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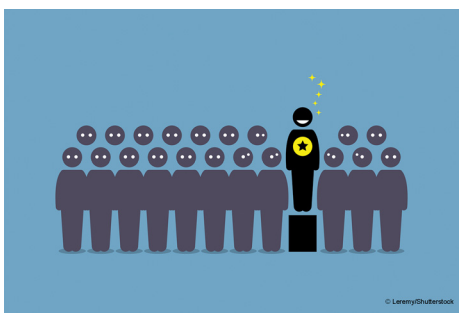
See Zhuwu Jiang, Yuanmei Chen *et al.*, pp. 12129–12138. Image reproduced by permission of Xiao Yao from *Phys. Chem. Chem. Phys.*, 2025, **27**, 12129.

EDITORIAL



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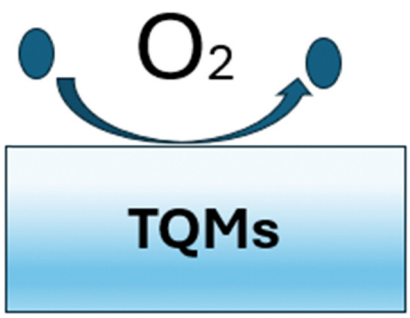

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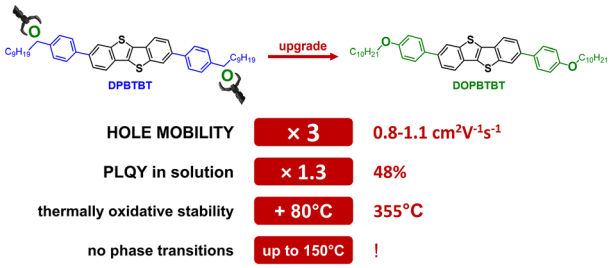

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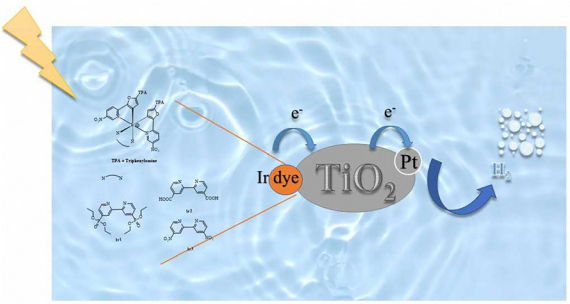

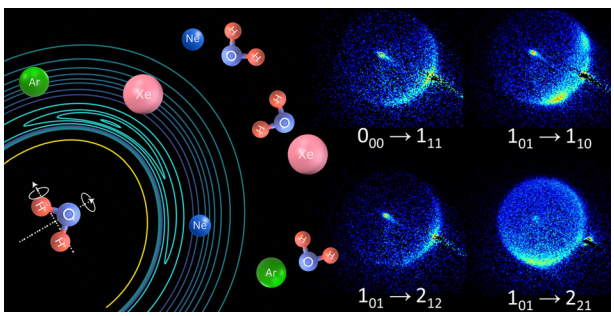

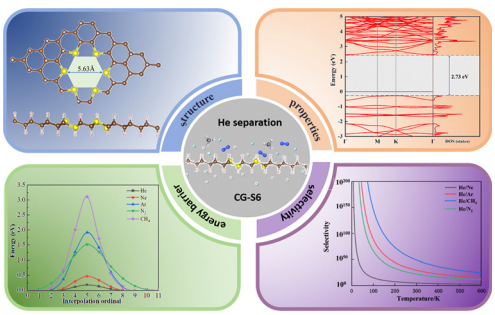

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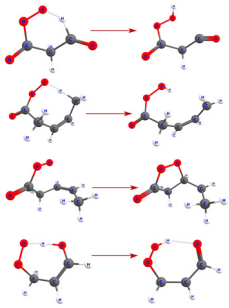

