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Cover

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Inside cover

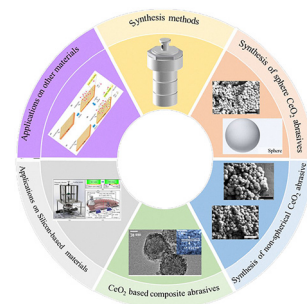
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REVIEW

13213

Recent advances in CeO₂ based abrasives for chemical mechanical polishing

Yongxin Wang, Yunhui Shi,* Jiabao Cheng, Yao Xu, Yizhan Wang and Jiawei Qiu

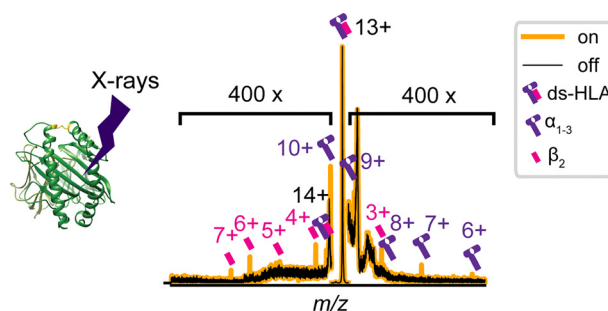


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X-ray spectroscopy meets native mass spectrometry: probing gas-phase protein complexes

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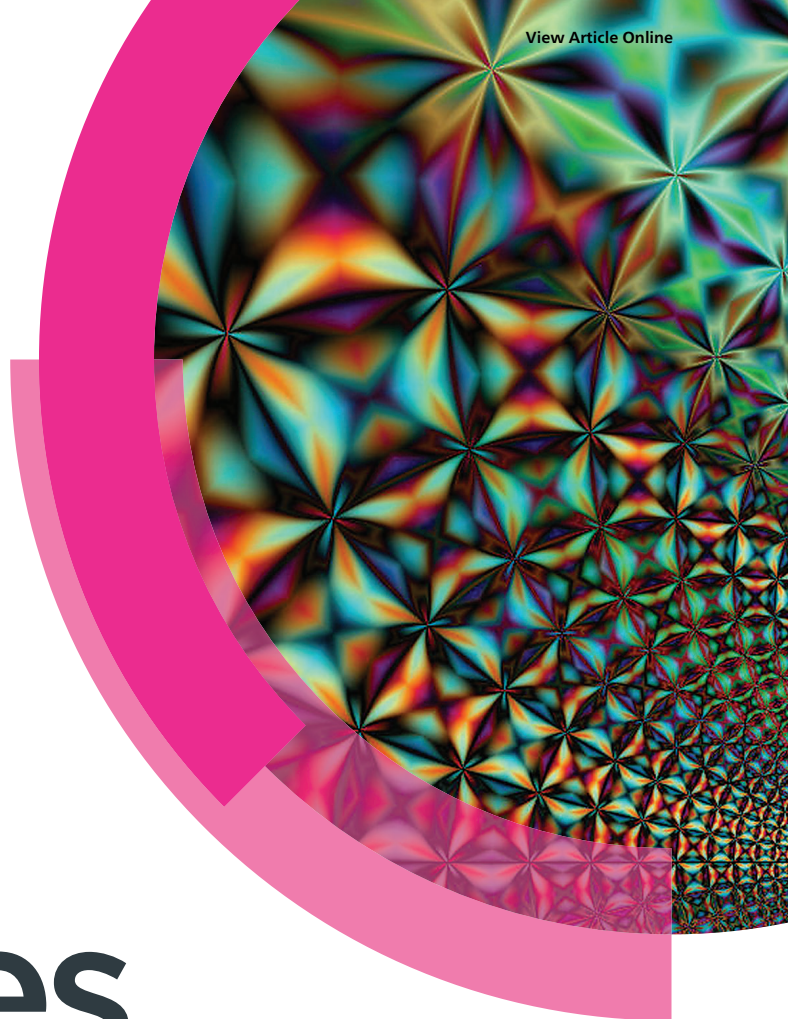


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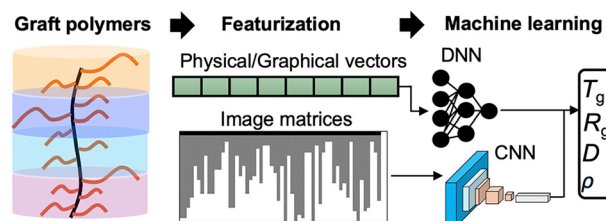


COMMUNICATIONS

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Machine learning of the architecture–property relationship in graft polymers

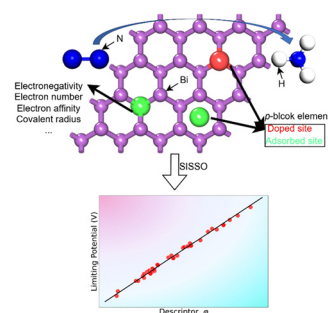
Kevin V. Bigting, Jordan J. Carden, Shubhadeep Nag, Jimmy Lawrence, Yen-Fang Su and Yaxin An*



