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Cover

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Inside cover

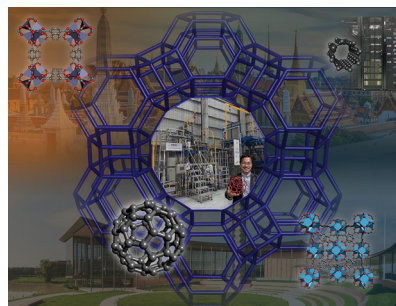
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EDITORIAL

12116

Advances in computational chemistry and catalysis: honouring Jumras Limtrakul's 72nd birthday

Thana Maihom* and Chularat Wattanakit*

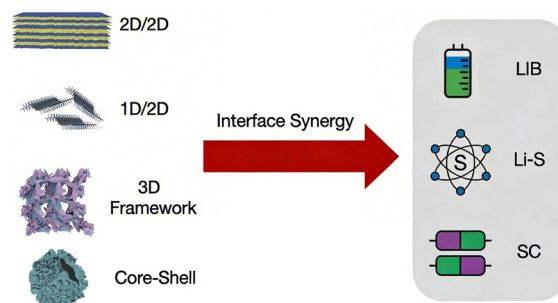


REVIEW

12118

Synergy and interface: design of MXene/LDH composites and their electrochemical energy storage applications

Xiaohui Zhang, Yaxin Zhu, Song Liu, Longyu Yang, Hongfu Cui, Miao Zhu, Shucun Li* and Yuqing Qiao*



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Fundamental questions
Elemental answers

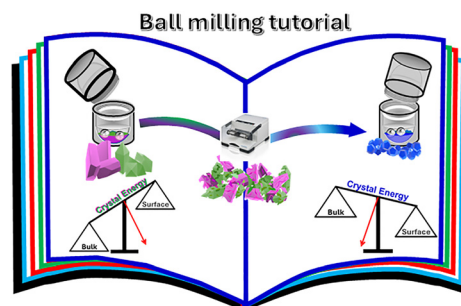


TUTORIAL REVIEWS

12138

Unravelling key phenomena in ball milling reactions toward fundamental principles—a minireview tutorial

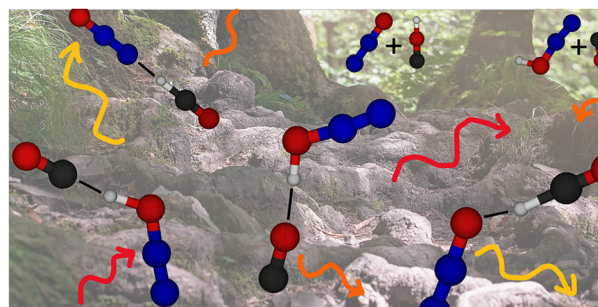
Ana M. Belenguer



12172

A practical guide to RRKM theory, its simplified multi-well version AWATAR and master equation modelling of radiative processes

Magdalena Salzburger, Marc Reimann, Jessica C. Hartmann, Milan Ončák and Martin K. Beyer*

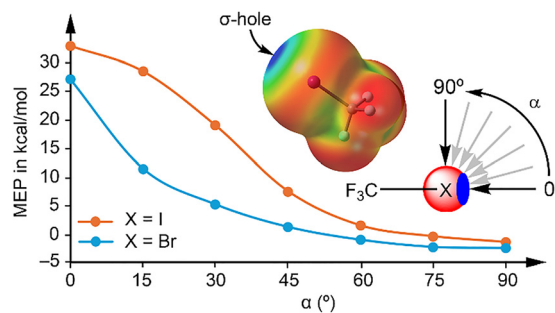


RESEARCH PAPERS

12188

Evaluation of the solvent competitive binding in halogen and chalcogen bonding: a theoretical study for supramolecular applications

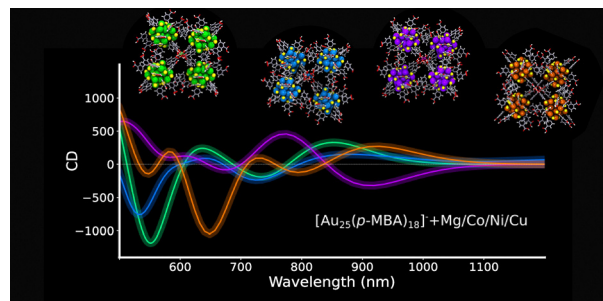
Eric Miguens, Mariana Rocha and Antonio Frontera*



