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IN THIS ISSUE

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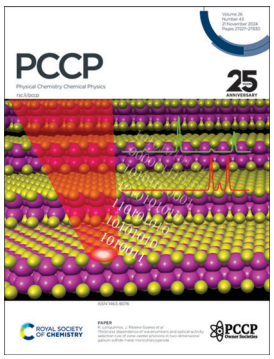
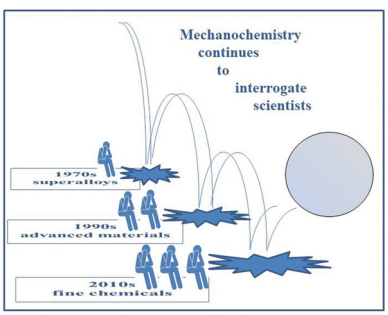
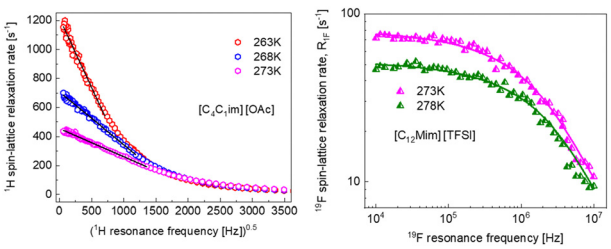


Cover
See R. Longuinhos, J. Ribeiro-Soares *et al.*, pp. 27260–27269. Image produced and designed by Raphael Longuinhos Monteiro Lobato, with the approval of the co-authors from *Phys. Chem. Chem. Phys.*, 2024, **26**, 27260.

EDITORIAL



REVIEW



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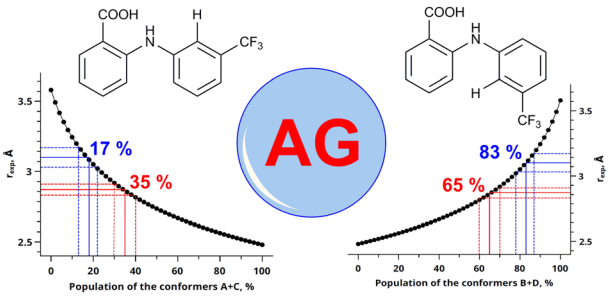
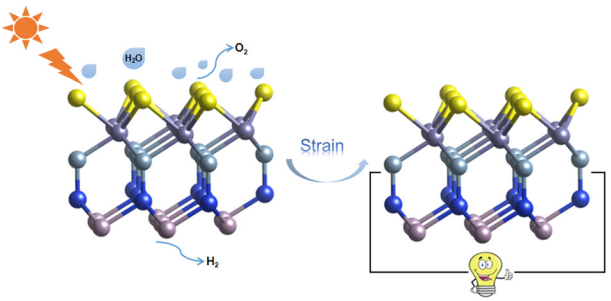


Structural and sorption characteristics of an aerogel composite material loaded with flufenamic acid: insights from MAS NMR and high-pressure NOESY studies

Valentina V. Sobornova, Valeriya V. Mulloyarova, Konstantin V. Belov, Alexey A. Dyshin, Peter M. Tolstoy, Mikhail G. Kiselev and Ilya A. Khodov*

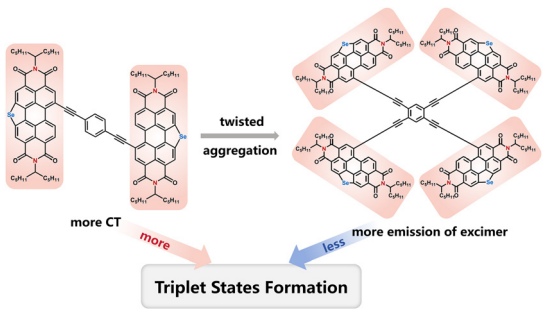
27314



Two-dimensional Janus XWZAZ′ (X = S, Se, Te; A = Si, Ge; Z, Z′ = N, P, As): candidates for photocatalytic water splitting and piezoelectric materials