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Proposing explainable descriptors towards enhanced N₂ reduction performance on the two-dimensional bismuthine nanosheets modified by p-block element-based electrocatalysts

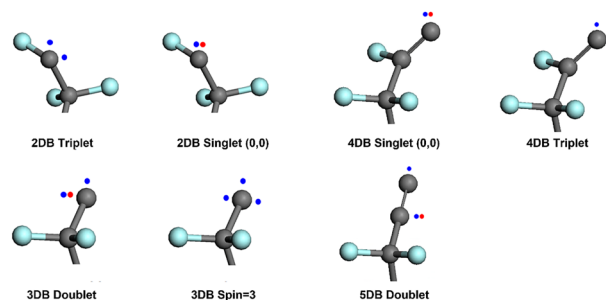
Dengning Sun, Xiaokun Du, Jing Chen, Tao Ye, Hao Shen, Ruirui Wang, Ying Wang,* Guoqiang Liu, Yangyang Wan* and Zhongti Sun*



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Roles of spin-state dangling bonds and strain in the electronic structure of polytetrafluoroethylene for charge transfer from first-principles

SeongMin Kim,* So-Hee Kim and Sang-Woo Kim*

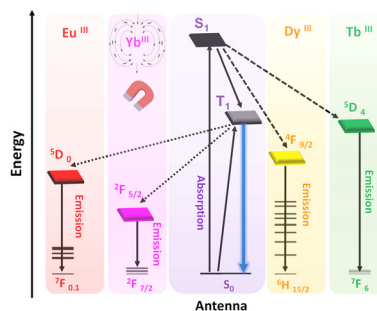


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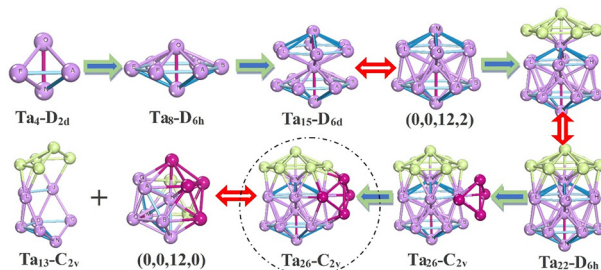
Different mechanisms for lanthanide(III) sensitization and Yb-field-induced single-molecule magnet behaviour in a series of pentagonal bipyramidal and octahedral lanthanide complexes with axial phosphine oxide ligands

Hadjer Allia, Ana Rodríguez-Expósito, María A. Palacios,* Juan-Ramón Jiménez, Albano N. Carneiro Neto, Renaldo T. Moura Jr., Fabio Piccinelli, Amparo Navarro, María Mar Quesada-Moreno* and Enrique Colacio*



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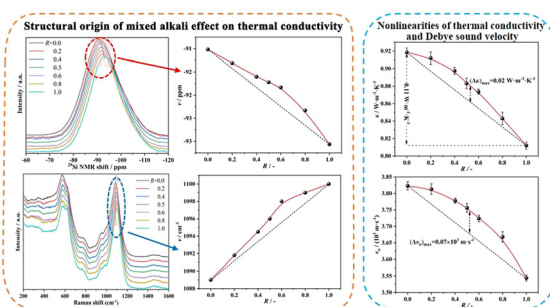
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The origin of the anomalous expansion of the first peak in the radial distribution function during the rapid solidification of tantalum metal

Yuanqi Jiang,* Dadong Wen, Qiang Xu, Jian Lv, Rui Zhao and Ping Peng

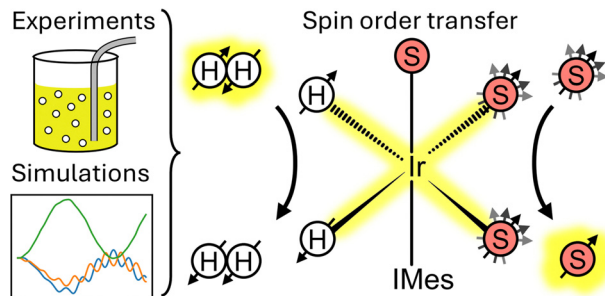
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Sodium and potassium mixed effect on thermal conductivity in a borosilicate glass

Qing Zhang, Shenglin Chen, Yingting Cai, Chao Huang, Ang Qiao and Haizheng Tao*

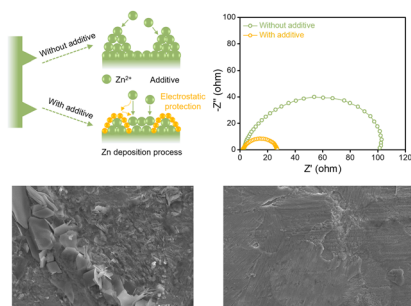
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Characterisation of the polarisation transfer to fluorinated pyridines in SABRE