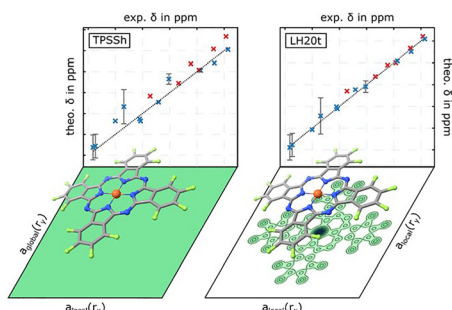
12196

Optical properties of metal-ion-mediated Au_{25} nanocluster-based assemblies

Hanna Jääskö, Sami Malola and Hannu Häkkinen*



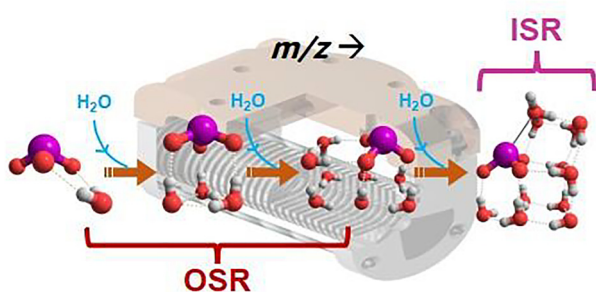
12203



Accurate ^{19}F NMR chemical shifts in Fe(II) complexes with the LH20t local hybrid functional

Justin Krampe, Timon Zankel, Roman Kornievskii, Kilian Heckenberger, Christina M. Thiele* and Vera Krewald*

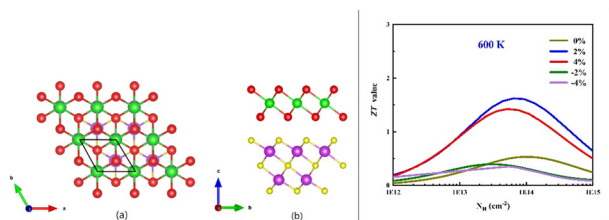
12216



Ion vibrational spectroscopy of the microhydrated iodate anion: unveiling the onset of heterogeneous ion solvation

Arghya Chakraborty, Huiyan Li, Zhi-Feng Liu* and Knut R. Asmis*

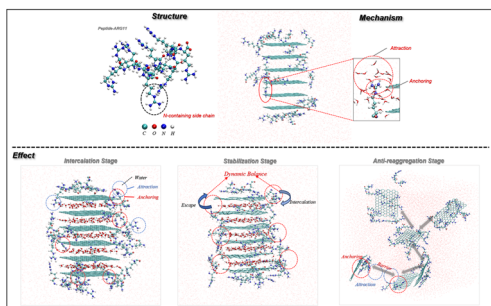
12228



Synergistic optimization of the thermoelectric properties of the 2D $\text{MgI}_2/\text{Bi}_2\text{S}_3$ heterostructure via biaxial strain

Chunwei Zhang,* Kangjia Lv, Xiaobo Jiang, Qian Lu, Liang Li, Haixiang Huan, Linzhen Zhou and Cui Bo

12242



The dominant role of N-containing side chains in peptide-mediated graphene dispersion and stabilization: a molecular dynamics simulation study

Rongqing Xia, Xiaoping Zeng, Dawei Wang, Qianqian Liu, Jiangyu Wu* and Lu Cai*

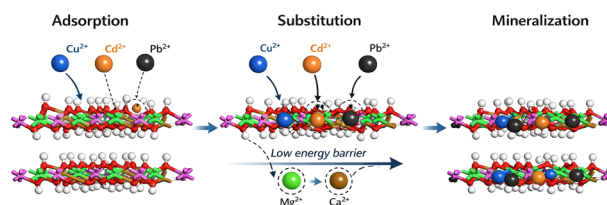


RESEARCH PAPERS

12256

Theoretical study on the mechanism of super-stable mineralization of heavy metal cations by ternary layered double hydroxides for soil remediation