Zhen Gao, Hongbo Wu, Yao He* and Kai Xiong*

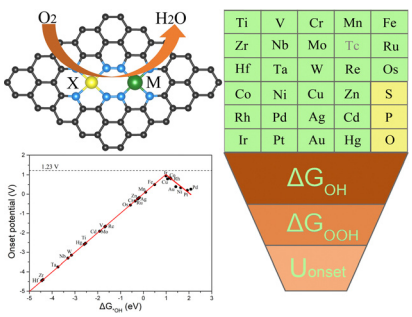
27325



The efficient triplet states formation of Se-modified PDI dimers and tetramers in solvents

Feijun Huang, Wenli Su, Yubo Yang, Hang Wang, Zhishan Bo, Pengfei Jing and Wenkai Zhang*

27332



Theoretical screening of the metal-nonmetal pair anchored on N-doped graphene for the oxygen reduction reaction

Ji Zhang, Peng Zhang, Aimin Yu, Dong-sheng Li and Chenghua Sun*

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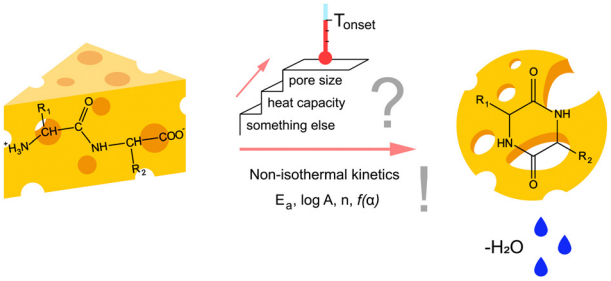

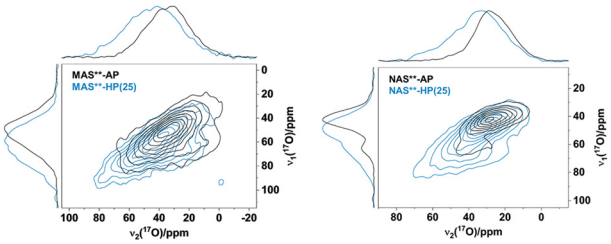

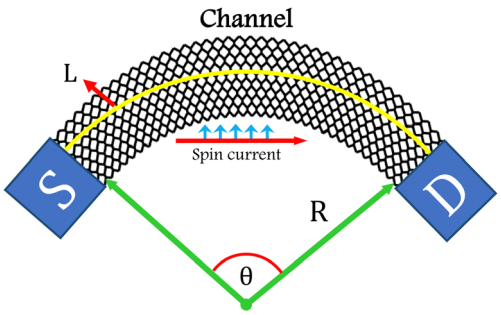

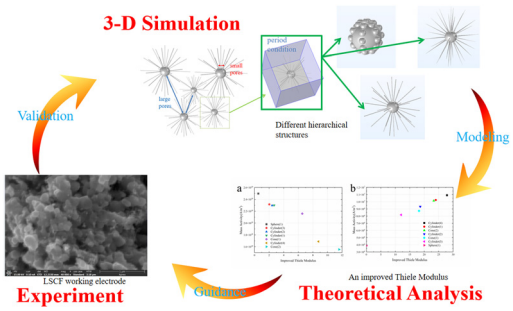

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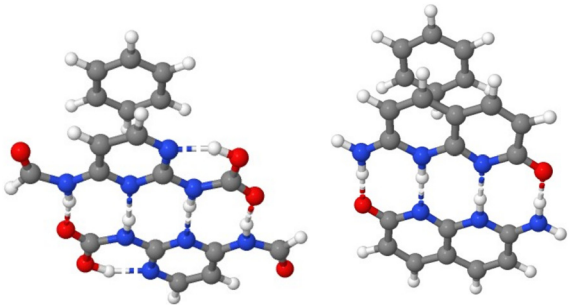