Joni Eronen,* S. Karl-Mikael Svensson, Nazmul Hossain, Vladimir V. Zhivonitko, Juha Vaara and Anu M. Kantola*

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A facile and eco-efficient additive strategy enables high-performance aqueous zinc-ion batteries

Kai Yang,* Jiuzhou Yu, Xu Zhang, Shaoting Wang, Qiang Wang, Ci Gao, Yiyao Song and Xingxing Guo

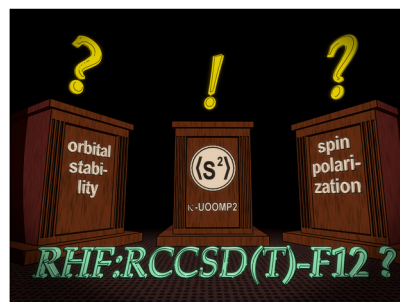


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Revisiting a large and diverse data set for barrier heights and reaction energies: best practices in density functional theory calculations for chemical kinetics

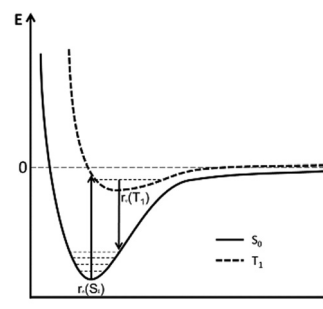
Xiao Liu, Kevin A. Spiekermann, Angiras Menon, William H. Green and Martin Head-Gordon*



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Unusually high spin–orbit coupling in the methionine singlet–triplet transition and the role of magnetic perturbations in amino acids

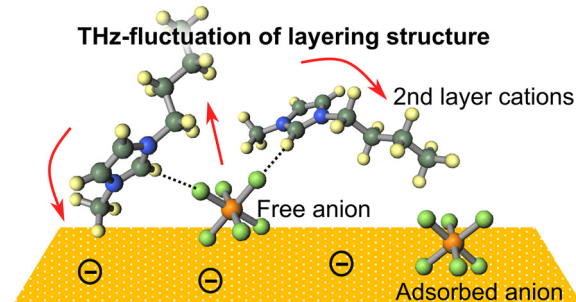
B. Minaev,* M. Sukhyna, P. Stakhira, V. Minaeva and H. Ågren



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Structures and terahertz dynamics of an imidazolium-based ionic liquid on a gold electrode studied using surface-enhanced Raman scattering

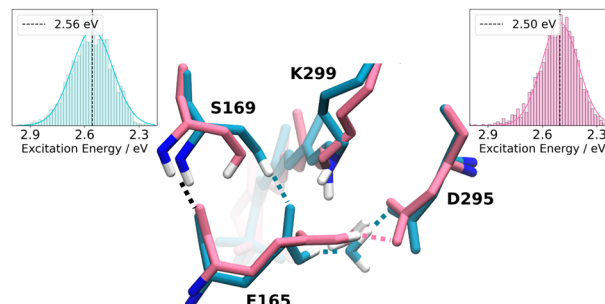
Ryo Ueno, Kenta Motobayashi and Katsuyoshi Ikeda*



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Complex active site structures influence absorption spectrum of Chrimson wild type and mutants

Katharina Spies,* Beatrix M. Bold and Marcus Elstner



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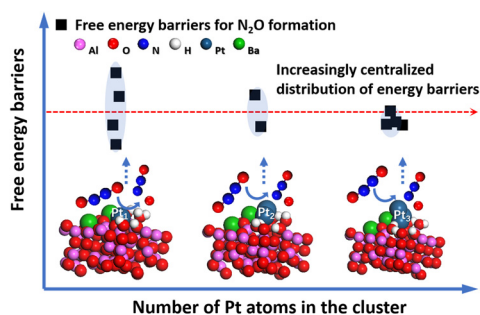
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DFT and SISSO studies on the CO₂ cycloaddition reaction to ethylene oxide catalyzed by intraframework M(II)-BEA zeolites

Winyoo Sangthong and Jakkapan Sirijaraensre*

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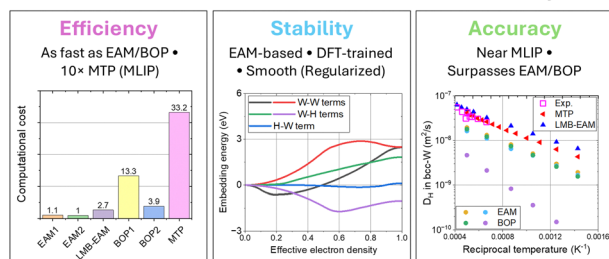


Mechanism of N₂O formation in catalytic after-treatment systems of ammonia/hydrogen-fuelled engines

Shilong Li, Gong Cheng, Haoran Chen, Ruichao Li, Peng Xia, Yue Li, Xingyu Liang and Kun Wang*

