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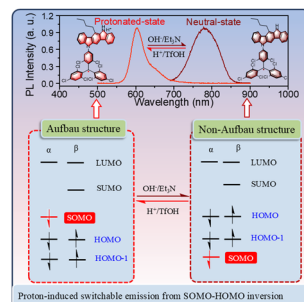
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## COMMUNICATIONS

9943

### A near-infrared luminescent organic radical with switchable emission and SOMO–HOMO inversion via a protonation/deprotonation process

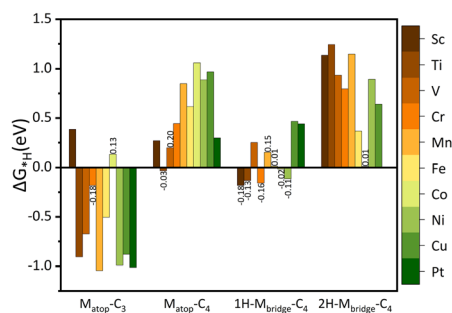
Ablikim Obolda,\* Parida Hazretomar, Mehrgul Abdulahat, Fudong Ma, Ayixiemuguli Tuersun, Zhaoze Ding and Zhuoyang Hu



9949

### Predicting a new class of diamond-supported transition-metal single-atom catalysts for hydrogen evolution

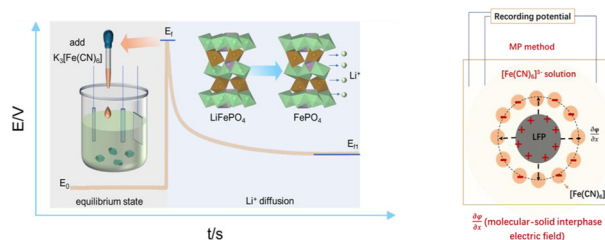
Sheng Qin, Ke Ding, Kaiye Zheng, Bifa Ji,\* Yongping Zheng\* and Yongbing Tang\*



9954

### A molecular titration strategy: utilizing a built-in electric field to measure the lithium diffusion coefficient in LiFePO<sub>4</sub>

Zexin Lin, Zhihao Deng, Xianrun Cao, Lu Guo, Feifei Zhang, Sheng Liu,\* Juezhi Yu\* and Gangfeng Ouyang

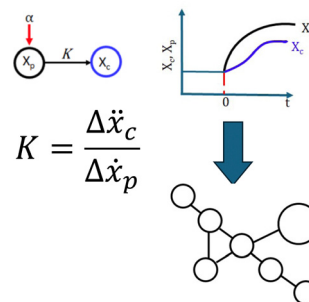


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9962

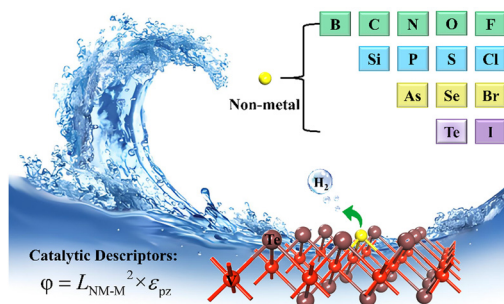
### Inferring networks of chemical reactions by curvature analysis of kinetic trajectories

Vignesh Narayanan, Lawrence K. Bordoh, István Z. Kiss\* and Jr-Shin Li



## RESEARCH PAPERS

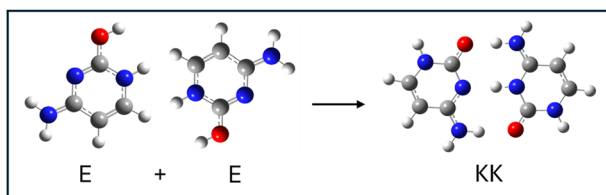
9970



### A non-metal doped VTe<sub>2</sub> monolayer: theoretical insights into the enhanced mechanism for the hydrogen evolution reaction

Yanwei Wang,\* Guofeng Li, Jisong Hu, Ge Gao, Ying Zhang, Guangxia Shi, Xu Yang, Lei Zhang, Ling Fang\* and Yinwei Li\*