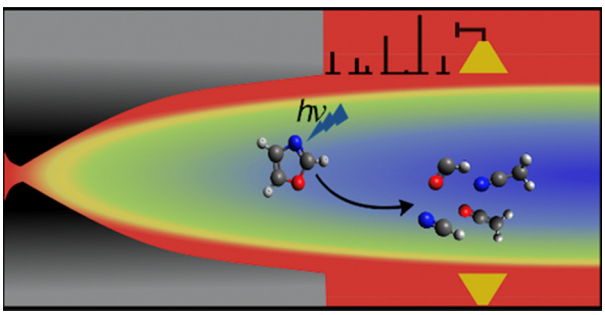

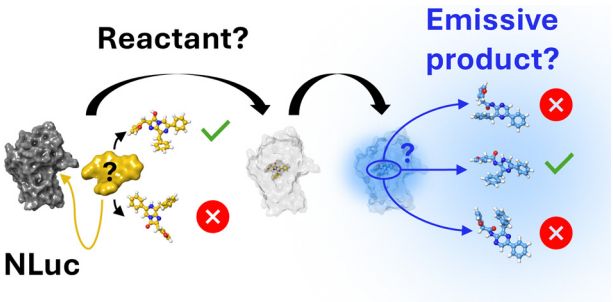

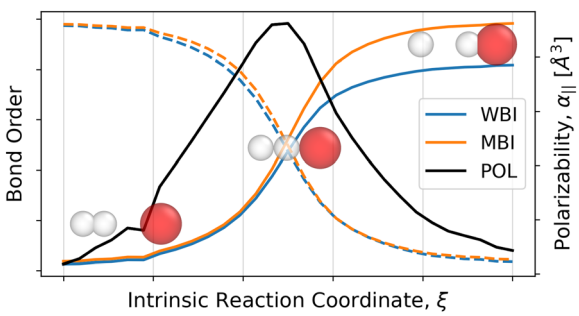

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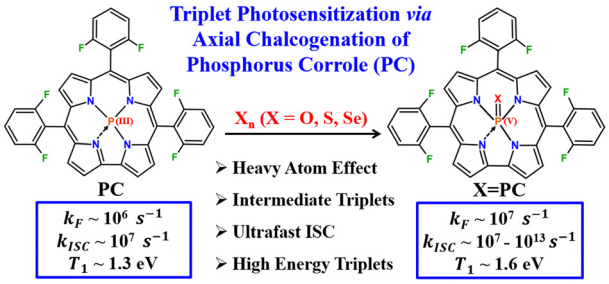
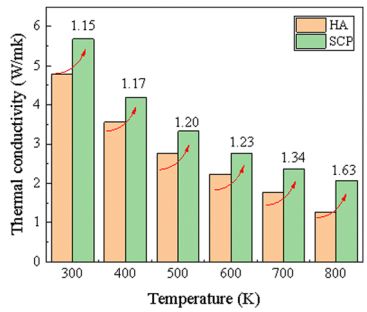


Tailoring intersystem crossing in phosphorus corroles through axial chalcogenation: a detailed theoretical study

Annette Mariya Tedy and Arun K. Manna*

27478



Thermal conductivity study of 2D Si_4C_8 materials by anharmonic phonon renormalization

Peng Gao, Xihao Chen,* Xingwu Yan, Longxin Zhang, Xiang Meng, Fuqiang Zhai* and Donglin Guo*

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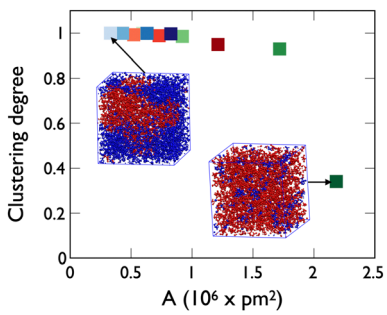

Structural insights into carboxylic-acid based DES across H-bond donor ratios: impact of CL&Pol refinement

Jon Zubeltzu* and Elixabete Rezabal

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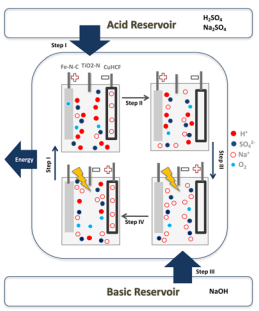