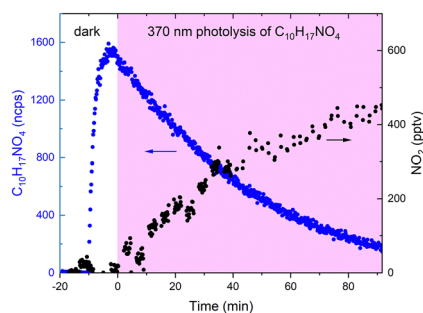
Jia-lin Guan, Yao Jie, Yi-Fan Zhang, Dan-Ni Chen, Yan-Jing Ren, Xin-Yi Du, Xiao-Heng Zhang and Hong Yan*



12266

Formation and photolysis of multifunctional organic nitrates from the reaction of limonene and NO₃ radicals

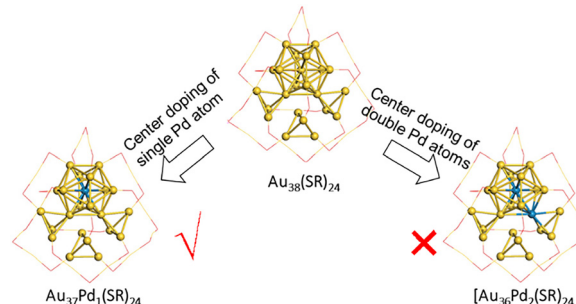
Laura Wüst, Lasse Moormann, Patrick Dewald, Eunyeong Jin, Jan Schuladen, Jonathan Williams, Frank Drewnick, Ulrich Pöschl, Jos Lelieveld and John N. Crowley*



12281

Tuning the electronic structure and stability of Au₃₈(SR)₂₄ nanoclusters via site-selective palladium doping

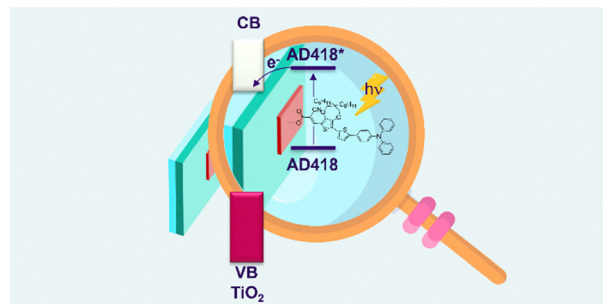
Qingyao Gong, Xiaxi Lei, Wenhui Zhao, Gang Wang and Wen Wu Xu*



12290

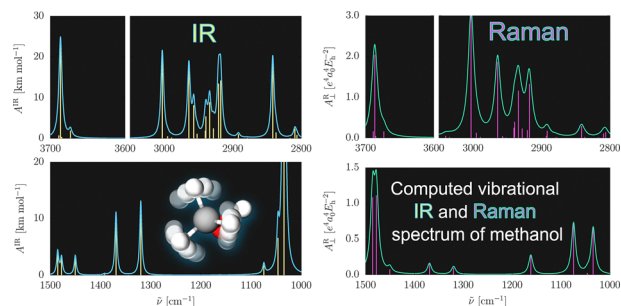
Fast and ultrafast charge transfer dynamics in organic dye sensitizers anchored on TiO₂ for photoelectrochemical cells

Federica Ruani, Matteo Bartolini, Elena Ermini, Elisa Bandini, Andrea Barbieri, Adalgisa Sinicropi, Alessandro Mordini, Lorenzo Zani* and Barbara Ventura*



RESEARCH PAPERS

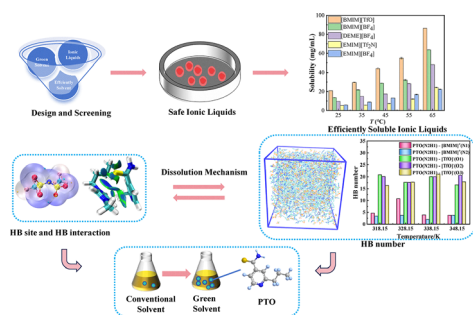
12299



Vibrational infrared and Raman spectra of the methanol molecule with equivariant neural-network property surfaces

Ayaki Sunaga, Albert P. Bartók and Edit Mátyus*

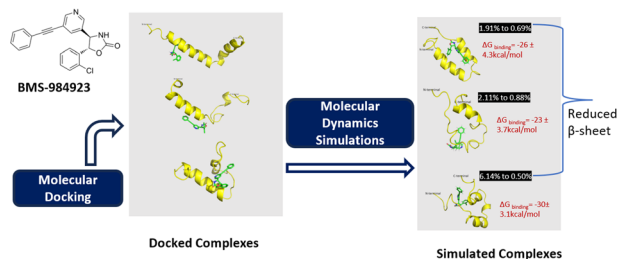
12314



Unraveling prothionamide solubility enhancement by ionic liquids: from molecular screening to microscopic insights