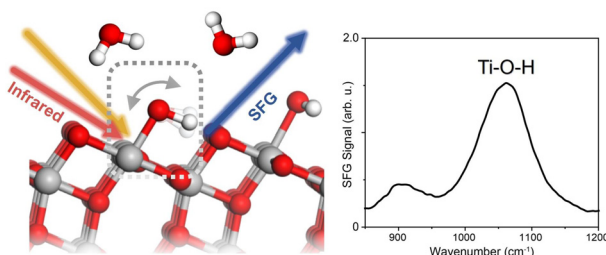
9980



### i-Motif DNA in isolated hemiprotonated cytosine dimers, studied using IR spectroscopy and theoretical calculations

Ana D. Parejo Vidal, Yuika Okura, Keisuke Hirata, Vijay Madhav Miriyala, Pavel Hobza,\* Shun-ichi Ishiuchi,\* Masaaki Fujii and Mattanjah S. de Vries\*

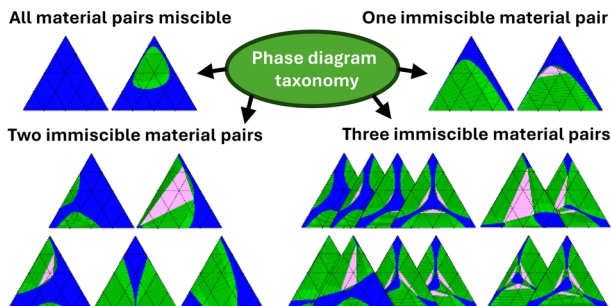
9991



### Auto-dissociation of atmospheric water on TiO<sub>2</sub>: insights from sum-frequency spectroscopy of Ti–O vibrations

Hui Li, Wenqi Zheng, Xinyi Liu, Jiashi Li, Lianbing Wen, Fujie Tang and Wei-Tao Liu\*

9998



### Taxonomy of amorphous ternary phase diagrams: the importance of interaction parameters

Yasin Ameslon, Hao Liu, Jens Harting, Olivier J. J. Ronsin and Olga Wodo\*

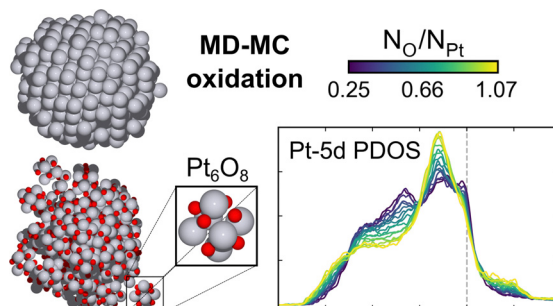


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10011

### Multi-scale modeling and experimental investigation of oxidation behavior in platinum nanoparticles

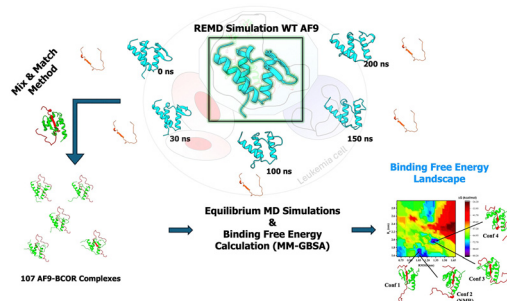
Tom Demeyere, Husn U. Islam, Tom Ellaby, Misbah Sarwar, David Thompsett and Chris-Kriton Skylaris\*



10023

### Exploring the binding free energy landscape of intrinsically disordered protein–protein interactions: insights into the AF9–BCOR complex implicated in leukemia

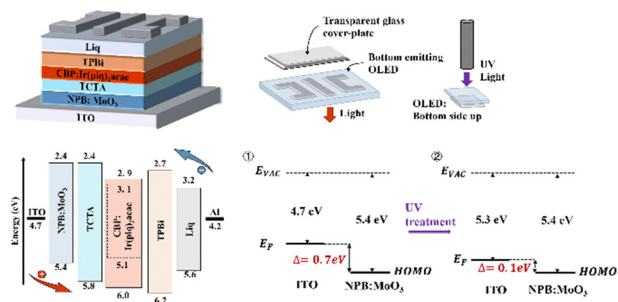
Shilpa Sharma and Arjun Saha\*



10036

### Research on the influence of ultraviolet radiation on OLEDs and the luminance attenuation model of light aging

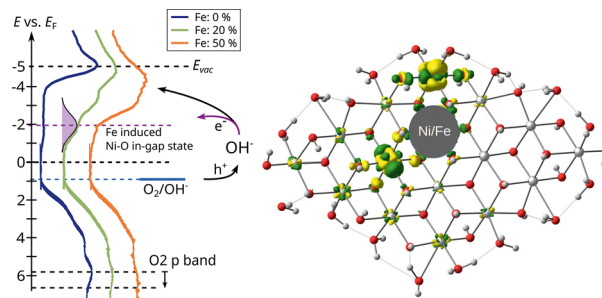
Lulu Zhou, Zhanhan Hu, Wei Shi,\* Yixiao Zhang, Yangyang Zhu, Yi Liao, Yachen Xu, Jialu Gu, Weixia Lan and Bin Wei\*



