

IN THIS ISSUE

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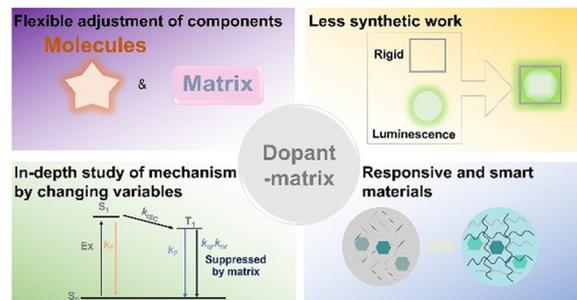
Inside cover
See Yanwei Wang, Ling Fang, Yinwei Li *et al.*, pp. 9970–9979. Image reproduced by permission of Yanwei Wang from *Phys. Chem. Chem. Phys.*, 2025, 27, 9970.

REVIEW

9913

Recent advances in dopant–matrix afterglow systems: high-performance organic afterglow materials and the critical role of organic matrices in materials fabrication

Yue Zhang, Zhe Mo, Zi Ye, Qianqian Yan, Xixi Piao, Jialiang Jiang, Biao Xu and Kaka Zhang*

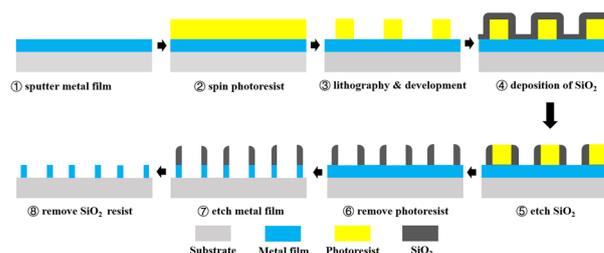


COMMUNICATIONS

9937

Nano-wire spin Hall nano-oscillator fabricated by novel sidewall transfer lithography

Jialin Shi, Chenglong Zhang, Zhenhu Jin and Jiamin Chen*



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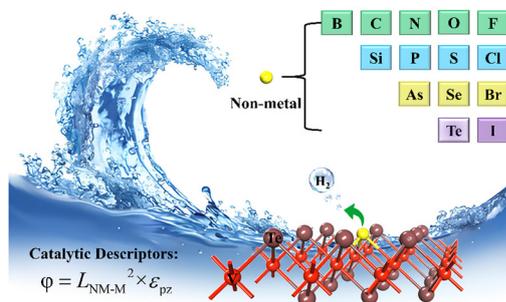
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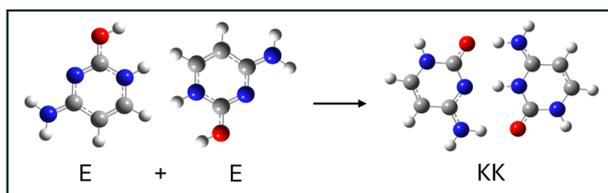
9970



A non-metal doped VTe₂ 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*

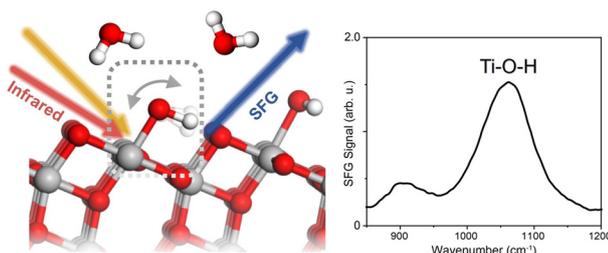
9980



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*

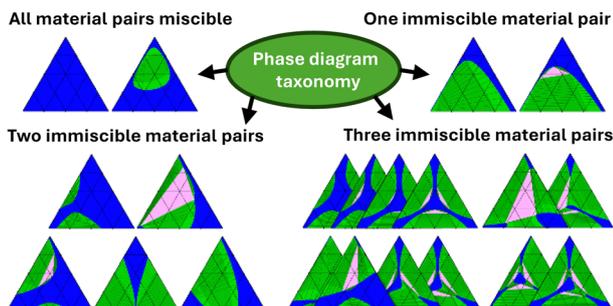
9991



Auto-dissociation of atmospheric water on TiO₂: 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*