Xiaowen Sun, Junqi Bai, Chuanrun Li, Zhigang Lei, Chengmin Gui,* Yichun Dong, Xiaoyi Gao and Yanyan Guo*

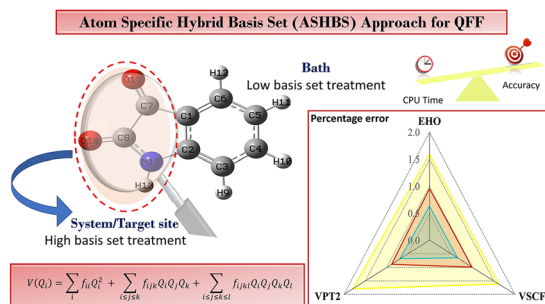
12329



Computational investigation of BMS-984923 against Alzheimer's amyloid-beta (Aβ) structures: insights into their molecular interactions and inhibition of aggregation

Smita Patir and Anupaul Baruah*

12348



Hybrid quartic force fields with atom-specific basis sets: an efficient route to calculate anharmonic vibrational spectra

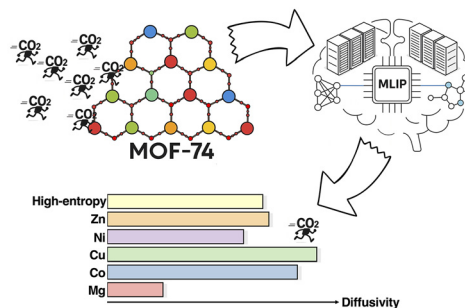
Mokshi Sharma and Tapta Kanchan Roy*



12362

Elucidating CO₂ dynamics in high-entropy MOF-74 via machine learning interatomic potentials

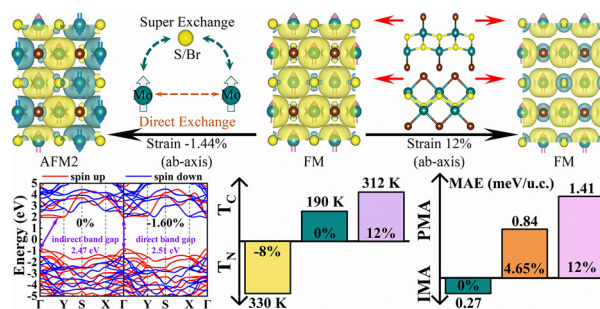
Klichchupong Dabsamut* and Ching-Ming Wei*



12379

Biaxial strain-mediated magnetic phase transition and anisotropy engineering in the MoSBr monolayer: a first-principles approach for room-temperature spintronics

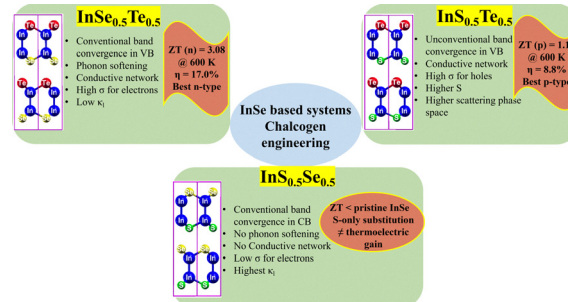
Yifan Zhao, Xinyi Wang, Peng Li and Ruilin Han*



12391

Designing high-performance thermoelectrics through chalcogen engineering in InSe-based layered materials

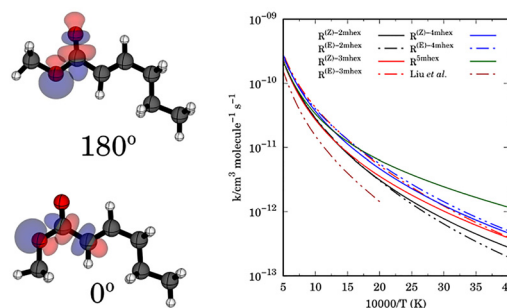
Shivani Vinod, Tanu Choudhary and Raju K. Biswas*



