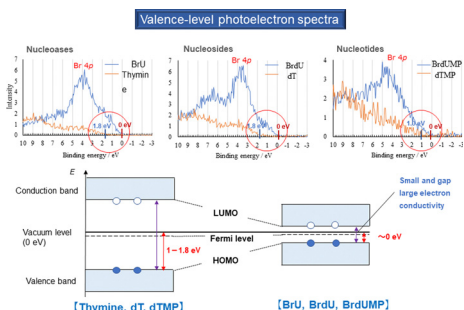
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Sergio Rampino, Mirco Zerbetto\* and Antonino Polimeno

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

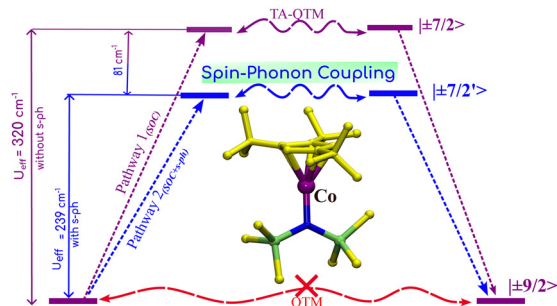


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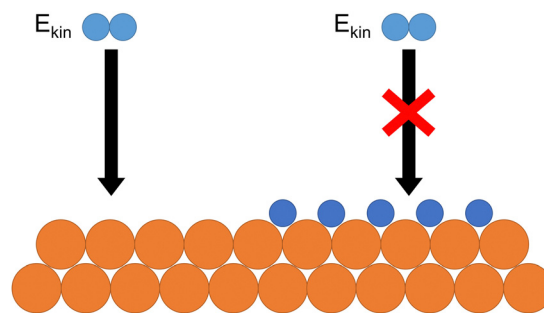
Sakshi Nain, Manish Kumar and Md. Ehesan Ali\*



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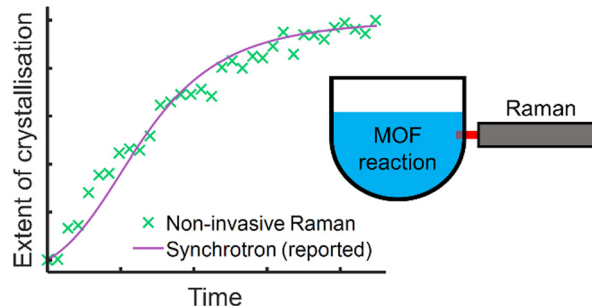
Diyu Zhang, Charlotte Jansen, Aart W. Kleyn and Ludo B. F. Juurlink\*



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

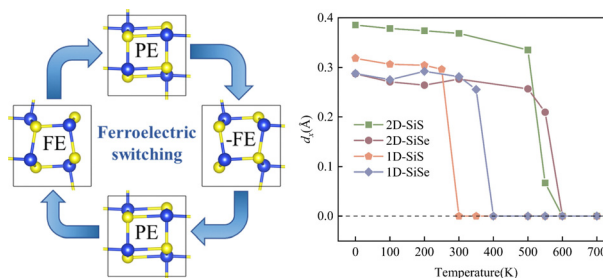
Magdalene W. S. Chong,\* Andrew J. Parrott,\* David J. Ashworth, Ashleigh J. Fletcher and Alison Nordon



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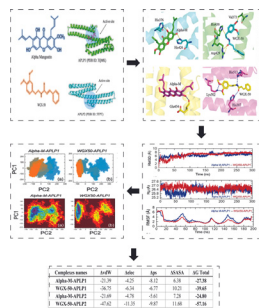
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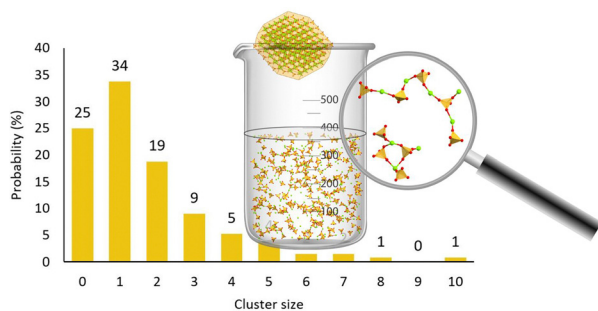
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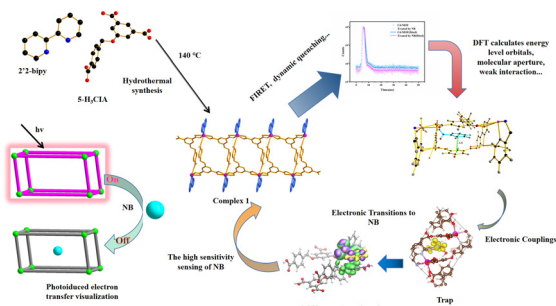
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Daniel J. M. Irving, Mark E. Light,\* Matilda P. Rhodes, Terence Threlfall and Thomas F. Headen