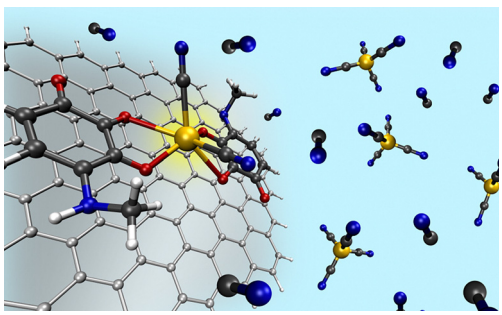

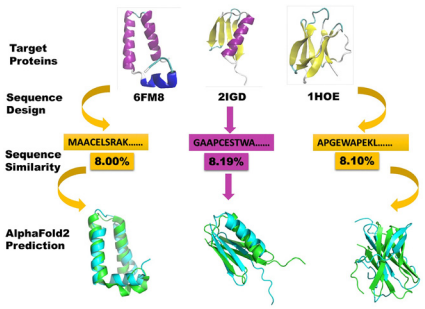

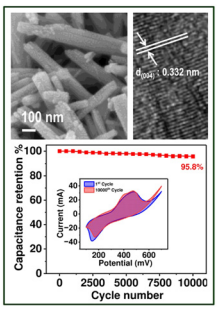

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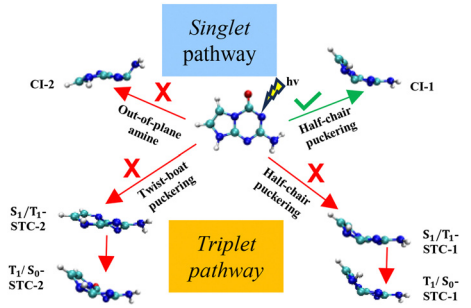
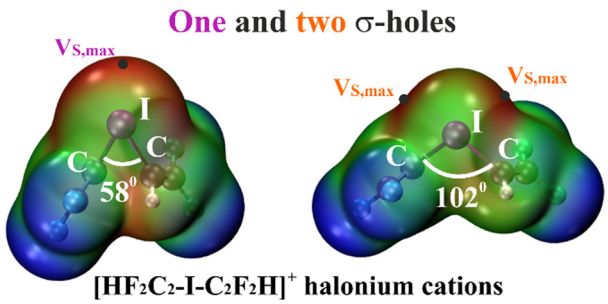


Efficient photodeactivation mechanism in an unnatural nucleic acid base

Somsuta Ray and Debashree Ghosh*

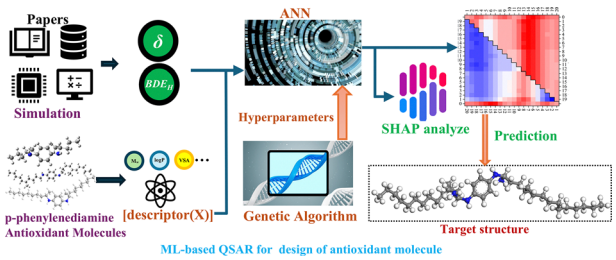
12248



Arrangement of σ-holes at the halogen atom in halonium cations

Mariusz Michalczyk* and Wiktor Zierkiewicz

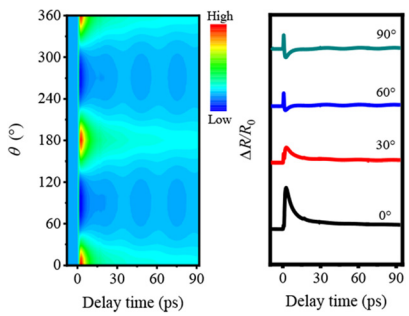
12256



Machine learning-assisted design of the molecular structure of *p*-phenylenediamine antioxidants

Zongya Wu, Shuai Sun, Chaokun Huang, Li Zhou, Yanlong Luo and Xiujuan Wang*

12267



Anisotropic ultrafast hot carrier dynamics of two-dimensional SnS single crystals

Zanxiong Peng, Borong Cong, Jiajun Cao, Chunlian Li, Xiaodong Shen and Weizheng Liang*