12411

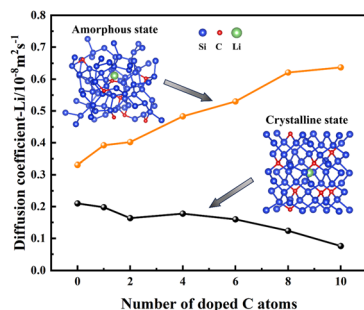
Unsaturated C₆ fatty acid methyl esters as reference molecules for biodiesel: kinetics of H-atom abstraction and addition

Joel Leitão Nascimento, Antonio Fernández-Ramos* and Tiago Vinicius Alves*



RESEARCH PAPERS

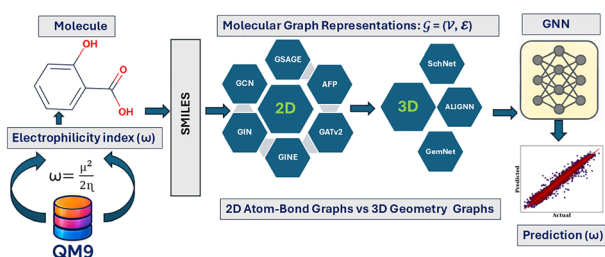
12424



Structures and properties of carbon-doped amorphous silicon as an anode for lithium ion batteries: a first-principles study

Wangyang Ruan, Caimeng Yu, Zhe Li, Shu Luo, Daosong Zha, Cen Wang and Min Wu*

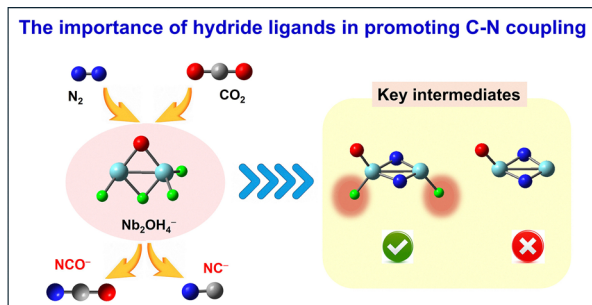
12432



Graph neural network architectures for predicting the electrophilicity index: insights from 2D and 3D molecular graph representations

Sandeep Kumar* and Annika Bande

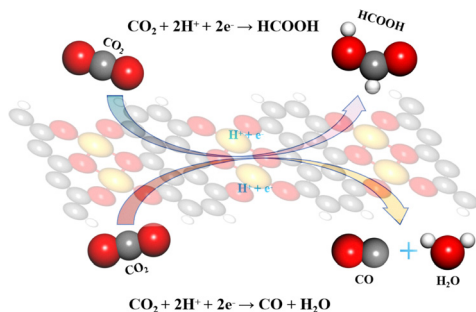
12444



C–N bond formation from co-conversion of N_2 and CO_2 mediated by Nb_2OH_4^- cluster anions: importance of hydride ligands

Xiao-Xiao Liu, Qing-Yu Liu, Zi-Yu Li* and Sheng-Gui He

12451



Theoretical design of one-dimensional dual site metal–organic framework ribbons for the CO_2 RR

Zhen Feng,* Weihui Wang, Xiangrui Ren, Chengyan Li, Shu Zheng, Zhiyuan Zhang, Zhanyong Guo* and Xianqi Dai*

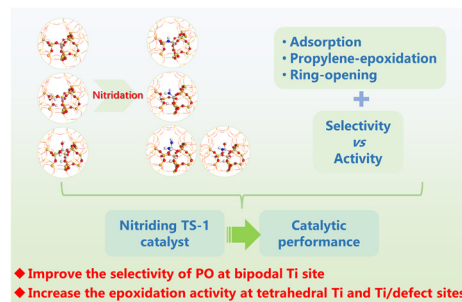


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12462

Mechanistic investigation of nitridation-promoted reactivity and selectivity for propylene epoxidation in TS-1 catalysts: a theoretical study

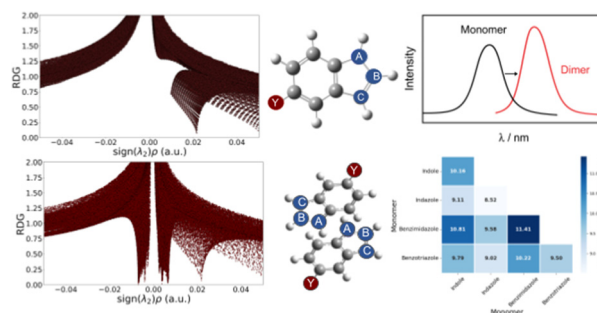
Qiaoyun Qin, Kai An, Hongxia Liu, Xueqiang Qi* and Baohe Wang*