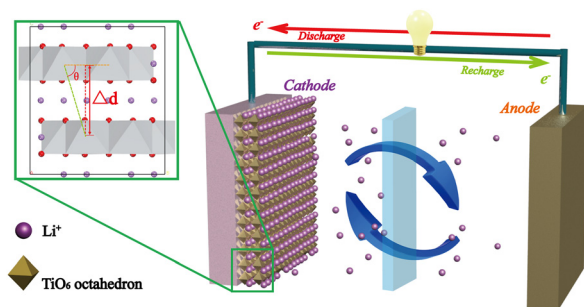
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### Pressure-induced phase transition toward high symmetry in zero-strain $\text{Li}_2\text{TiO}_3$

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



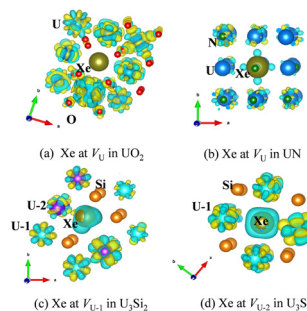


## RESEARCH PAPERS

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

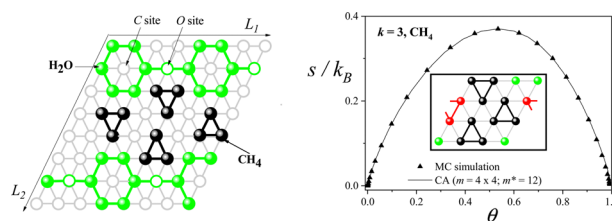
Jiajun Zhao, Dan Sun, Liu Xi, Ping Chen, Jijun Zhao and Yuanyuan Wang\*



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

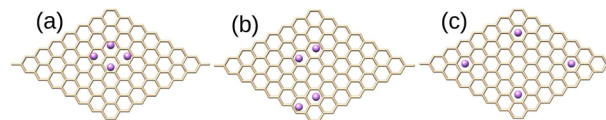
Noris M. De La Cruz Feliz, Pablo J. Longone, Fabricio O. Sanchez-Varretti, Fernando M. Bulnes and Antonio J. Ramirez-Pastor\*



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

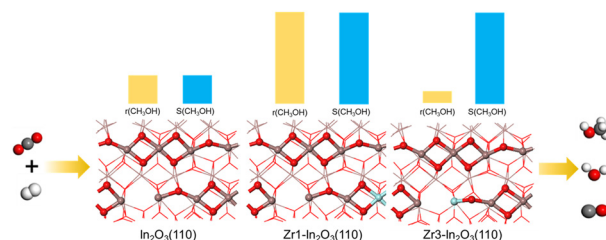
Hamed Abbasian



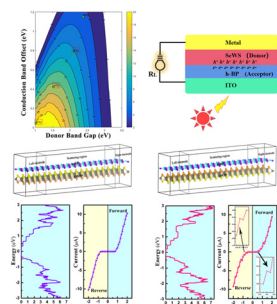
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DFT-based microkinetic studies on methanol synthesis from  $\text{CO}_2$  hydrogenation over  $\text{In}_2\text{O}_3$  and  $\text{Zr-In}_2\text{O}_3$  catalysts

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



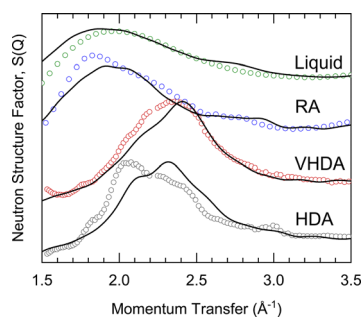
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### Reconfigurable band alignment of SWSe/h-BP heterostructures for photoelectric applications