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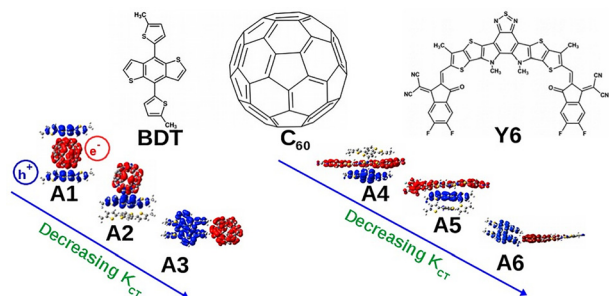
LMB-EAM: Fast, Stable, Near-MLIP Accuracy



Efficient calculations of impurity diffusivity in metals by linearized multi-band embedded atom method potentials

Sehyeok Park and Takuji Oda*

13403



Influence of molecular orientation on photovoltaic performance in double donor with fullerene and non-fullerene acceptor-based heterojunctions

Mohd Shavez and S. Mahapatra*

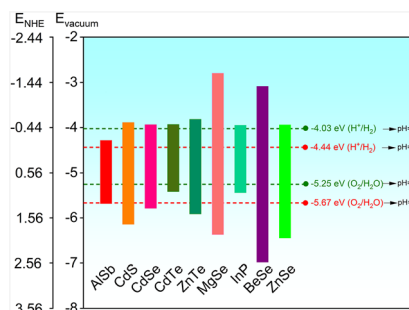


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Square octagon haeckelites as efficient photocatalysts with enhanced solar-to-hydrogen conversion and high carrier mobilities

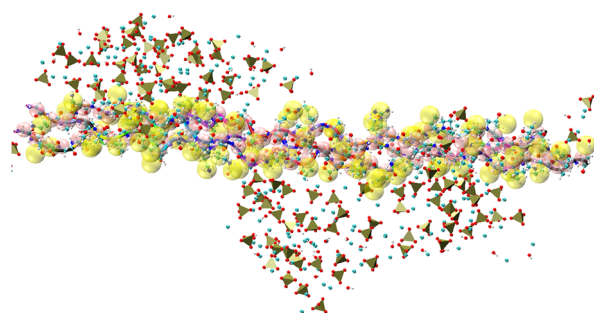
Ismail Shahid, Iqtidar Ahmad, Anwar Ali, Abid Raza, Xiaoliang Zhang,* Dawei Tang, Mohamed Kallel* and Shaimaa A. M. Abdelmohsen



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Nucleation of biomimetic hydroxyapatite nanoparticles on the surface of human type I collagen using a hybrid all-atom and coarse-grained model

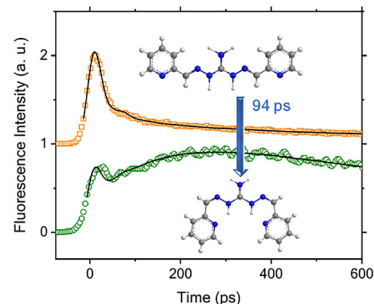
Zhiyu Xue, Xing Ye, Yao Cai, Xinyun Tan, XiaoMeng Wu, Fang Wu, Fei Li,* Dingguo Xu* and Bailing Zhou*



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Photoswitching dynamics of a guanidine anion receptor

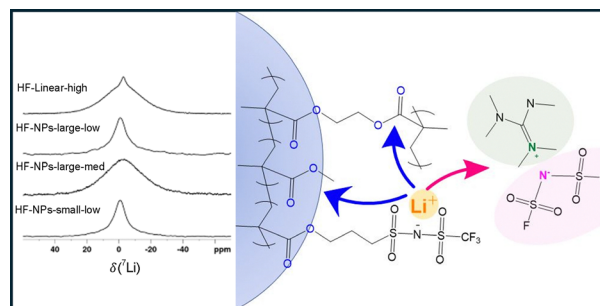
Ying-Zhong Ma,* Jeffrey D. Einkauf, Xinyou Ma, Duy-Khoi Dang, Paul M. Zimmerman, Radu Custelcean, Benjamin Doughty and Vyacheslav S. Bryantsev*



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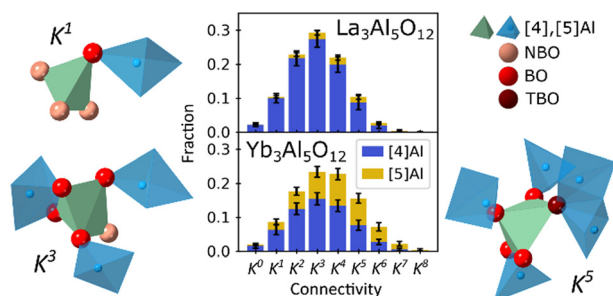
Effect of the polymer nature on the properties of composite solid electrolytes based on the organic ionic plastic crystal HMGFSI