10043

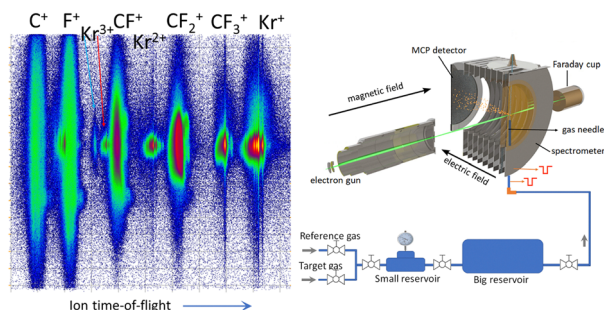
### The role of iron in the electronic configuration of mixed nickel iron oxides for the oxygen evolution reaction

Christopher Gort,\* Gustavo T. Feliciano, Alexander A. Auer, Bernhard Kaiser, Wolfram Jaegermann and Jan P. Hofmann\*



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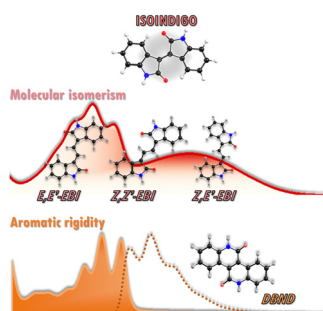
10057



### Electron impact single and double ionization and dissociation: revisiting $\text{CF}_4$ and $\text{CHF}_3$ with an improved experimental method

M. Dogan, W. Wolff, D. M. Mootheril, T. Pfeifer and A. Dorn\*

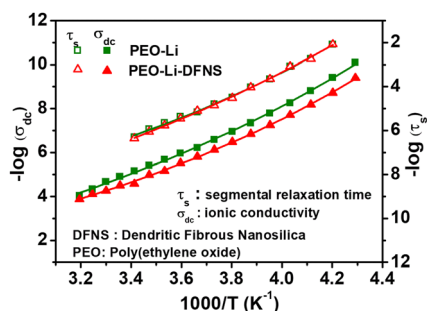
10073



### Exploring the decay mechanisms of isoindigo from indolin-2-one-based derivatives: molecular isomerism vs. aromatic rigidity

Carla Cunha, Marta Pineiro and J. Sérgio Seixas de Melo\*

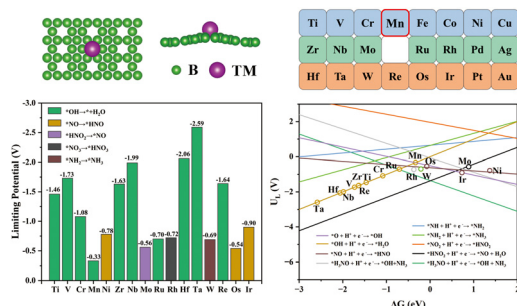
10082



### Correlation between free volume structure and ionic conductivity of a poly(ethylene oxide) and dendritic fibrous nanosilica composite-based electrolyte: an investigation using positron annihilation and broadband dielectric spectroscopy

Jaideep Mor, Kanaklata L. Pandey and Sandeep Kumar Sharma\*

10091



### Theoretical exploration of a single-atom catalyst anchored on $\beta_{12}$ -borophene for electrochemical nitrate reduction: catalyst screening and mechanistic insight

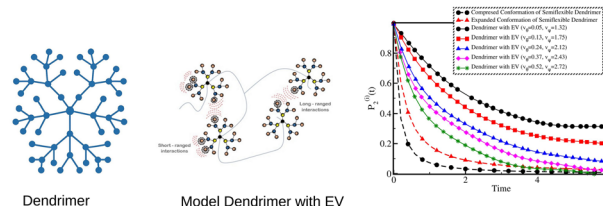
Yuqing Liu, Junjie Zhao, Ming Zhang,\* Longteng Qu, Tian Wang, Jian Wu, Zhuoran Xu and Ruzhi Wang