Electrochemical system of nitrogen-doped TiO_2, Fe–N–C, and copper hexacyanoferrate electrodes for photo-assisted energy conversion in acidic wastewater treatment

Bianca Tainá Ferreira, Matheus Martins and Fritz Huguenin*

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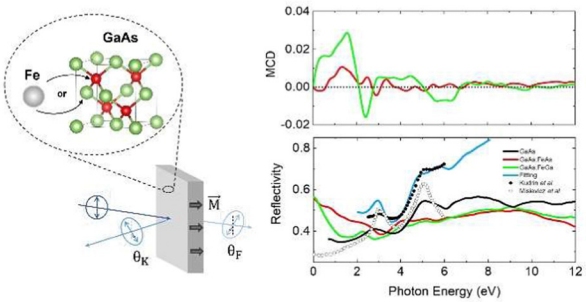

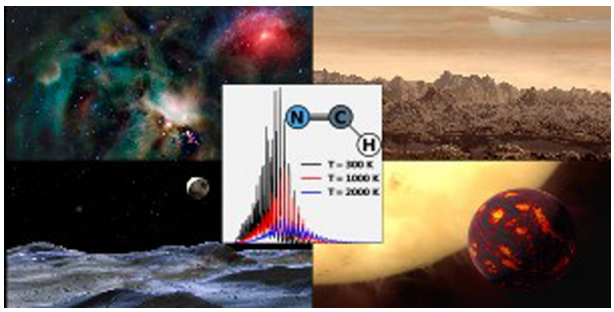

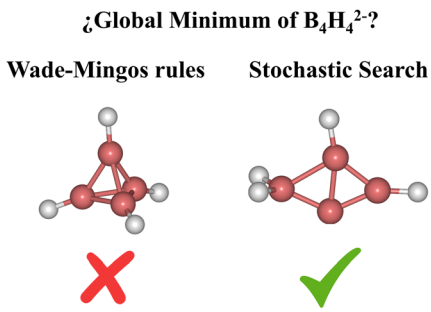

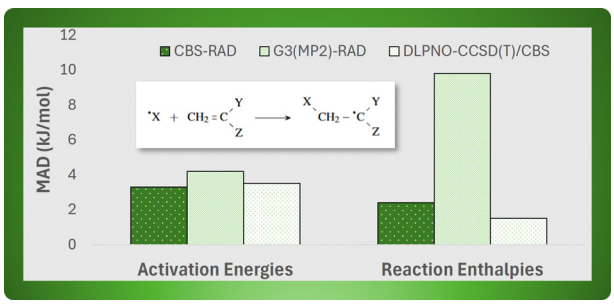

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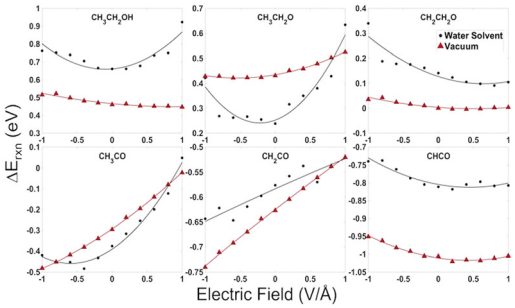

Modeling interfacial electric fields and the ethanol oxidation reaction at electrode surfaces

Yuhan Mei, Fanglin Che and N. Aaron Deskins*

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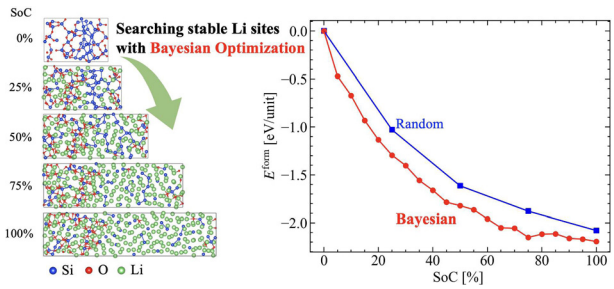