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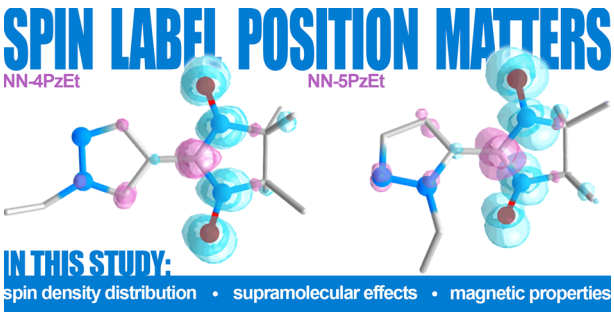
Specific features of the spin density distribution and magnetic properties in a series of pyrazolyl-substituted nitronyl nitroxides: a magnetochemical and quantum chemical study

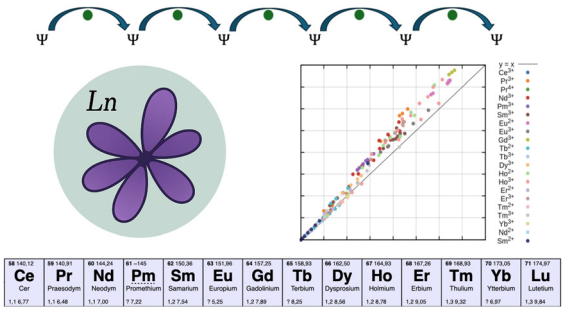
G. A. Letyagin,* P. A. Chernavin, K. Yu. Maryunina, S. E. Tolstikov, E. V. Tretyakov, G. V. Romanenko and A. S. Bogomyakov



12284

Excitations in lanthanide ions: a systematic evaluation of two-component CAS-CI and GW

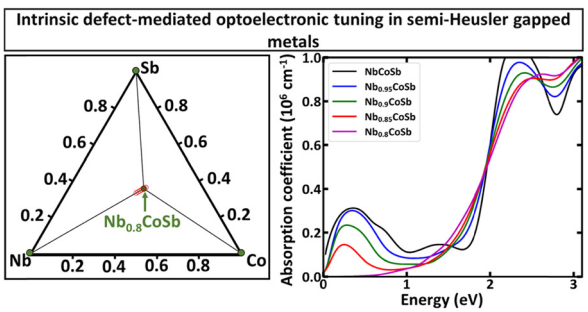
Roman Zielke, Florian Weigend* and Christof Holzer*



12294

Interplay between intrinsic defects and optoelectronic properties of semi-Heusler gapped metals

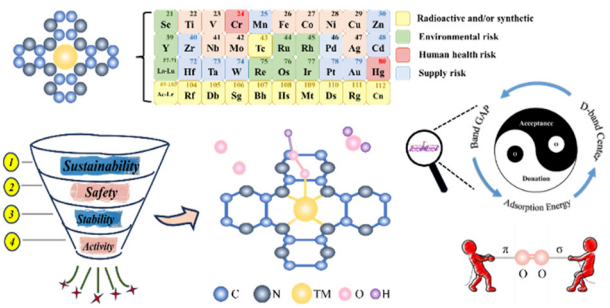
Muhammad Rizwan Khan, Jin Yang, Jincheng Kong,* Xiaoguang Li* and Zheng Wang*



12303

Computational high-throughput screening of high-performance transition metal C_8N_8 single-atom electrocatalysts for the oxygen reduction reaction

Keyuan Chen, Xingkao Zhang, Yongzhi Wu, Li Ma, Hanqing Li, Jueyi Ye, Ju Rong,* Xiaohua Yu* and Zhaohua Liu