10101

## Unraveling the influence of excluded volume on orientational relaxation dynamics in dendrimers

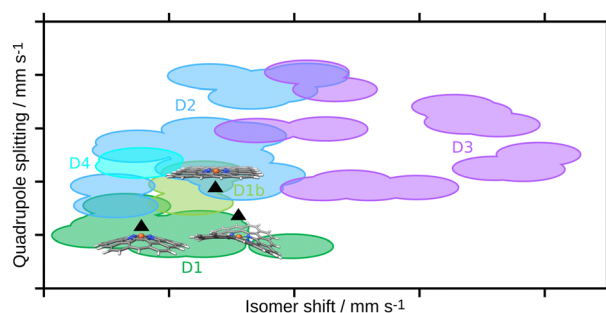
Shelly Bhardwaj and Amit Kumar\*



10111

## Pyrrolic FeN<sub>4</sub> models for FeNC catalysts: the influence of planarity on electronic properties and Mössbauer parameters

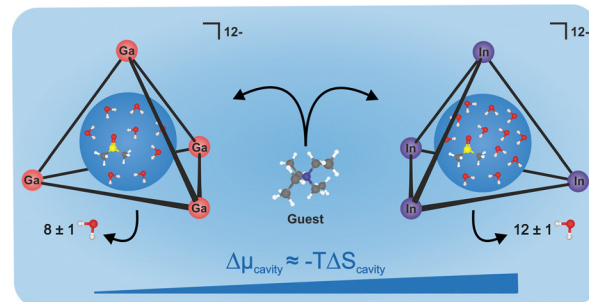
Niklas von Rhein, Jian Liang Low, Charlotte Gallenkamp,\* Beate Paulus and Vera Krewald\*



10120

## Tuning the free energy of host–guest encapsulation by cosolvent

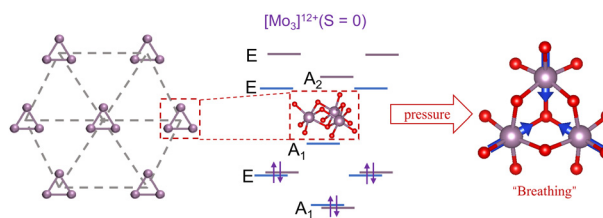
Melinda Nolten, Kay T. Xia, Simone Pezzotti, Gerhard Schwaab, Robert G. Bergman,\* Kenneth N. Raymond,\* F. Dean Toste,\* Teresa Head-Gordon,\* Wan-Lu Li\* and Martina Havenith\*



10129

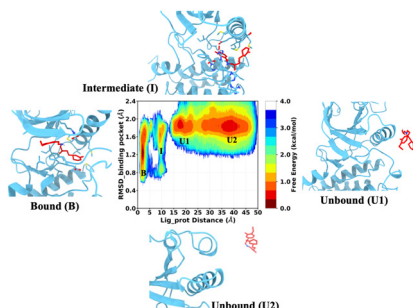
## Pressure-induced symmetry breaking and robust Mo<sub>3</sub> clusters (S = 0) in kagome compounds M<sub>2</sub>Mo<sub>3</sub>O<sub>8</sub> (M = Zn, Fe)

En Chen, Chen Li, Dequan Jiang, Yingying Ma, Haoming Cheng, Tianyao Pei, Chuanlong Lin and Yonggang Wang\*



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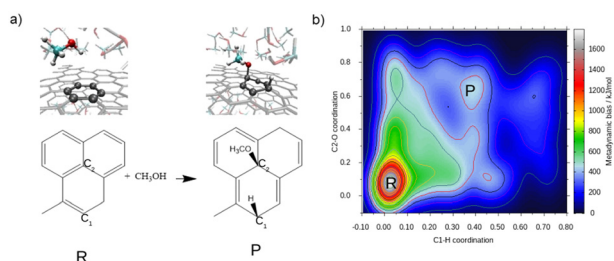
10137



### Identification and characterization of binding thermodynamics and kinetics of inhibitors targeting FGFR1 via molecular modelling and ligand Gaussian accelerated molecular dynamics simulations

Subhasmita Mahapatra and Parimal Kar\*

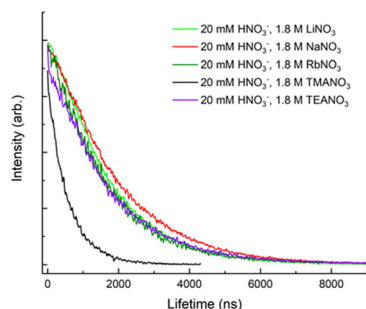
10153



### Structural transitions at the bilayer graphene-methanol interface from *ab initio* molecular dynamics

Flavio Siro Brigiano,\* Thomas Thévenet, Alexis Markovits, Julia Contreras-García, Alfonso San Miguel and Fabio Pietrucci

