

IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 27(25) 13197–13756 (2025)



Cover

See María A. Palacios, María Mar Quesada-Moreno, Enrique Colacio *et al.*, pp. 13266–13279. Image reproduced by permission of Ana Rodríguez-Expósito and María Elena Pestaña-Ocaña from *Phys. Chem. Chem. Phys.*, 2025, 27, 13266.



Inside cover

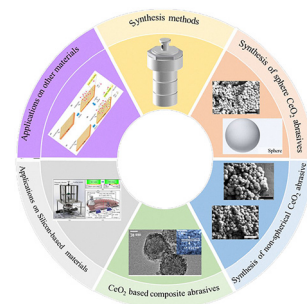
See Thomas Kierspel, Charlotte Uetrech *et al.*, pp. 13234–13242. Image reproduced by permission of Lara Flacht, Charlotte Uetrech, Thomas Kierspel from *Phys. Chem. Chem. Phys.*, 2025, 27, 13234.

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

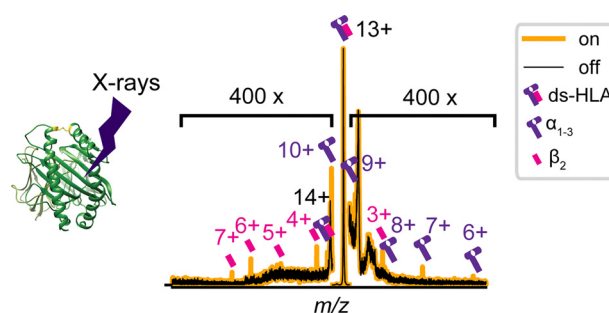


PERSPECTIVE

13234

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

Jocky C. K. Kung, Alan Kádek, Knut Kölb, Steffi Bandelow, Sadia Bari, Jens Buck, Carl Coleman, Jan Commandeur, Tomislav Damjanović, Simon Dörner, Karim Fahmy, Lara Flacht, Johannes Heidemann, Khon Huynh, Janine-Denise Kopicki, Boris Krichel, Julia Lockhauserbäumer, Kristina Lorenzen, Yinfei Lu, Ronja Pogan, Jasmin Rehmann, Kira Schamoni-Kast, Lucas Schwob, Lutz Schweikhard, Sebastian Springer, Pamela H. W. Svensson, Florian Simke, Florian Trinter, Sven Toleikis, Thomas Kierspel* and Charlotte Uetrech*



RSC Advances

At the heart of open access for
the global chemistry community

Editor-in-chief

Russell J Cox

Leibniz Universität Hannover, Germany

We stand for:



Breadth We publish work in all areas of chemistry and reach a global readership



Affordability Low APCs, discounts and waivers make publishing open access achievable and sustainable



Quality Research to advance the chemical sciences undergoes rigorous peer review for a trusted, society-run journal