First-principles study on the lithiation process of amorphous SiO anode for Li-ion batteries with Bayesian optimization

Ryoya Shintaku, Tomoyuki Tamura,* Shogo Nogami, Masayuki Karasuyama and Takakazu Hirose

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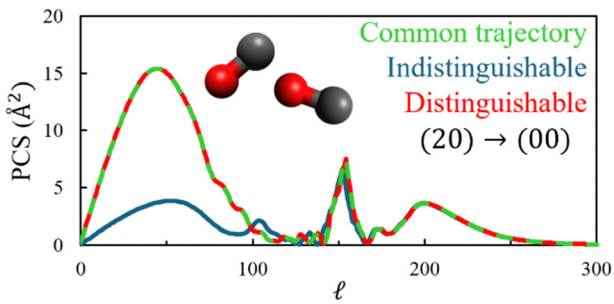

Mixed quantum/classical theory for rotationally inelastic scattering of identical collision partners revised

D. Bostan, B. Mandal and D. Babikov*

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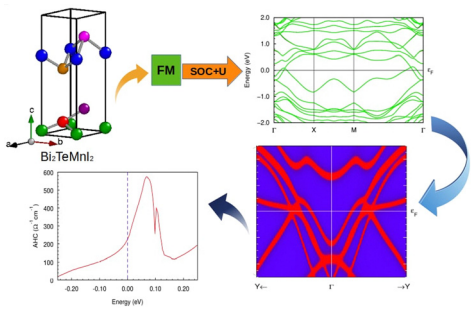

Emergence of Weyl points and large anomalous Hall conductivity in layered Bi_2TeMnI_2

Dipak Bhattarai, Deergh Bahadur Shahi, Dipendra Prasad Kalauni and Madhav Prasad Ghimire*

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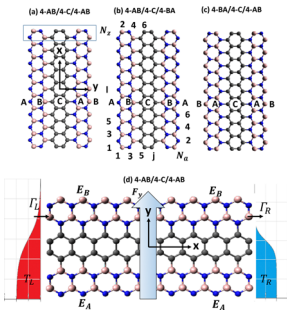