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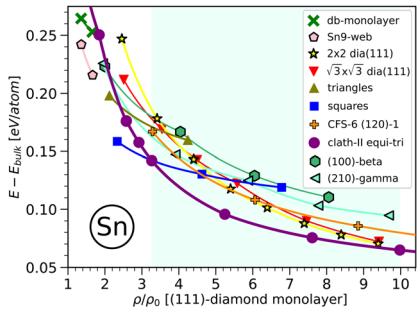
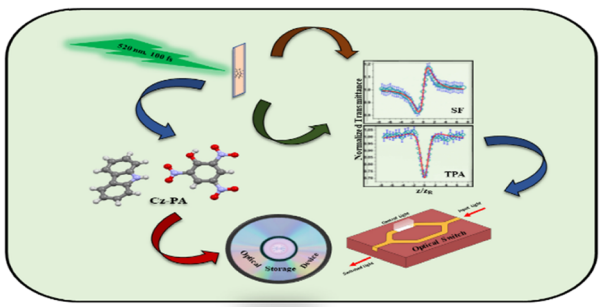


Stable thin clathrate layers

Eva Pospíšilová

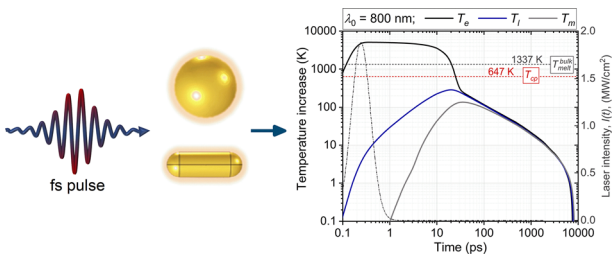
12331



Enhanced ultrafast cubic nonlinearity in the carbazole–picric acid complex for potential applications in photonic devices: Kerr nonlinearity with two-photon absorption

Mohd Mehkoom, Farman Ali, Amit Kumar Pradhan, Prasanta Kumar Datta* and Umakanta Tripathy*

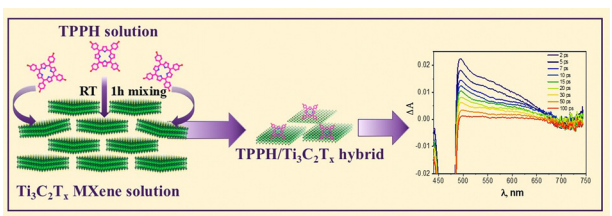
12343



Probing ultrafast heat transfer mechanisms in plasmonic gold nanostructures: FEM analysis of core–shell configurations under femtosecond laser irradiation

Joshua Fernandes and Myoung-Jin Kim*

12368



Coupling porphyrin with MXene nanosheets: exploring non-covalent interactions and photophysical characteristics

Marina Smirnova, Blazej Scheibe, Marcin Jarek, Alexandra Siklitskaya, Adam Kubas and Anna Lewandowska-Andralojc*

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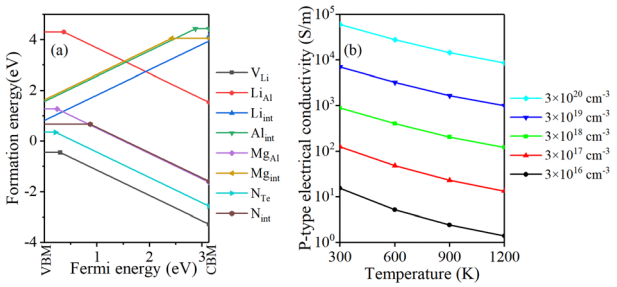