12472

Photophysics and complexation of indolic compounds: the effect of intra-annular and extra-annular substitution

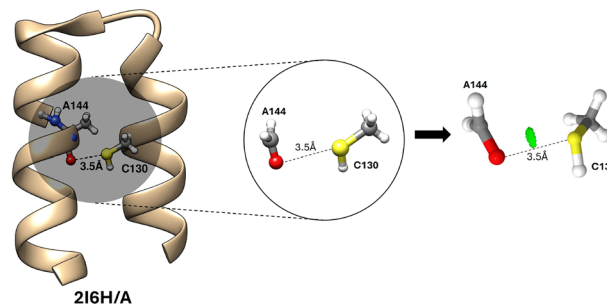
Soumyadip Ray, Atheena Krishna D. and Padmabati Mondal*



12483

Chalcogen bond interactions involving sulphur atoms of methionine or cysteine residues and backbone carbonyl oxygen atoms in protein structures

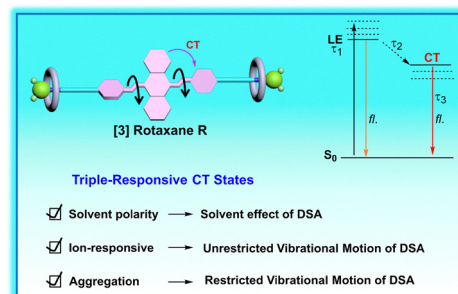
Prathvi Singh, Venkatnarayan Ramanathan and Ramasubbu Sankararamkrishnan*



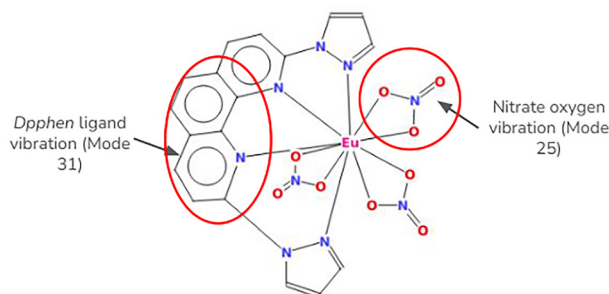
12491

A tunable charge-transfer-state rotaxane gated by solvent, anions, and aggregation

Wei-Liang Hu, Yuan Yuan, Gui-Yuan Wu,* Xian-Yi Zhang, Wei-Jian Li* and Zhou Lu*



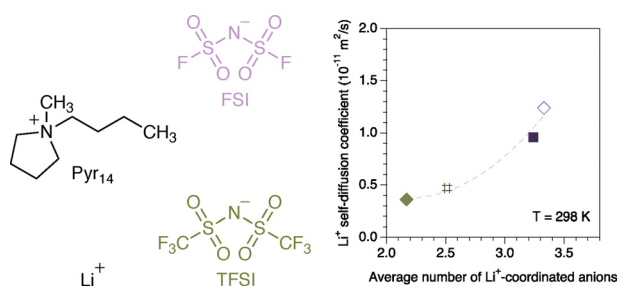
12500



Dominant vibronic relaxation channels in a europium-based molecular qubit

Neil Iyer

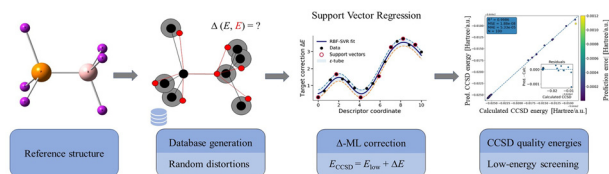
12508



The impact of anion mixing on Li⁺ coordination and transport properties in pyrrolidinium-based ionic liquid electrolytes

Nicole Abdou,* Quan Wu, Lars Evenäs, Anna Martinelli and Aleksandar Matic*

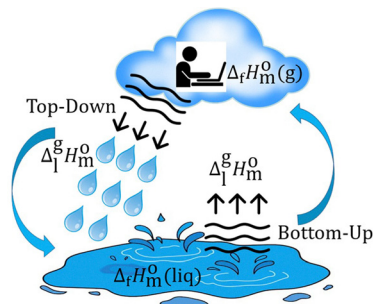
12517



Δ-Machine learning toward CCSD accuracy for homohalogenated borane–phosphine adducts: screening low-energy structures from DFT and MP2 libraries