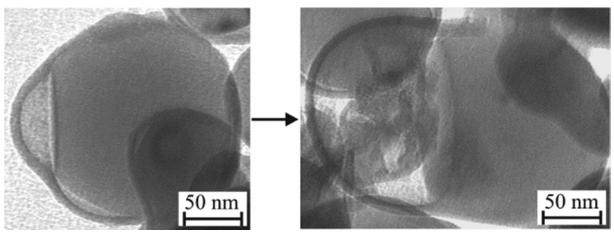

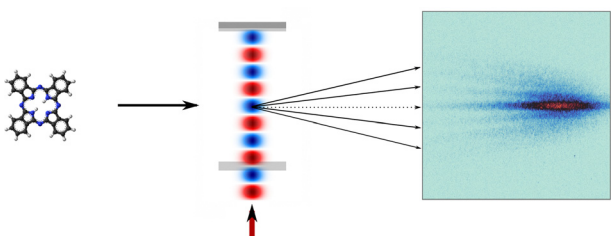

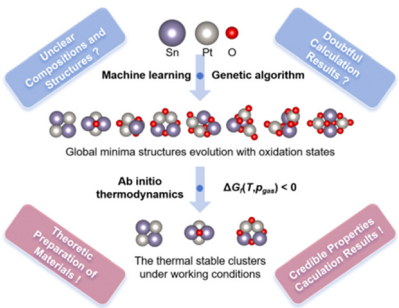

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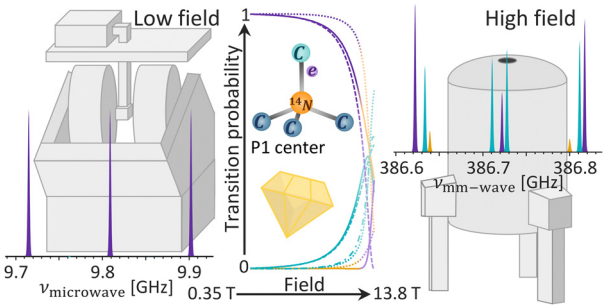
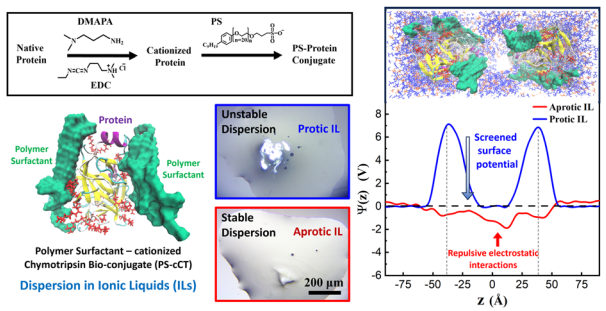


On the peculiar EPR spectra of P1 centers at high (12–20 T) magnetic fields

Orit Nir-Arad, Eyal Laster, Mais Daksi, Nurit Manukovsky and Ilia Kaminker*

27648



Cation effects and charge inversion contribute to the electrostatic stabilisation of protein bioconjugates in neat ionic liquids

Lokesh Soni, Raj Kumar, Kamendra P. Sharma* and Ajay Singh Panwar*

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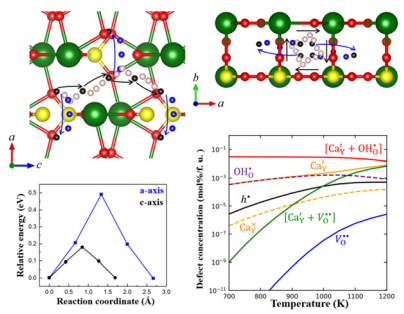

First-principles calculations of proton defect properties in Ca-doped YPO_4

Gyeongseo Lee,* Takafumi Ogawa, Kazuki Shitara and Akihide Kuwabara*

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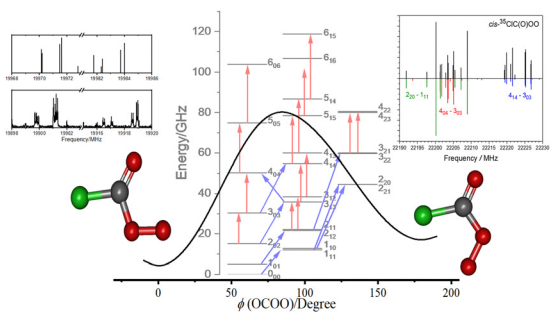

Insights of the peroxychloroformyl radical ClC(O)OO *via* microwave spectrum

Ching-Hua Chang, Wen Chao, Cheng-Han Tsai, Mitchio Okumura, Frank A. F. Winiberg and Yasuki Endo*

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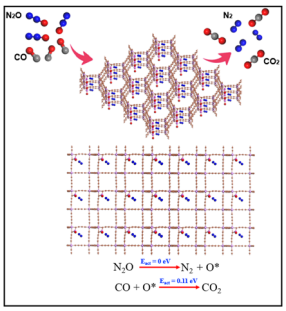