Yady García,* Antonela Gallastegui, Vera Bocharova, Luca Porcarelli, Colin Kang, Haijin Zhu, David Mecerreyes, Maria Forsyth and Luke A. O'Dell*



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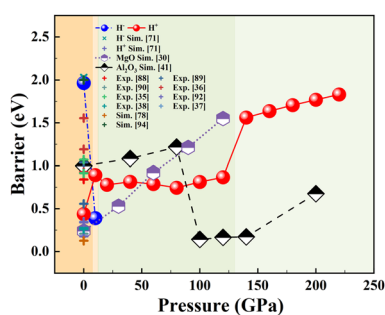
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Effect of rare earth size on network structure and glass forming ability in binary aluminum garnets

Stephen K. Wilke,* Chris J. Benmore, Randall E. Youngman, Benjamin J. A. Moulton, Abdulrahman Al-Rubkhi and Richard Weber

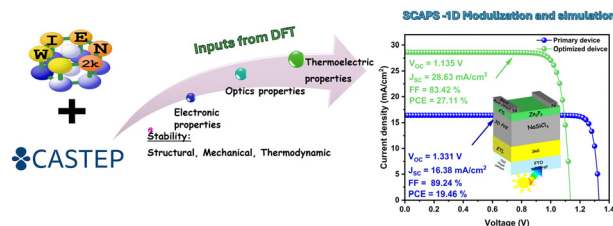
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Investigation of hydrogen diffusion in zirconia under extreme conditions

Fengqi Wang, Yuanqin Zhu and Xianlong Wang*

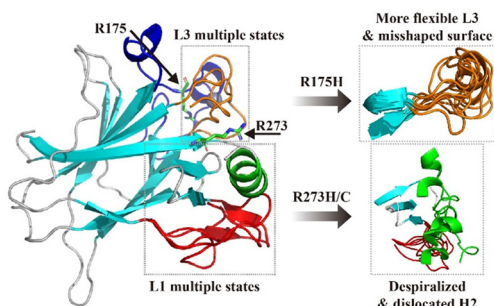
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Insight into NaSiCl₃: a lead-free perovskite for the next generation revealed by DFT and SCAPS-1D

Selma Rabhi,* Asif Nawaz Khan, Oualid Chinoune, Rania Charif, Nabil Bouri, Samah Al-Qaisi,* Shima Sadaf,* Amal BaQais and Mir Waqas Alam

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Structural dynamics of the wild-type p53 DNA-binding domain and hotspot mutants reveal oncogenic conformational shifts

Ziqian Zhao, Gang Wang, Xiaoxiao Wu and Zhenyu Qian*

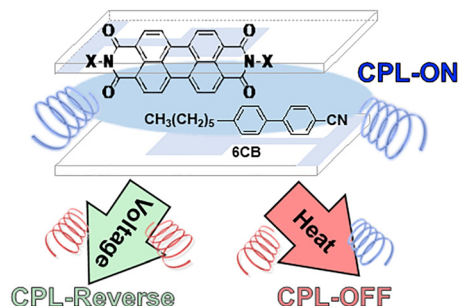


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Switching of circularly polarised luminescence in perylene-diimide-based chiral liquid crystals induced by electric fields and heating

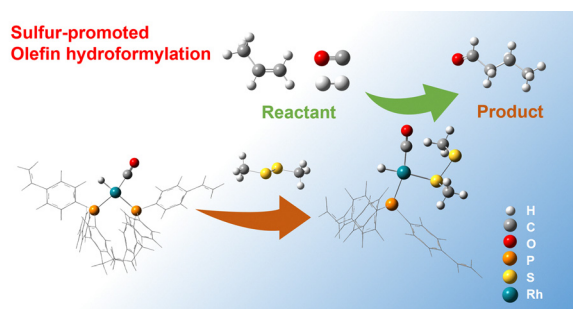
Daiya Suzuki, Seika Suzuki, Kosuke Kaneko, Tomonori Hanasaki, Motohiro Shizuma and Yoshitane Imai*



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Propylene hydroformylation catalyzed by rhodium-based catalysts with phosphine-sulfur ligands: a combined theoretical and experimental study

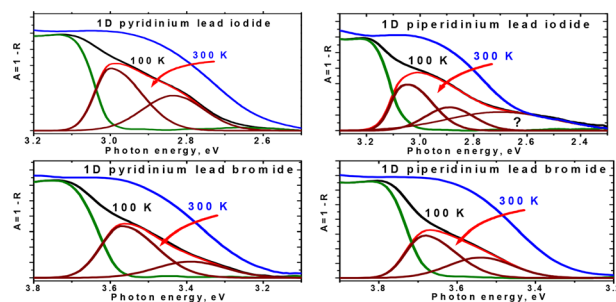
Yuxuan Zhou, Siquan Feng, Cunyao Li, Xiangen Song, Li Yan, Yunjie Ding and Xue-Qing Gong*



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Origin of the absorption edge fine structure in Pb-based organic-inorganic 1D perovskites