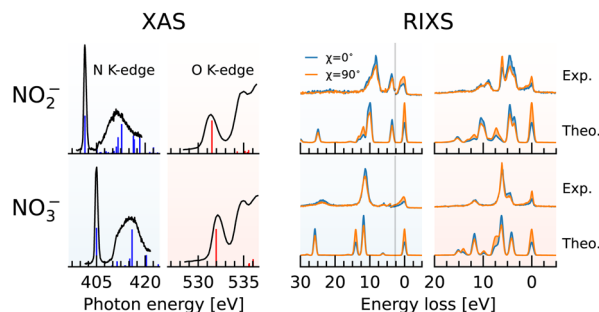
10166



### Uranyl fluorescence in acidic solution: quenching effects by tetramethylammonium (TMA<sup>+</sup>)

Thomas D. Persinger,\* Michael C. Heaven and Richard E. Wilson

10174



### Electronic structure of aqueous nitrite and nitrate ions from resonant inelastic X-ray scattering

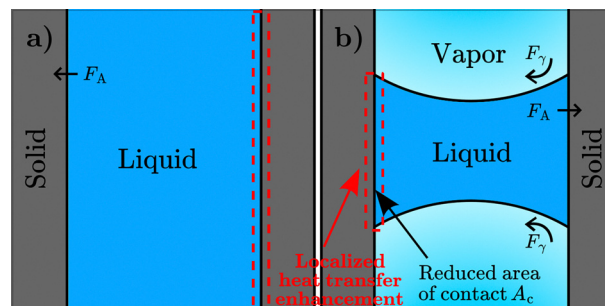
Sebastian Eckert,\* Laurenz Otto, Eric J. Mascarenhas, Annette Pietzsch, Rolf Mitzner, Mattis Fondell, Vinicius Vaz da Cruz and Alexander Föhlisch



10185

### Spectral mechanisms of solid/liquid interfacial heat transfer in the presence of a meniscus

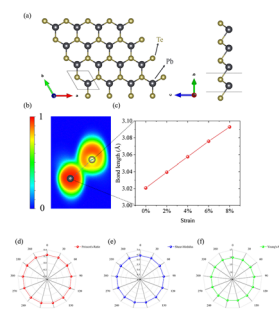
Abdullah El-Rifai,\* Liudmyla Klochko, Viktor Mandrolko, Sreehari Perumanath, David Lacroix, Rohit Pillai\* and Mykola Isaiev\*



10198

### Theoretical investigation of the ultralow thermal conductivity of 2D PbTe via a strain regulation method

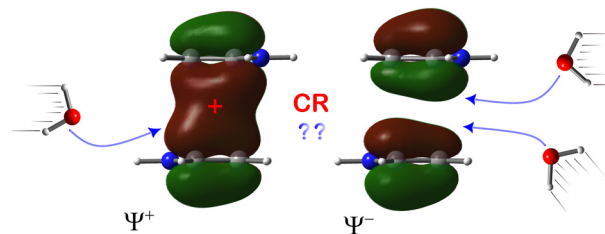
Peng Gao, Xihao Chen,\* Zonghang Liu, Wengang An\* and Ning Wang\*



10209

### Effect of microhydration on the aromatic charge resonance interaction: the case of the pyrrole dimer cation

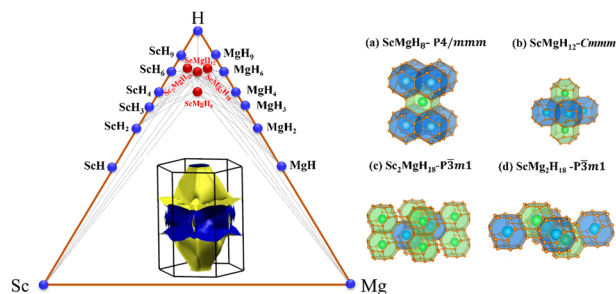
Dashjargal Arildii, Yoshiteru Matsumoto and Otto Dopfer\*



10227

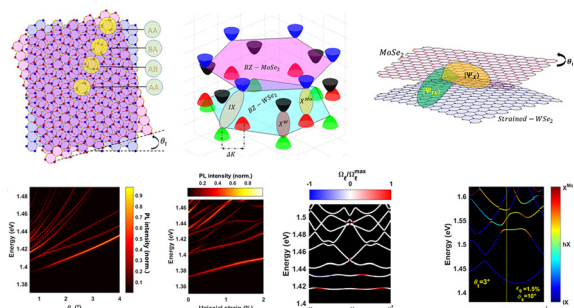
### First-principles investigation of the phase diagram and superconducting properties of the Sc–Mg–H system under high pressure