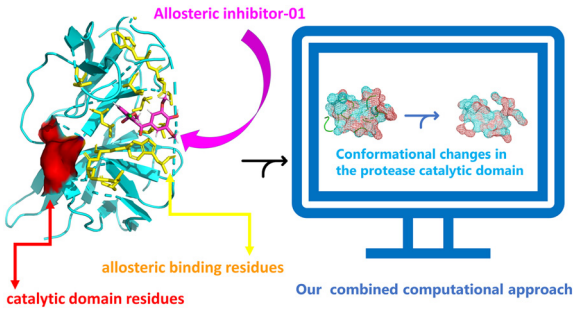

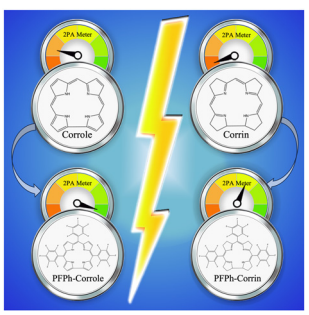

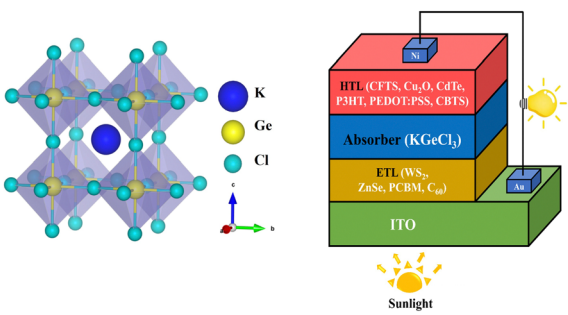

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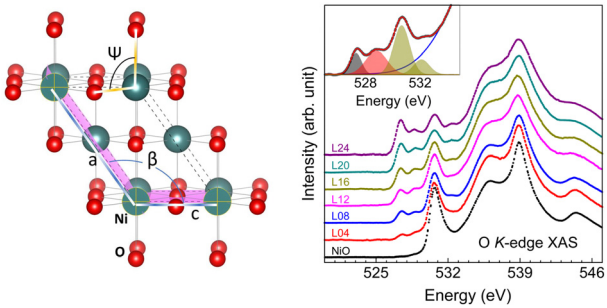

Hole-states in Li doped NiO: doping dependence of Zhang-Rice spectral weight

Suman Mandal* and Krishnakumar S. R. Menon

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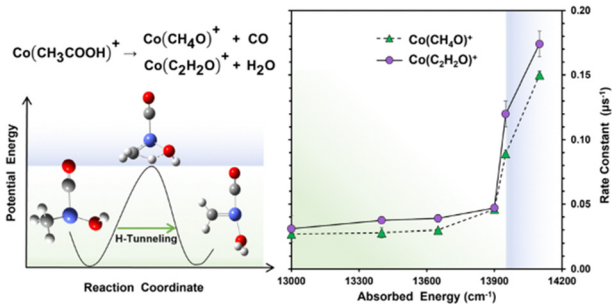
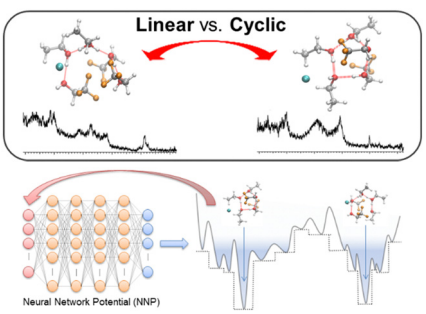


Hydrogen tunneling with an atypically small KIE measured in the mediated decomposition of the $Co(CH_3COOH)^+$ complex

Simon U. Okafor, Gabriele Pinto, Michael Brdecka, William Smith, Tucker W. R. Lewis, Michael Gutierrez and Darrin J. Bellert*

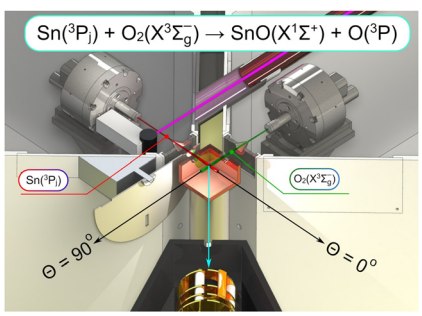
27751



Hydrogen bond network structures of protonated 2,2,2-trifluoroethanol/ethanol mixed clusters probed by infrared spectroscopy combined with a deep-learning structure sampling approach: the origin of the linear type network preference in protonated fluoroalcohol clusters

Po-Jen Hsu, Atsuya Mizuide, Jer-Lai Kuo* and Asuka Fujii*

27763



Experimental and theoretical study of the Sn–O bond formation between atomic tin and molecular oxygen