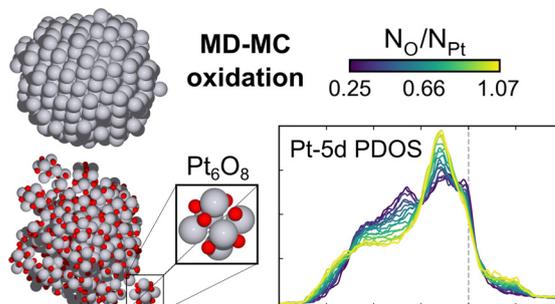


RESEARCH PAPERS

10011

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

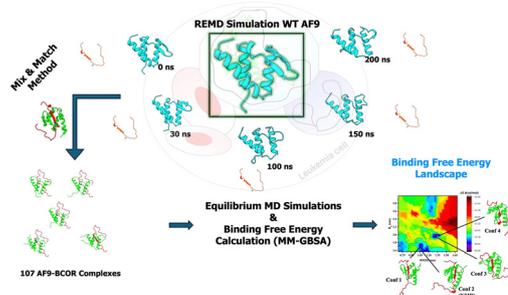
Tom Demeyere, Husn U. Islam, Tom Ellaby, Misbah Sarwar, David Thompsett and Chris-Kriton Skylaris*



10023

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

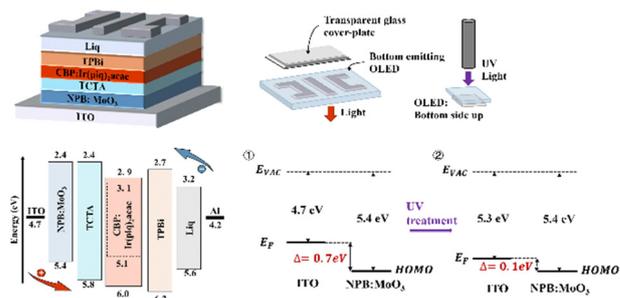
Shilpa Sharma and Arjun Saha*



10036

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

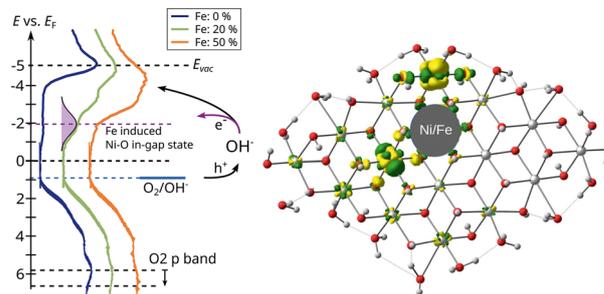
Lulu Zhou, Zhanhan Hu, Wei Shi,* Yixiao Zhang, Yangyang Zhu, Yi Liao, Yachen Xu, Jialu Gu, Weixia Lan and Bin Wei*



10043

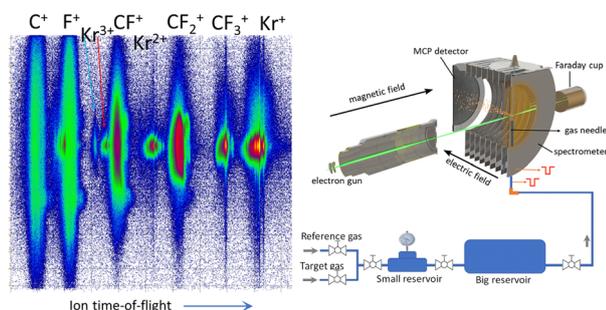
The role of iron in the electronic configuration of mixed nickel iron oxides for the oxygen evolution reaction

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



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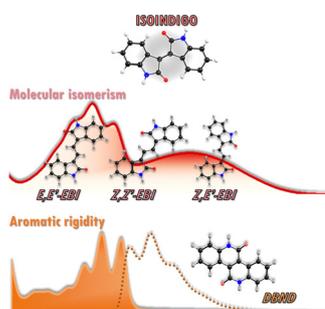
10057