Okan Köksal

12530



Top-down and bottom-up evaluation of thermochemistry of α,ω -alkanediols

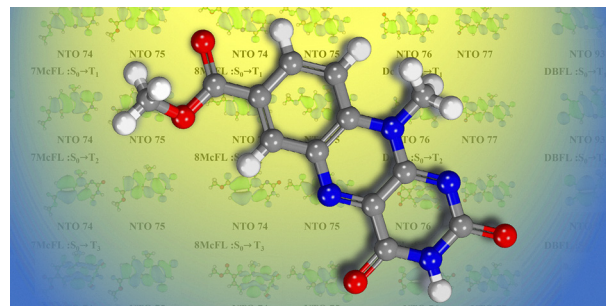
Riko Siewert, Olga V. Dorofeeva, Artemiy A. Samarov, Arina V. Elbakari, Karsten Müller, Peter Wasserscheid and Sergey P. Verevkin*



12551

Carboxyl-functionalized flavin as efficient heavy-atom-free triplet photosensitizers: a theoretical investigation

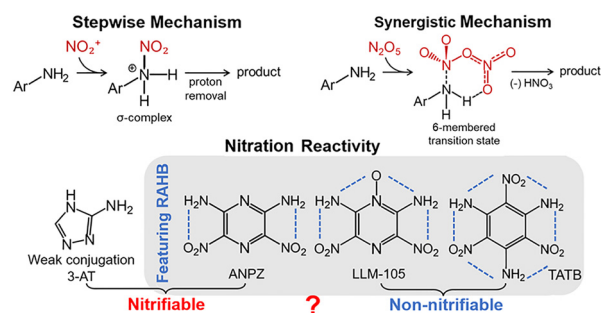
Huimin Guo,* Heping Li and Chengyu Yang



12563

Aromatic amine nitration mechanisms: reactivity governed by resonance-assisted hydrogen bonds

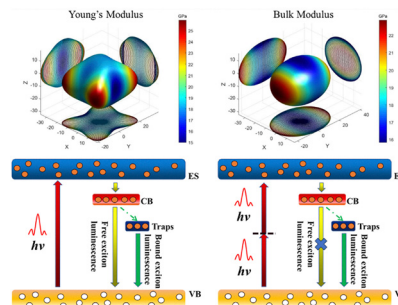
Tianlong Wu, Zhe Wu, Guo-Ping Lu, Hua Guan, Dabin Liu, Yingzhe Liu and Baojing Zhou*



12573

The structural stability and temperature-dependent exciton dynamics of CsPbBr₃ millimeter crystals

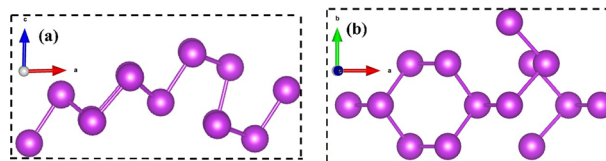
Hailong Yu,* Jia Liu, Jijuan Jiang, Yang Jia, Guan Wang, Wenqiang Shi and Hongyan Meng



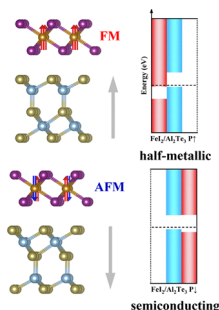
12584

Near-zero Poisson's ratio monolayer bismuthene

Lingling Bai, Runqing Zhang, Huafeng Dong* and Huan Ma



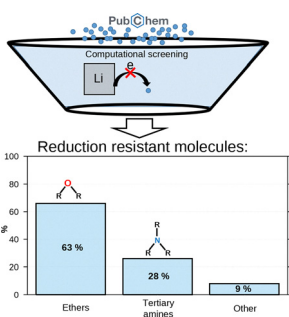
12592



Reversible switching of half-metallicity and magnetic order in 2D $\text{Fe}_2/\text{Al}_2\text{Te}_3$ van der Waals multiferroics tailored by ferroelectric polarization