Iakov A. Medvedkov, Anatoliy A. Nikolayev, Shane J. Goettl, Zhenghai Yang, Alexander M. Mebel* and Ralf I. Kaiser*

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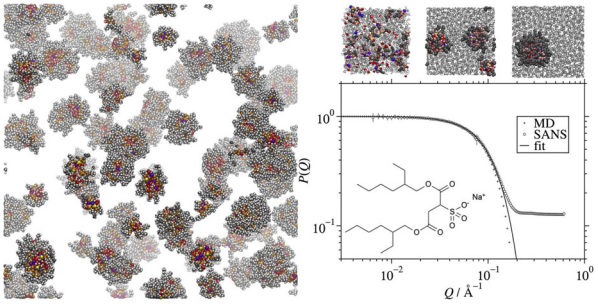
Experimental and simulation study of reverse micelles formed by aerosol-OT and water in non-polar solvents

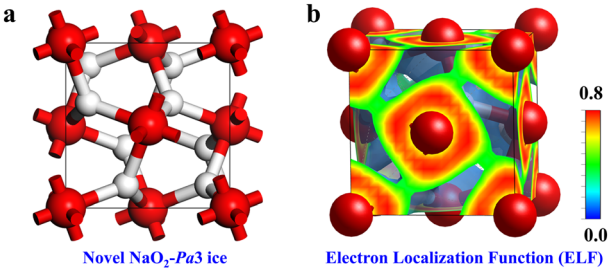
Angie Mat'usová, Georgina Moody, Peter J. Dowding, Julian Eastoe and Philip J. Camp*



27783

New metallic ice phase under high pressure

Yingying Huang,* Liuyuan Zhu, Hanlin Li, Haiping Fang, Ruoyang Chen* and Shiqi Sheng*



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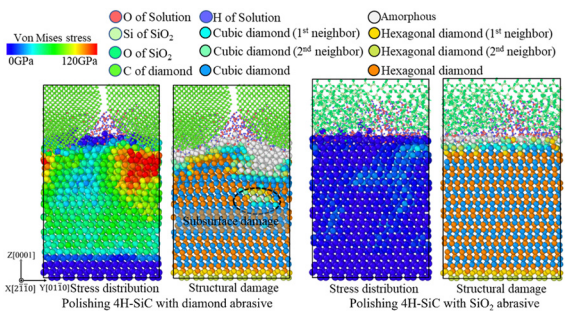
Effects of oxidizer concentration and abrasive type on interfacial bonding and material removal in 4H-SiC polishing processes

Yuqi Zhou, Kezhong Xu, Yuhan Gao, Ziniu Yu and Fulong Zhu*



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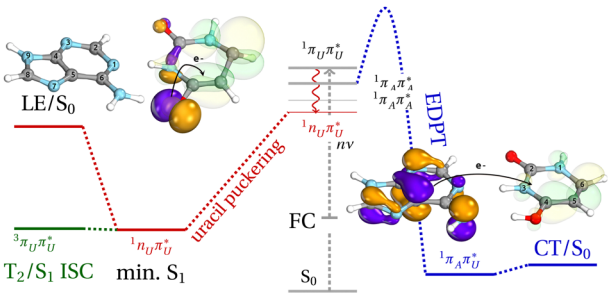
Theoretical insight into photodeactivation mechanisms of adenine–uracil and adenine–thymine nucleobase pairs

Kinga Szkaradek* and Robert W. Góra*



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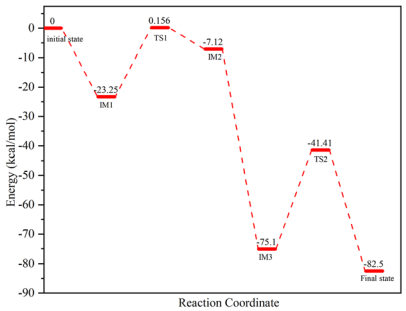

Performance of functionalized graphene oxide with organic radical scavengers in proton exchange membranes

Yu Hu, Jiaxing Wang, Shuai Wang* and Yuan Feng