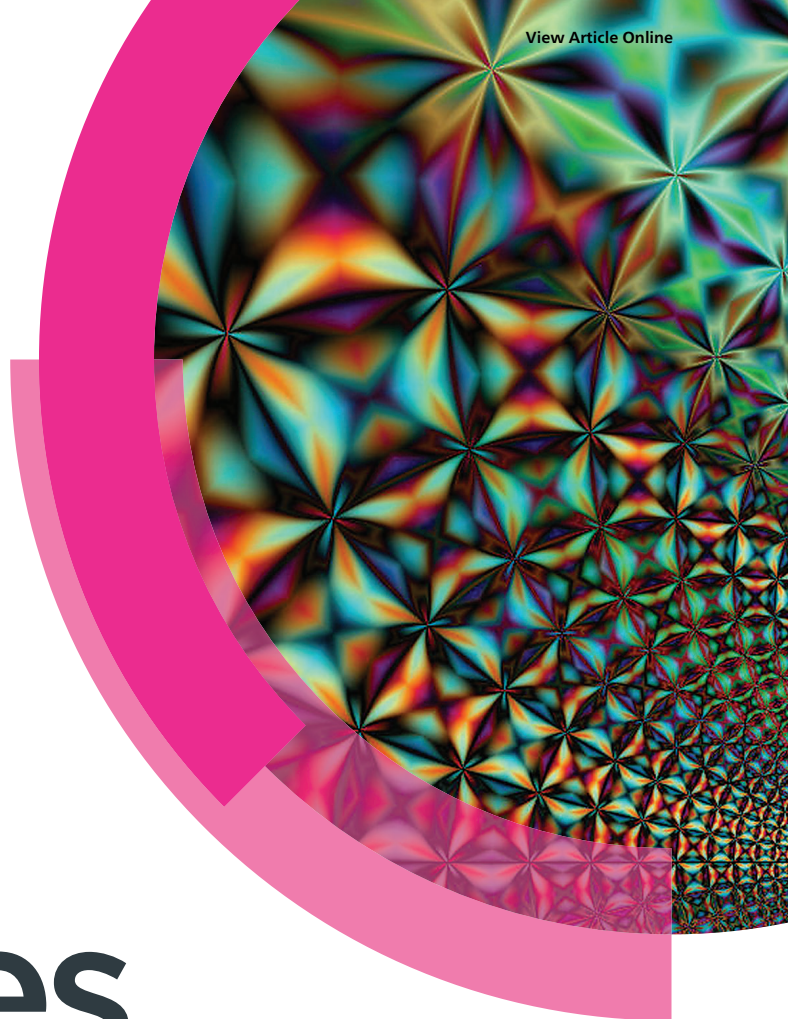


Community Led by active researchers, we publish quality work from scientists at every career stage, and all countries

Submit your work now

rsc.li/rsc-advances

@RSC_Adv

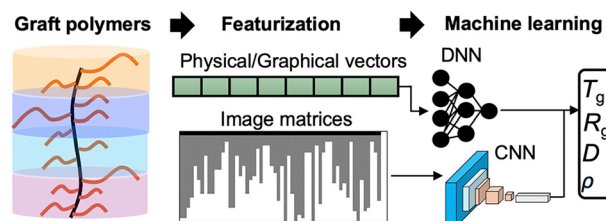


COMMUNICATIONS

13243

Machine learning of the architecture–property relationship in graft polymers

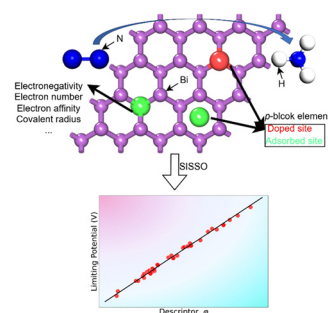
Kevin V. Bigting, Jordan J. Carden, Shubhadeep Nag, Jimmy Lawrence, Yen-Fang Su and Yaxin An*



13248

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

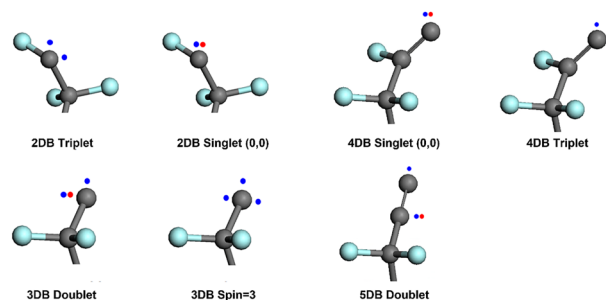
Dengning Sun, Xiaokun Du, Jing Chen, Tao Ye, Hao Shen, Ruirui Wang, Ying Wang,* Guoqiang Liu, Yangyang Wan* and Zhongti Sun*



13257

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*

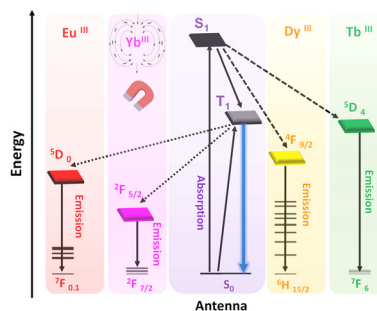


RESEARCH PAPERS

13266

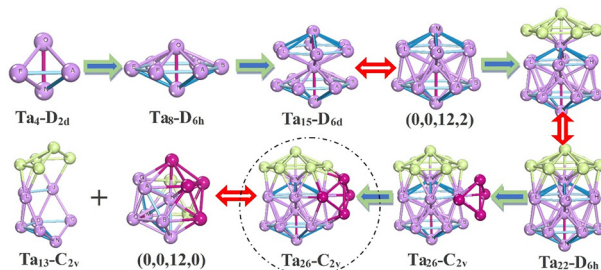
Different mechanisms for lanthanide(III) sensitization and Yb-field-induced single-molecule magnet behaviour in a series of pentagonal bipyramidal and octahedral lanthanide complexes with axial phosphine oxide ligands