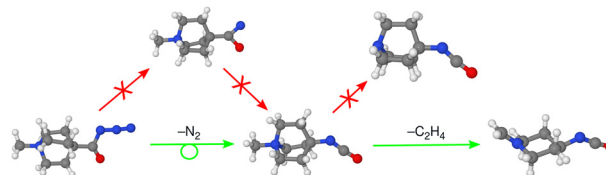
Vyacheslav N. Kuznetsov,* Yuri V. Chizhov, Nadezhda I. Glazkova, Ruslan V. Mikhaylov, Vladimir K. Ryabchuk, Alexei V. Emeline and Nick Serpone*



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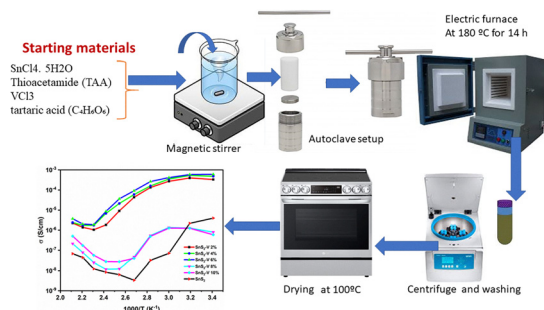
Gas-phase Curtius and Wolff rearrangement reactions investigated by tandem-MS, IR ion spectroscopy and theory

Wacharee Harnying, Hui-Chung Wen, Jonathan Martens, Giel Berden, Jos Oomens, Jana Roithová, Albrecht Berkessel, Mathias Schäfer* and Anthony J. H. M. Meijer*



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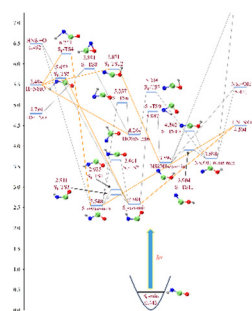
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Ionic conductivity of vanadium-doped tin disulfide for photovoltaic applications

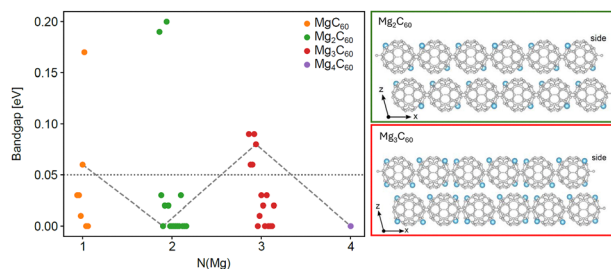
Shafi Ullah, Hanif Ullah, Abel García-Bernabé, Andreu Andrio, Bernabe Mari Soucase and Vicente Compañ*

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Full-dimensional neural network potential energy surface for the multi-channel photodissociation of HNSiO via its S_1 band

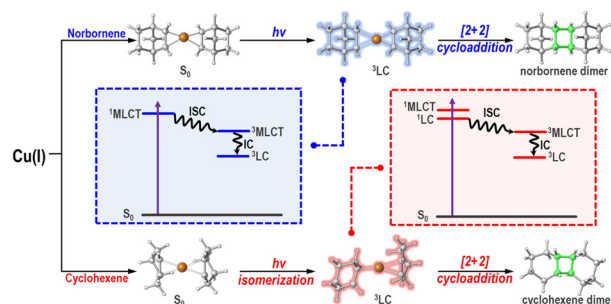
Tingchuan Shang, Siting Hou, Huixian Han* and Changjian Xie*

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Trends in the electronic and geometric structures of doped two-dimensional quasi-hexagonal C_{60}

Alexander E. Barnes, Stephanie Lambie and Nicola Gaston*

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Photodimerization of norbornenes and cyclohexenes catalyzed by Cu(I) complexes: mechanistic similarities and differences

Xin-Xin Liu, Jia-Jia Ma, Guo Li, Ling-Ya Peng,* Qiu Fang,* Wei-Hai Fang and Ganglong Cui*

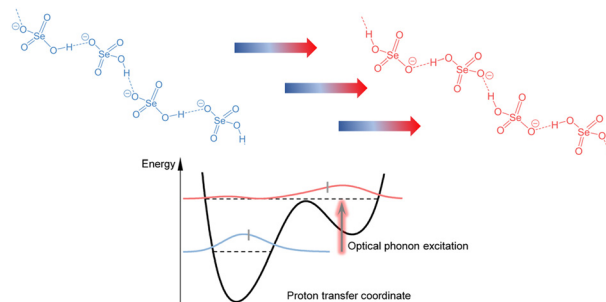


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Proton delocalization in short hydrogen bonds assembling HSeO_4^- anions into supramolecular adducts

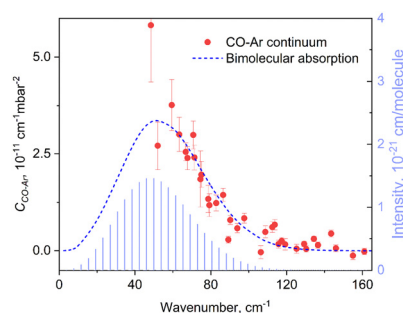
Roberta Beccaria, Andrea Pizzi, Edem Chakalov, Giuseppe Resnati* and Peter Tolstoy*



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CO–Ar continuum under the rotational band: can super-Lorentzian wings be involved?