Electron impact single and double ionization and dissociation: revisiting CF_4 and CHF_3 with an improved experimental method

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

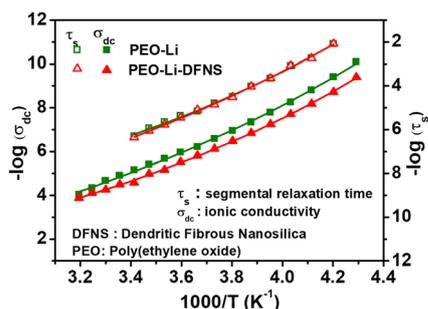
10073



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*

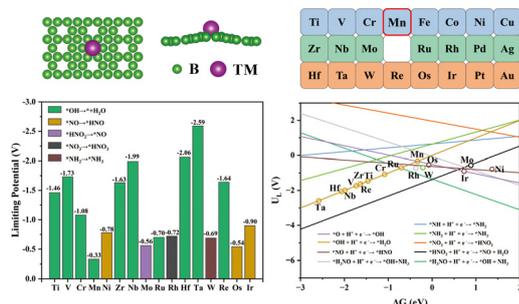
10082



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 β_{12} -borophene for electrochemical nitrate reduction: catalyst screening and mechanistic insight

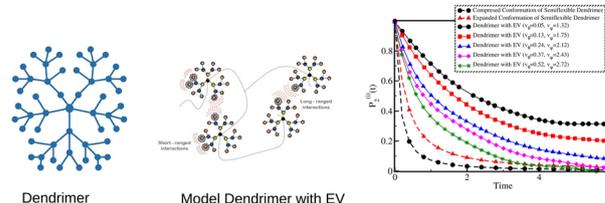
Yuqing Liu, Junjie Zhao, Ming Zhang,* Longteng Qu, Tian Wang, Jian Wu, Zhuoran Xu and Ruzhi Wang



10101

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

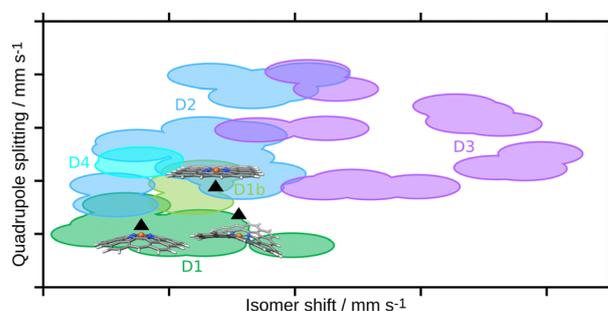
Shelly Bhardwaj and Amit Kumar*



10111

Pyrrolic FeN₄ models for FeNC catalysts: the influence of planarity on electronic properties and Mössbauer parameters

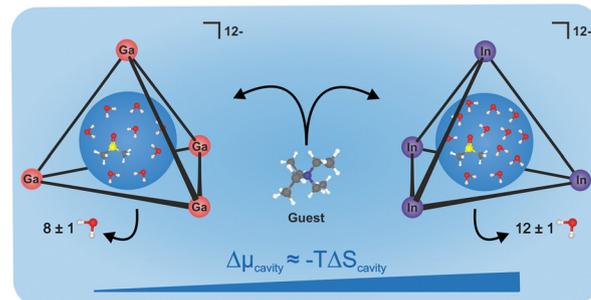
Niklas von Rhein, Jian Liang Low, Charlotte Gallenkamp,* Beate Paulus and Vera Krewald*



10120

Tuning the free energy of host–guest encapsulation by cosolvent

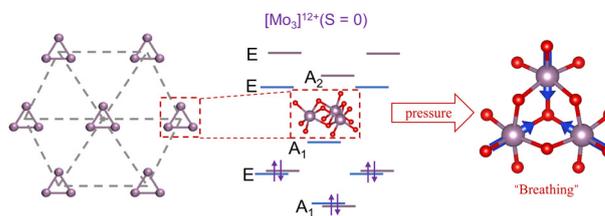
Melinda Nolten, Kay T. Xia, Simone Pezzotti, Gerhard Schwaab, Robert G. Bergman,* Kenneth N. Raymond,* F. Dean Toste,* Teresa Head-Gordon,* Wan-Lu Li* and Martina Havenith*