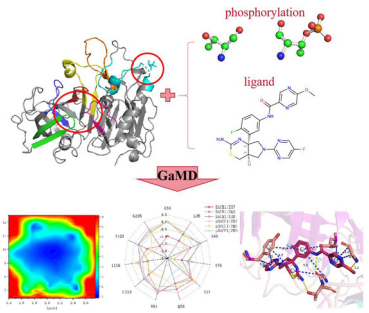

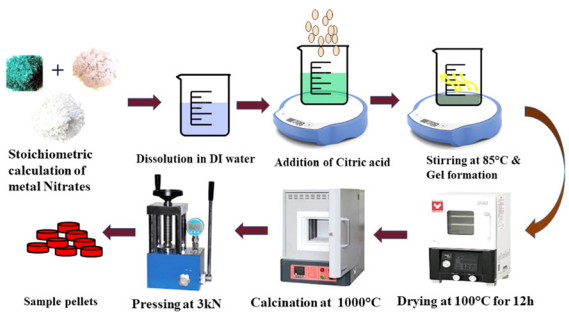

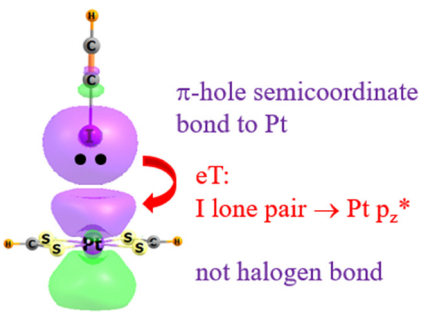

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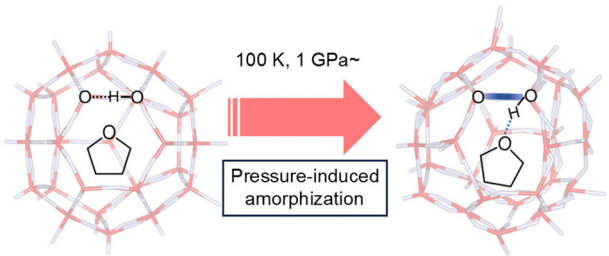

Similarities between the tetrahydrofuran clathrate hydrate after pressure-induced amorphization and aqueous tetrahydrofuran solution: an *in situ* Raman and infrared spectroscopic study

Naoki Noguchi,* Haruki Fujii and Hidekazu Okamura

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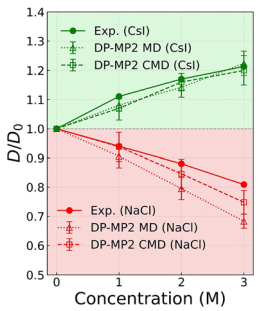
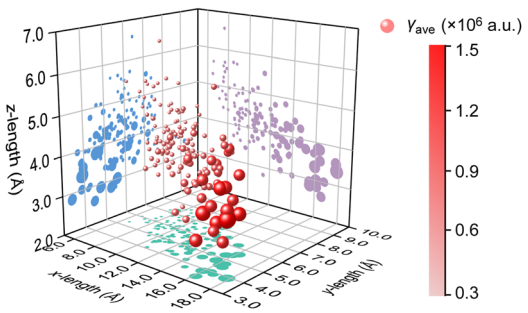


Structure making and breaking effects of ions on the anomalous diffusion of water revealed by machine learning potentials

Jinfeng Liu,* Xuchao Zhou and Xiao He*

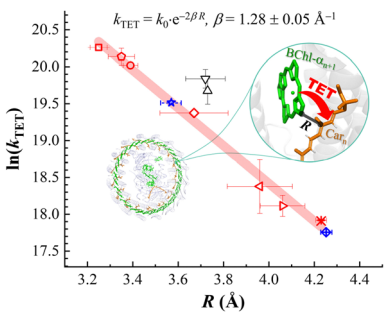
12453



A length descriptor to measure the linear and third-order nonlinear optical responses of atomic-cluster isomers

Quanjie Zhong

12462



Triplet excitation dynamics of photosynthetic light-harvesting antennae: mechanistic insights into the conjugation regulated carotenoid functionality

Yu-Qian Li, Yi-Hao Yan, Rong-Yao Gao, Jian-Wei Zou, Yu-Lu Wu, Xing-Yu Yue, Yao Lu, Xiang-Ping Wang, Ming-Qing Chen, Qi-Wei Li, Hao-Yi Wang, Peng Wang, Long-Jiang Yu,* Junrong Zheng and Jian-Ping Zhang*

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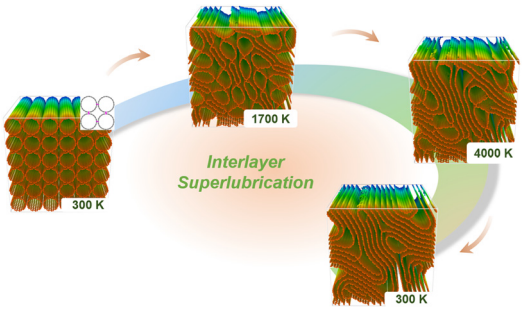