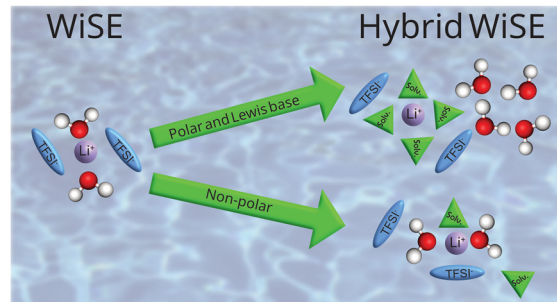
Aleksandra O. Koroleva,* Tatyana A. Galanina, Maksim A. Koshelev and Mikhail Yu. Tretyakov



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On the structure of hybrid water-in-salt electrolytes

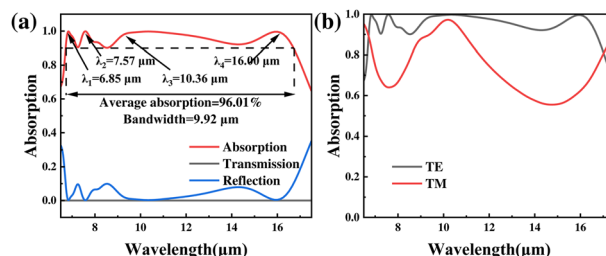
Raúl Lois-Cuns, Antía Santiago-Alonso, Martín Otero-Lema, Juan J. Parajó, Josefa Salgado, Hadrián Montes-Campos,* Trinidad Méndez-Morales* and Luis M. Varela



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Infrared band ultra-wideband metamaterial absorption device based on cylindrical multiscale resonator

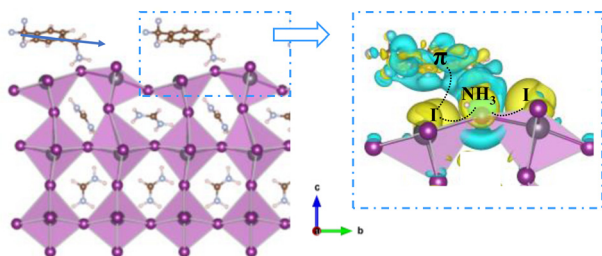
Jiao Wang, Qianju Song, Hua Yang, Chaojun Tang, Zao Yi* and Jianguo Zhang*



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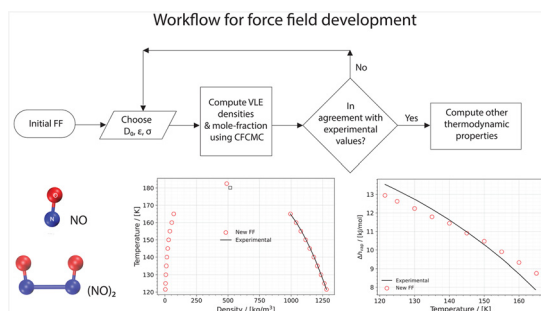
optimal orientation [2, 4, -1]



The orientation design of high-polarity ligand dipole CF₃-PEA for enhancing the surface stability and optoelectronic properties of the FAPbI₃ perovskite

Xiuchen Han, Qi Yang, Shuning Wang, Xinyue Zhang, Dongmeng Chen, Peiwen Xiao, Wenjing Fang* and Bing Liu*

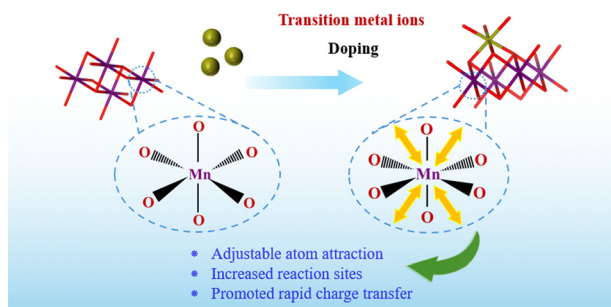
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Modeling nitric oxide and its dimer: force field development and thermodynamics of dimerization

Tijin H. G. Saji, Thijs J. H. Vlugt, Sofia Calero and Behnaz Bagheri*

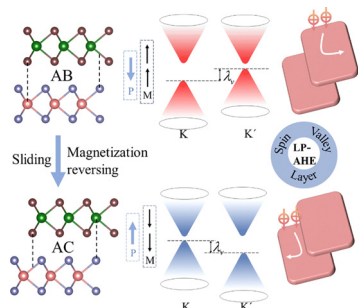
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Transition metal tailored δ -MnO₂ with optimized charge compensation for enhanced hydrogen evolution