10129

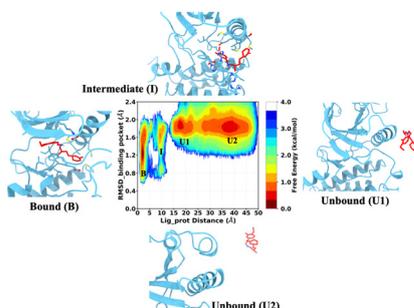
Pressure-induced symmetry breaking and robust Mo₃ clusters (S = 0) in kagome compounds M₂Mo₃O₈ (M = Zn, Fe)

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



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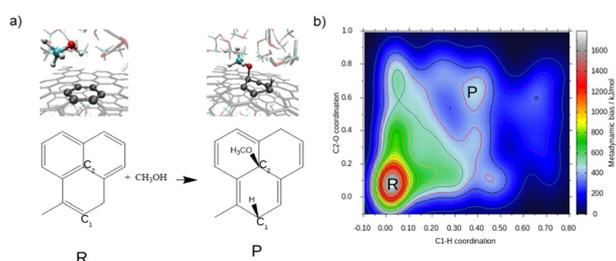
10137



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*

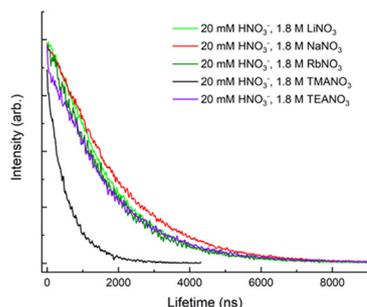
10153



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

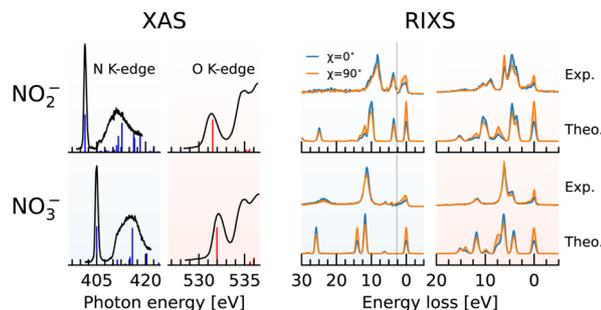
10166



Uranyl fluorescence in acidic solution: quenching effects by tetramethylammonium (TMA⁺)

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

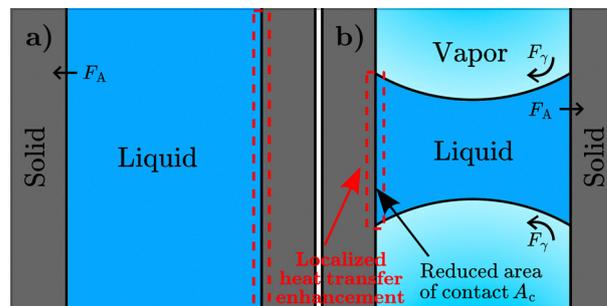
Sebastian Eckert,* Laurenz Otto, Eric J. Mascarenhas, Annette Pietzsch, Rolf Mitzner, Mattis Fondell, Vinicius Vaz da Cruz and Alexander Föhlisch



10185

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

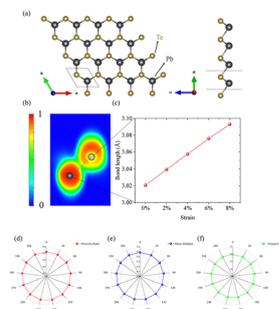
Abdullah El-Rifai,* Liudmyla Klochko, Viktor Mandrolko, Sreehari Perumanath, David Lacroix, Rohit Pillai* and Mykola Isaiev*