Guoan Ding, Zhijian He, Shuhong Xie* and Daifeng Zou*

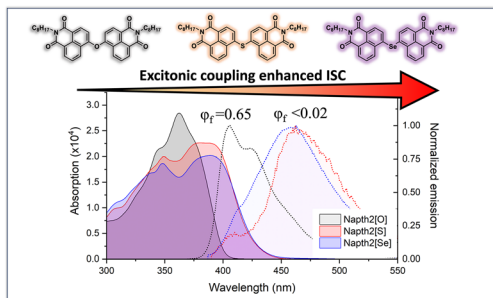
12601



Mapping the reduction-resistant solution components: ethers confirmed, tertiary amines revealed

M. A. Orekhov* and S. A. Kislenco

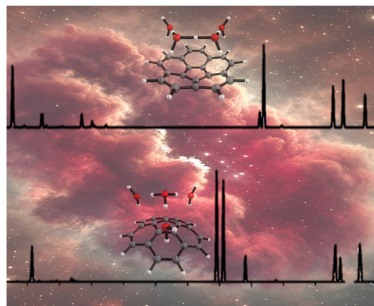
12609



Revisiting the intersystem crossing mechanisms in chromophore dimers through the lens of excitonic coupling: a case study of naphthalimide

Monika G. Mutovska, Dario Puchán Sánchez, Arthur H. G. David, Clément Cabanetos,* Tangui Le Bahers, Yulian Zagranyski,* Cyrille Monnereau* and Josene M. Toldo*

12623



Surface curvature effects in neutral and protonated water clusters: insights from DFT and energy decomposition analysis

Murillo H. Queiroz, Bruno S. Sampaio, Celine Nieuwland, Célia Fonseca Guerra, Tiago V. Alves and Roberto Rivelino*

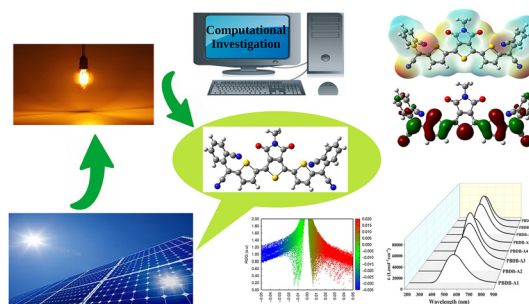


RESEARCH PAPERS

12632

Terminal group engineering in small molecule acceptors: a first-principles approach to improving organic solar cell performance

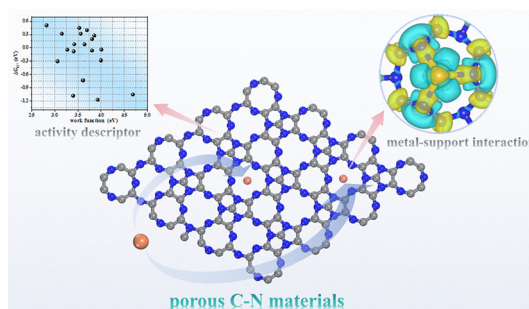
Rinki Deka and Dhruva Jyoti Kalita*



12643

Work function-regulated two-dimensional porous C₇N₆-based single-atom catalysts for the hydrogen evolution reaction

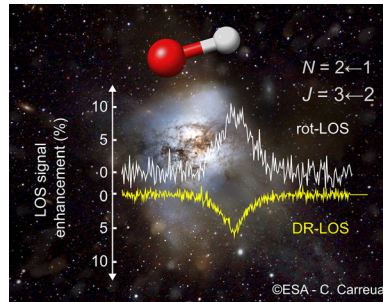
Wenli Xie, Bin Cui, Desheng Liu, Haicai Huang* and Chuanlu Yang*



12651

Hyperfine-resolved rovibrational and rotational spectroscopy of OH⁺ ($X^3\Sigma^-$)

Wesley G. D. P. Silva, Lea Schneider, Urs U. Graf, Holger S. P. Müller, Pavol Jusko, Arshia M. Jacob, Dominik Riechers, Stephan Schlemmer and Oskar Asvany*



CORRECTION

12660

Correction: Investigations of the structural, electronic, and optical properties of Ti₃XC₂ (X = Ge, Pb, or Bi) by DFT

Haider Hussain,* Zulfiqar Ali Shah, Syed Zafar Ilyas, Abdul Shakoor* and Zawar Hussain