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

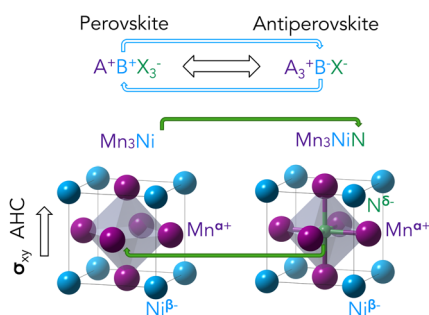
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### Neutron scattering study of polyamorphic THF·17(H<sub>2</sub>O) – toward a generalized picture of amorphous states and structures derived from clathrate hydrates

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

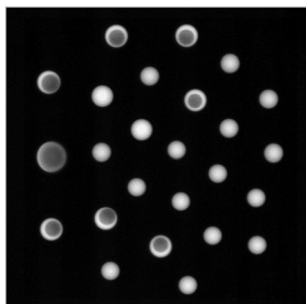
14992



### 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

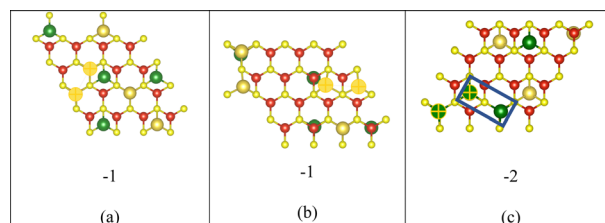


## RESEARCH PAPERS

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

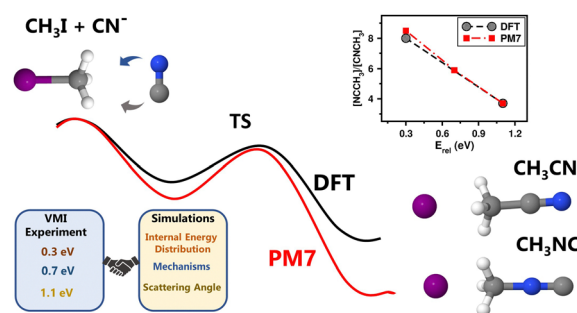
Darwin B. Putungan, Shaosen Su, Liang Gao, Ankit Goyal, Shi-Hsin Lin and Akhil Garg\*



15015

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

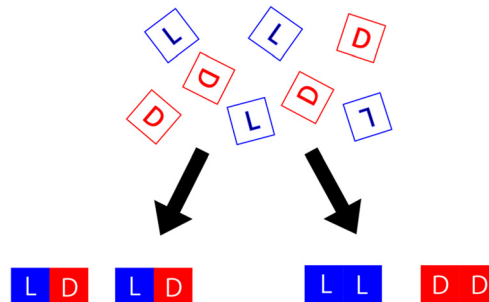
Akash Gutal and Manikandan Paranjothy\*



15023

### Enantioselective amino acid interactions in solution

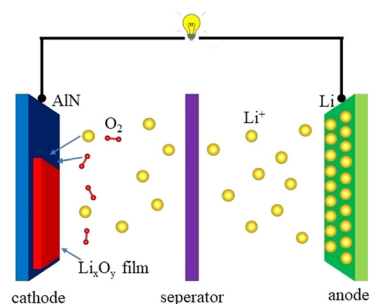
Natsuki Watanabe, Mitsuo Shoji,\* Koichi Miyagawa, Yuta Hori, Mauro Boero, Masayuki Umemura and Yasuteru Shigeta



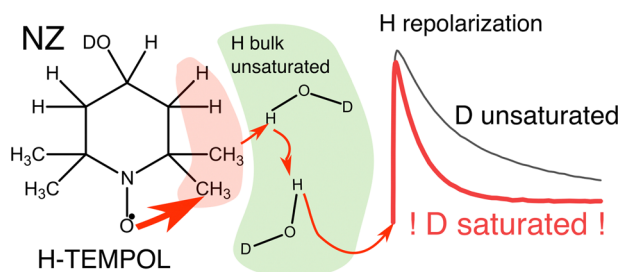
15030

### 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



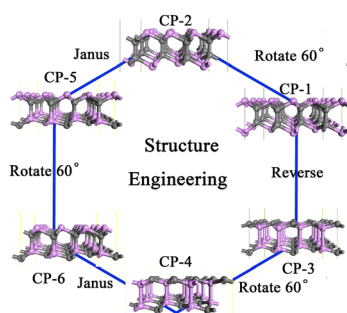
15040



### 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 C<sub>2</sub>P<sub>2</sub> monolayers

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