10198

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

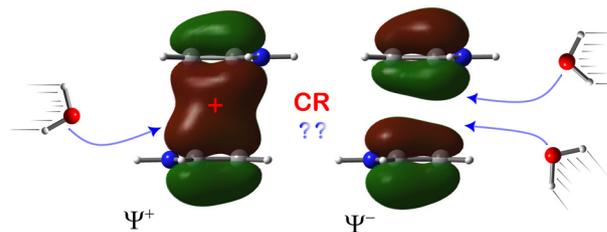
Peng Gao, Xihao Chen,* Zonghang Liu, Wengang An* and Ning Wang*



10209

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

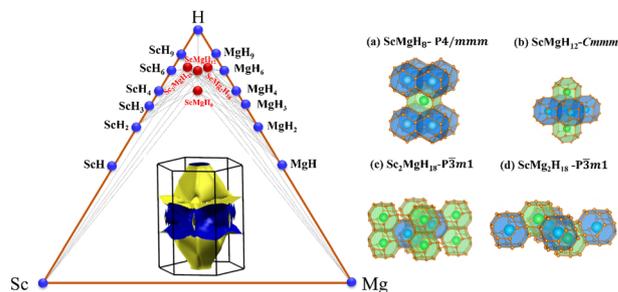
Dashjargal Arildii, Yoshiteru Matsumoto and Otto Dopfer*



10227

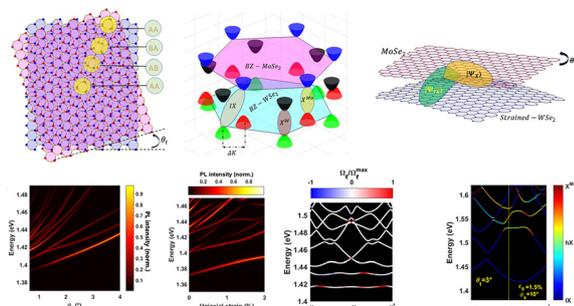
First-principles investigation of the phase diagram and superconducting properties of the Sc–Mg–H system under high pressure

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



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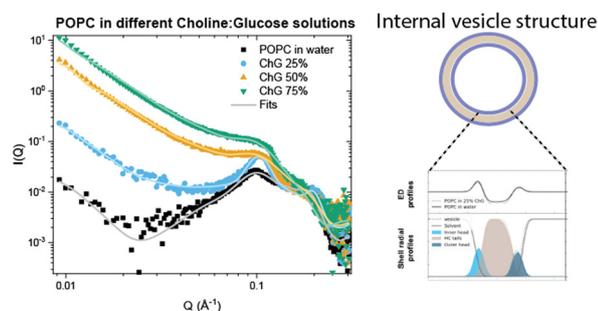
10235



Hybrid moiré excitons in a strained heterobilayer of transition metal dichalcogenides