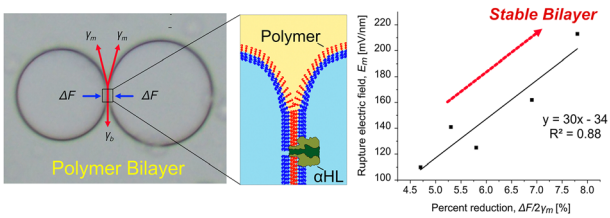

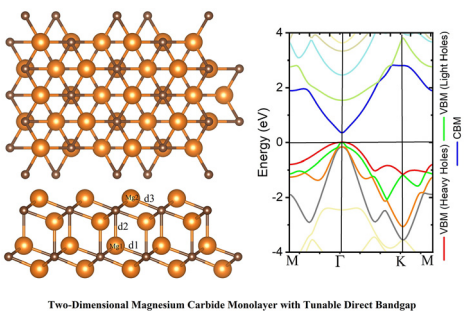

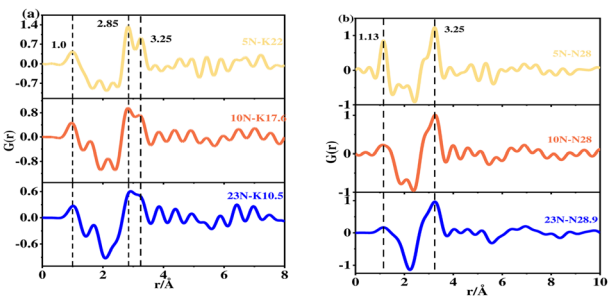

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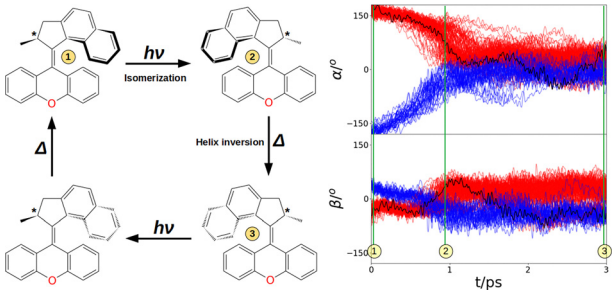
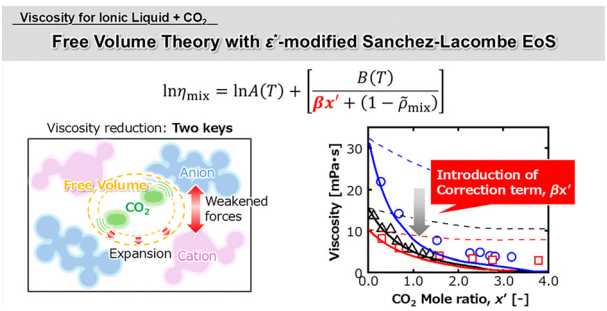


First principles prediction of wavelength-dependent isomerization quantum yields of a second-generation molecular nanomotor

Jesús Lucia-Tamudo, Michelle Menkel-Lantz and Enrico Tapavicza*

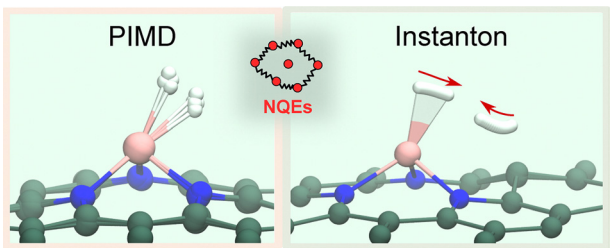
12532



Viscosity prediction of CO_2-saturated imidazolium-based ionic liquids using the ε*-modified Sanchez–Lacombe equation of state and free volume theory with a new correction term