Zhen Qin, Wenqing Zhang, Shichang Li,\* Ying Chang, Chunbao Feng, Bole Chen and Dengfeng Li\*



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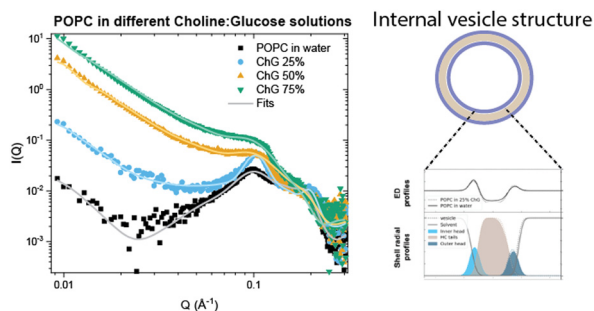
10235



### Hybrid moiré excitons in a strained heterobilayer of transition metal dichalcogenides

Houssem Eddine Hannachi\* and Sihem Jaziri

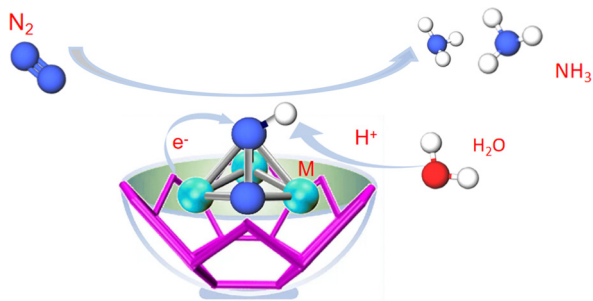
10248



### The integrity of the lipid bilayer structure is retained in natural occurring deep eutectic solvent water mixtures – a small angle X-ray scattering study

Marité Cárdenas,\* Victoria Ariel Bjørnstad, Kari Kristine Almåsvoold Borgos and Reidar Lund\*

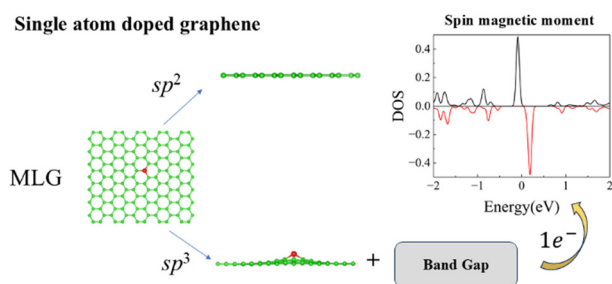
10259



### Theoretical study of ammonia synthesis catalysed by trimetallic clusters with or without a sumanene support

Xiao-Meng Huang, Zhi-Wen Ji, Xun-Lei Ding,\* Yan Chen, Wei Li, Jiao-Jiao Chen, Shao-Peng Xu and Lin-Lin Li

10275



### The role of local orbital hybridization in band gap opening and magnetism induced by single-atom doping in graphene

Jianfei Xiang, Huimin Hu\* and Jin-Ho Choi\*

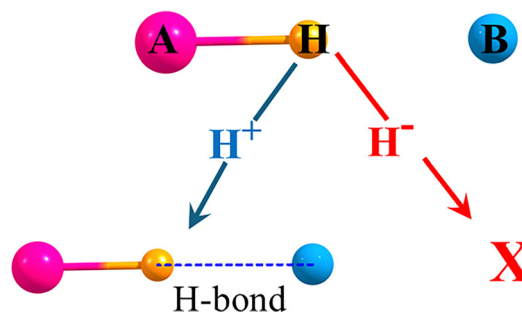


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10283

## Lower limits on hydrogen bond strength. Charge of bridging H atom

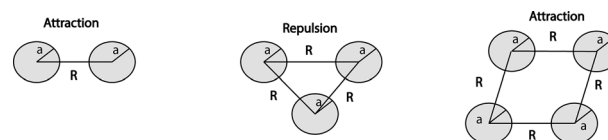
Steve Scheiner



10291

## Attractive and repulsive terms in multi-filament dispersion interactions

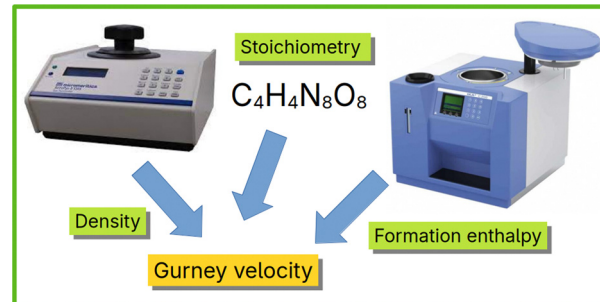
Subhojit Pal,\* John F. Dobson\* and Mathias Boström\*