Houssem Eddine Hannachi* and Sihem Jaziri

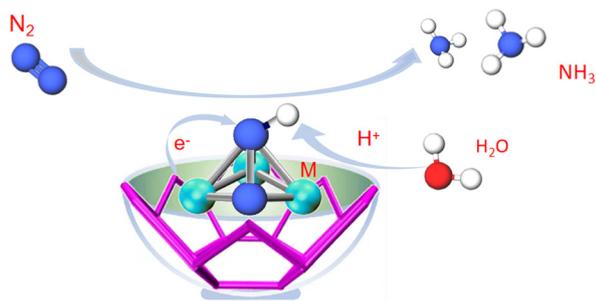
10248



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*

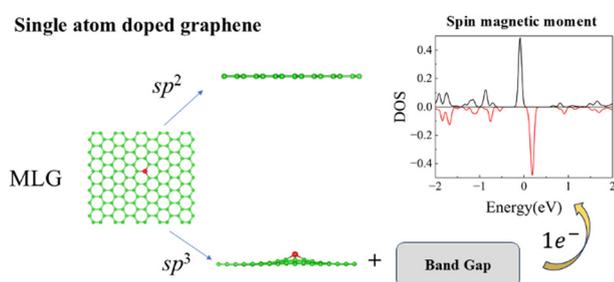
10259



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*

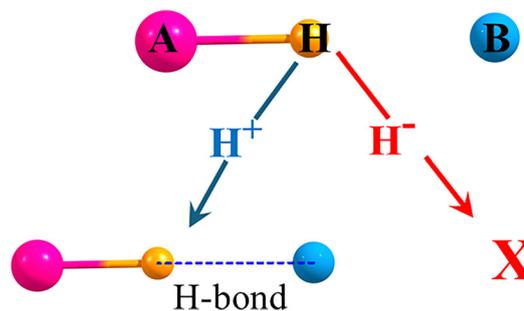


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10283

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

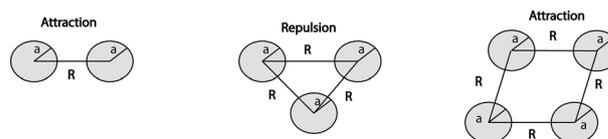
Steve Scheiner



10291

Attractive and repulsive terms in multi-filament dispersion interactions

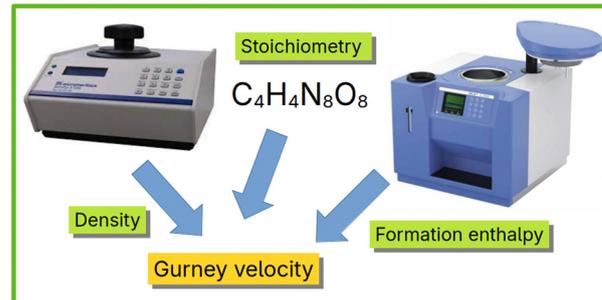
Subhojit Pal,* John F. Dobson* and Mathias Boström*



10302

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

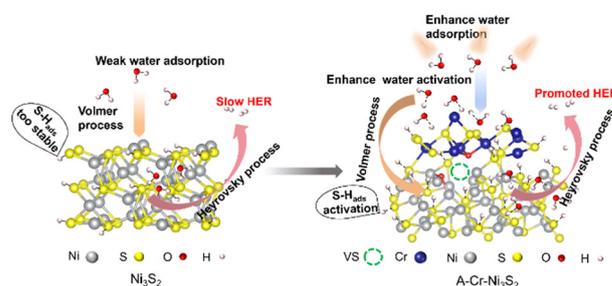
Didier Mathieu



10310

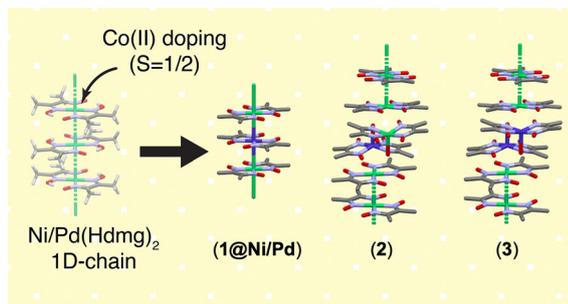
In situ activation-induced surface reconstruction on Cr-incorporated Ni₃S₂ for enhanced alkaline hydrogen evolution reaction

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



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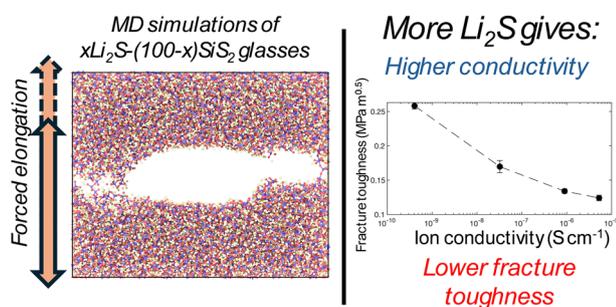
10321