Ryohei Otani, Yuya Hiraga* and Masaru Watanabe*

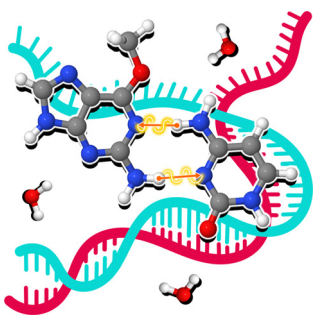
12542



Nuclear quantum effects in two-hydrogen intermediates on graphene-embedded transition metal atoms

Erxun Han, Wei Fang* and Ji Chen*

12550



Proton transfer in methylated G–C: nuclear quantum effects and water-assisted hopping

Juliana G. de Abrantes,* Adam P. Motala, Ian Riddlestone, Louie Slocombe and Marco Sacchi*

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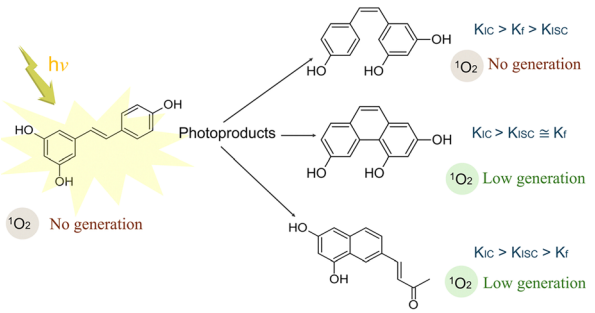

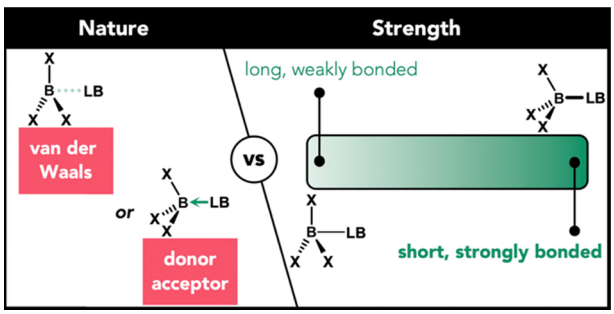

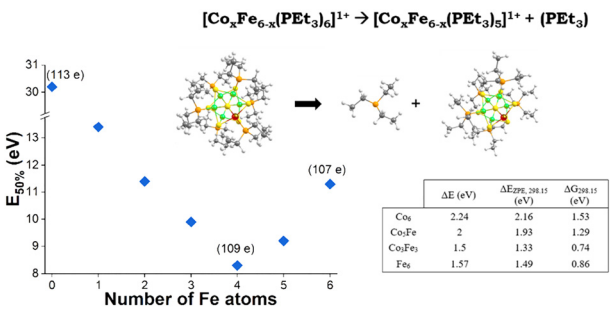

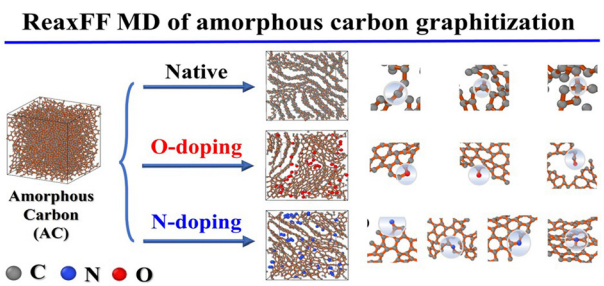

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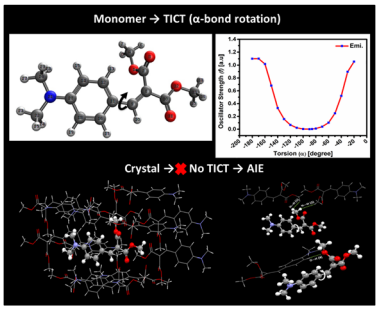

Aggregation-induced emission mechanism of styrene derivative: a theoretical study

Aarzoo, Kenichiro Saita, Masato Kobayashi, Takao Tsuneda,* Tetsuya Taketsugu and Ram Kinkar Roy*