Juyin Liu, Zhipeng Li, Jianze Chen, Xin Zhang,* Yao Zhang, Lijun Li, Hong Wang and Yanfang Gao*

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Interlayer coupling of valley and layer in the homostructure bilayer Scl₂

Xiao-Jing Dong and Chang-Wen Zhang*

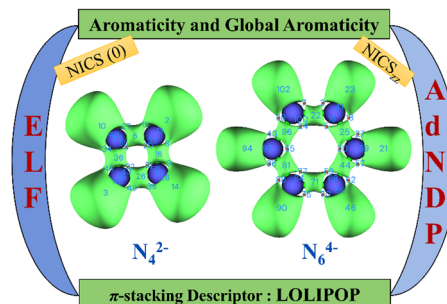


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A careful scrutiny of the aromaticity in anionic polynitrogen clusters

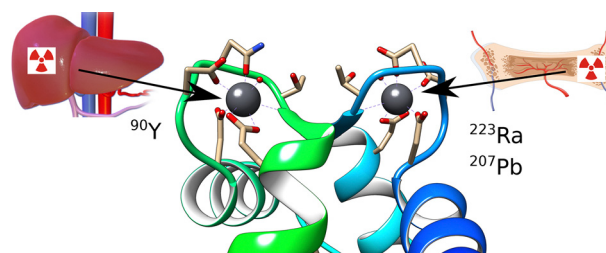
Gourhari Jana* and Pratim K. Chattaraj*



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Estimating protein binding upon treatment with radionuclide ions

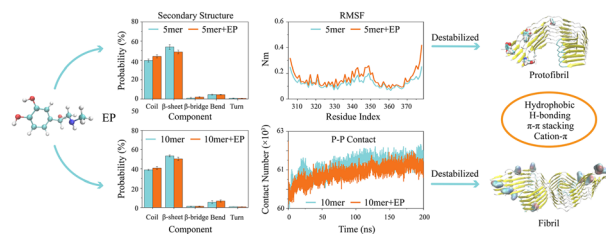
Ran Friedman



13714

Epinephrine destabilizes Alzheimer's disease-related tau protofibril and fibril: a computational study

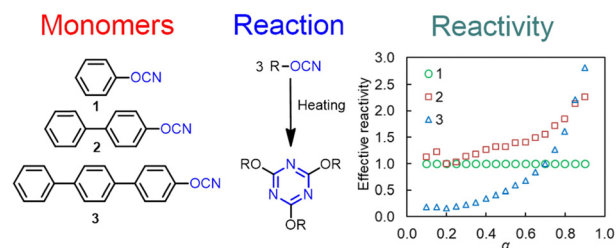
Jiaxing Tang, Dushuo Feng, Feng Wang, Lulu Guan, Zhengdong Xu and Yu Zou*



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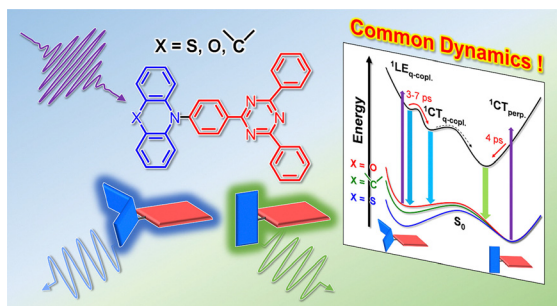
Assessing the reactivity of cyanate esters in [2+2+2] cyclotrimerization: meeting the challenge by augmenting differential scanning calorimetry with kinetic computations

Andrey Galukhin,* Ilya Nikolaev, Alexander Kachmarzhik, Roman Nosov and Sergey Vyazovkin*



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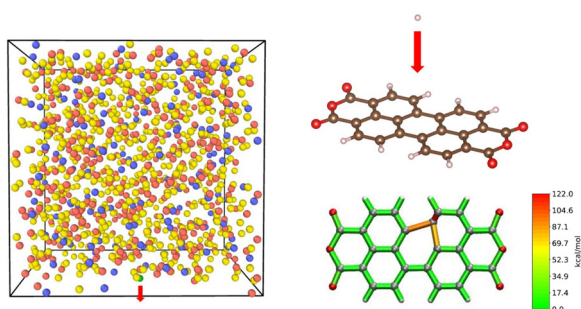
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Common mechanism of dual emission in linearly-linked donor–acceptor-type thermally activated delayed fluorescence molecules

Tomohiro Ryu, Arvydas Ruseckas, Masaki Saigo, Kiyoshi Miyata, Youichi Tsuchiya, Hajime Nakanotani, Chihaya Adachi, Ifor D. W. Samuel and Ken Onda*

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Modeling the projected range of protons in matter: insights from molecular dynamics and quantum chemistry

Chieh-Min Hsieh, Alexander Dellwisch and Tim Neudecker*