10302

## Gurney and cylinder wall velocities of explosives: analytical estimates and thermochemical simulations

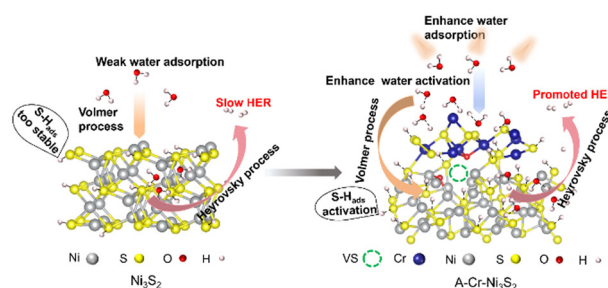
Didier Mathieu



10310

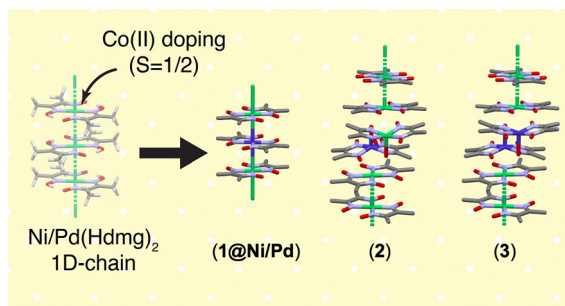
*In situ* activation-induced surface reconstruction on Cr-incorporated Ni<sub>3</sub>S<sub>2</sub> for enhanced alkaline hydrogen evolution reaction

Ruidi Li, Cong Chen,\* Junxia Shen, Zhihe Wei, Pierre-Yves Olu, Wen Dong, Yang Peng, Ronglei Fan\* and Mingrong Shen\*



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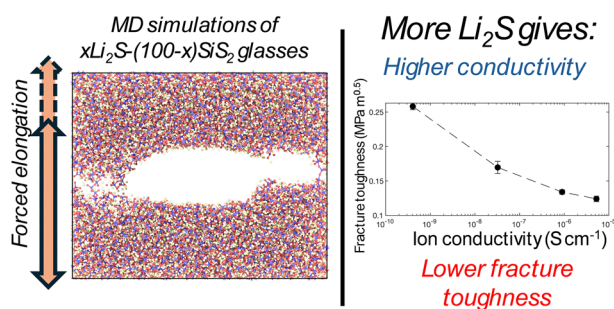
10321



### Revisiting cobaloxime(II) chemistry and clearing misconceptions of cobaloxime(II) in diamagnetic Ni(II) and Pd(II) matrixes using comprehensive magnetic measurements

Yukina Suzuki,\* Mirosław Arczyński, Masanori Wakizaka, Hisaaki Tanaka, Ryuta Ishikawa, Takefumi Yoshida, Takeshi Yamane, Kazunobu Sato, Ryota Sakamoto and Masahiro Yamashita\*

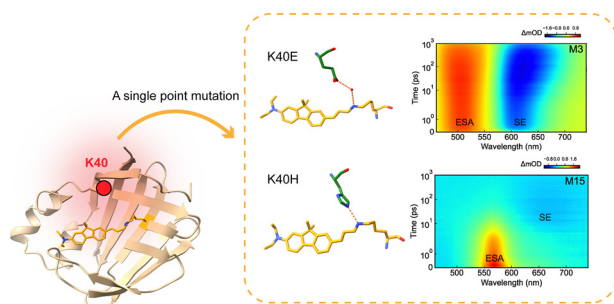
10331



### Balancing fracture toughness and ionic conductivity in lithium thiosilicate glassy electrolytes

Søren S. Sørensen, Daniel Boysen, Esben R. Lindbjerg, Helle N. Mortensen, Kaja T. Lippert, Sisse M. Diget, Zuzanna Konieczna, Matthieu Micoulaut and Morten M. Smedskjaer\*

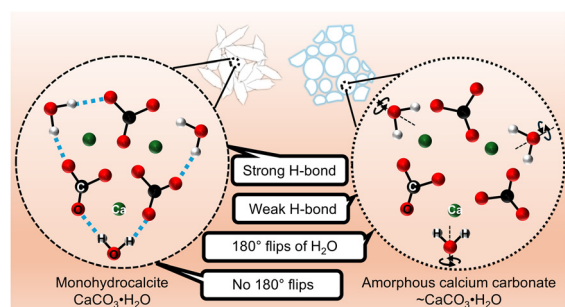
10342



### Proton transfer kinetics modulated by single-residue substitution in photobasic FR-1V/hCRABPII

Jiajia Meng, Gaoshang Li, Xiaolu Bai, Siteng Zhao, Jin Dai, Yin Song, Xubiao Peng\* and Qing Zhao\*