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*

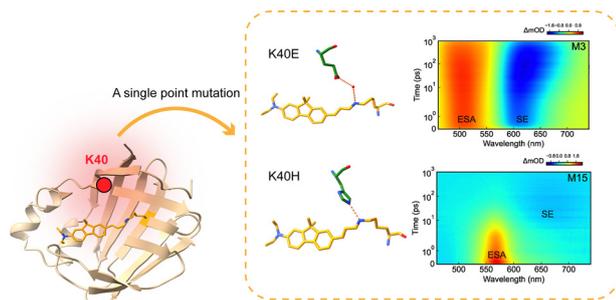
10331



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*

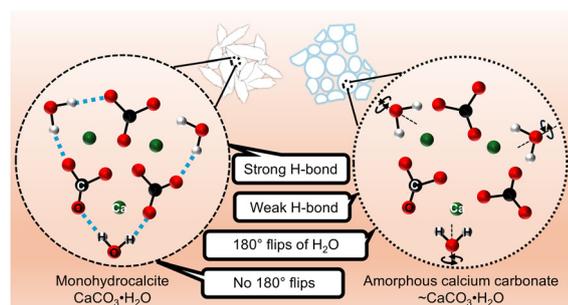
10342



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*

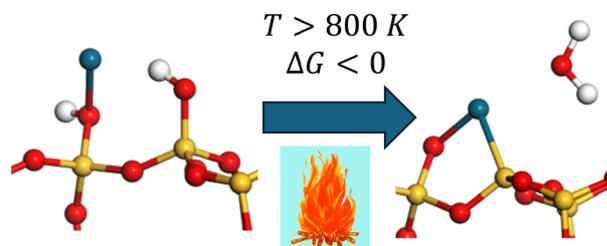


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10364

Computational investigation of silica-supported Pd_n and Pd_n(xO) nanoclusters

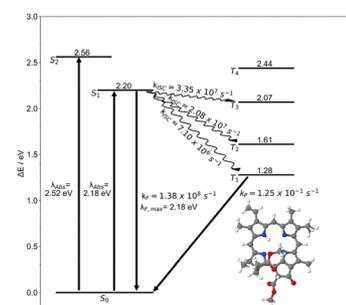
C. J. Lombard, C. G. C. E. van Sittert,* J. N. Mugo, C. Perry and D. J. Willock*



10376

A computational study on the photophysics of methylpheophorbide a

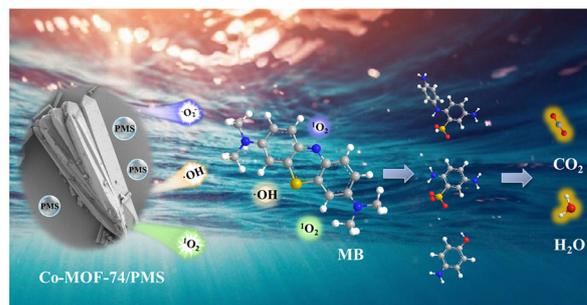
Hernán Rueda Bueno, Julio R. Pinzón, Martha C. Daza and Markus Doerr*



10387

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

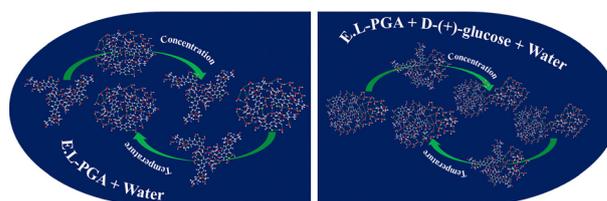
Jiaqi Li, Yidan Zhang, Pingyu Luo, Chun Li, Fanming Zeng,* Tiantian Sun,* Hanhui Lei, Xiaoteng Liu* and Chunbo Liu



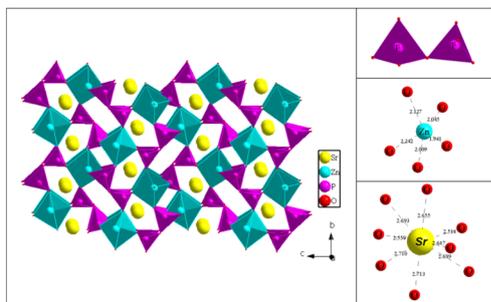
10399

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 SrZnP₂O₇ diphosphates compared to SrA^{II} P₂O₇ (A = Sr and Ni) with analysis of OLPT conduction mechanism

Krichen Marwa and Megdiche Makram*