10348



### Investigation of the structure and dynamics of amorphous calcium carbonate by NMR: stabilization by poly-aspartate and comparison to monohydrocalcite

Sanjay Vinod-Kumar, Albert A. Smith-Penzel, Venkata SubbaRao Redrouthu, Maxim B. Gindele, Denis Gebauer and Guinevere Mathies\*

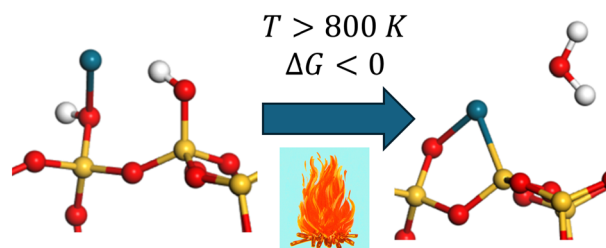


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10364

**Computational investigation of silica-supported Pd<sub>n</sub> and Pd<sub>n</sub>(xO) nanoclusters**

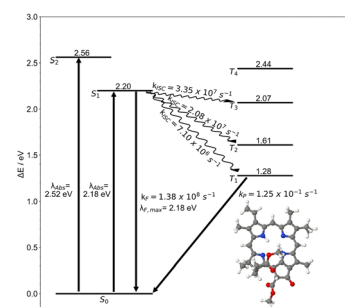
C. J. Lombard, C. G. C. E. van Sittert,\* J. N. Mugo, C. Perry and D. J. Willock\*



10376

**A computational study on the photophysics of methylpheophorbide a**

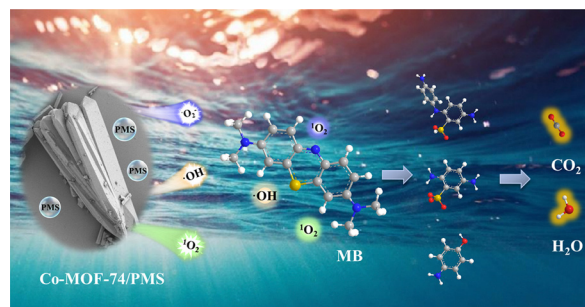
Hernán Rueda Bueno, Julio R. Pinzón, Martha C. Daza and Markus Doerr\*



10387

**Peroxymonosulfate activated M-MOF-74 (M = Co, Fe, Ni) visible light photocatalysts for methylene blue degradation enhancement**

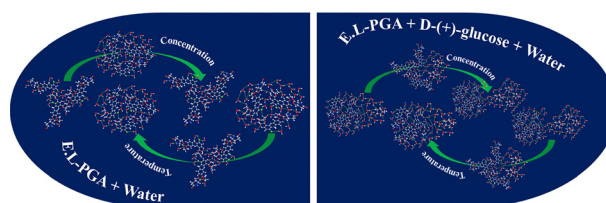
Jiaqi Li, Yidan Zhang, Pingyu Luo, Chun Li, Fanming Zeng,\* Tiantian Sun,\* Hanhui Lei, Xiaoteng Liu\* and Chunbo Liu



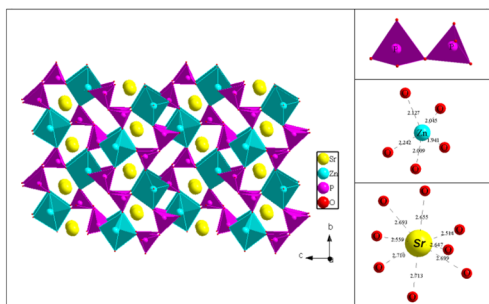
10399

**Revealing water structure modification by a sodium–glucose cotransporter-2 inhibitor-type antidiabetic drug with D-(+)-glucose in aqueous media**

Mohammad Hossain and Md. Abu Bin Hasan Susan\*



10413



**Structural, thermodynamic, electrical and dielectric properties of SrZnP<sub>2</sub>O<sub>7</sub> diphosphates compared to SrA<sup>II</sup> P<sub>2</sub>O<sub>7</sub> (A = Sr and Ni) with analysis of OLPT conduction mechanism**

Krichen Marwa and Megdiche Makram\*