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*



RESEARCH PAPERS

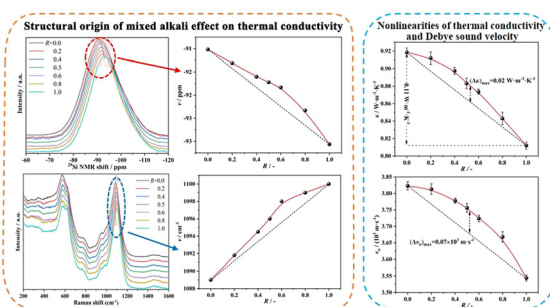
13280



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

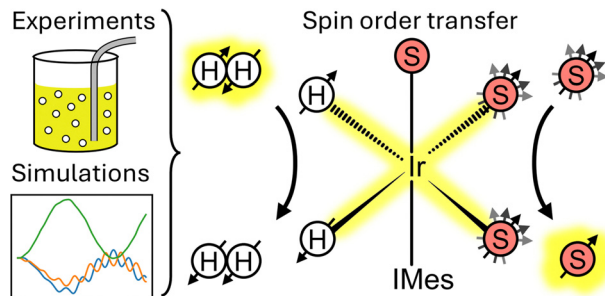
13295



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*

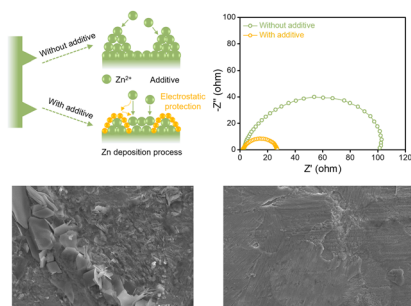
13305



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*

13315



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

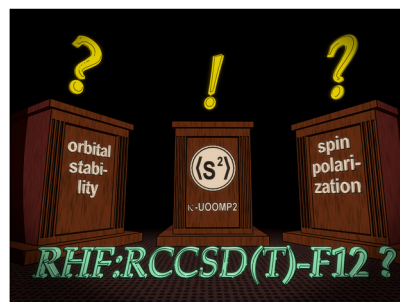


RESEARCH PAPERS

13326

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

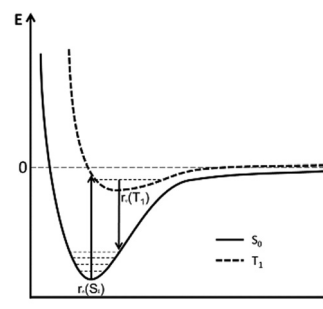
Xiao Liu, Kevin A. Spiekermann, Angiras Menon, William H. Green and Martin Head-Gordon*



13340

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

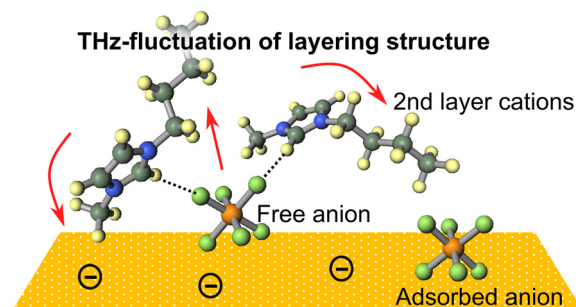
B. Minaev,* M. Sukhyna, P. Stakhira, V. Minaeva and H. Ågren



13352

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

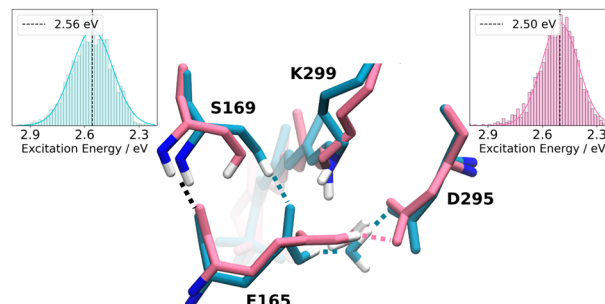
Ryo Ueno, Kenta Motobayashi and Katsuyoshi Ikeda*



13360

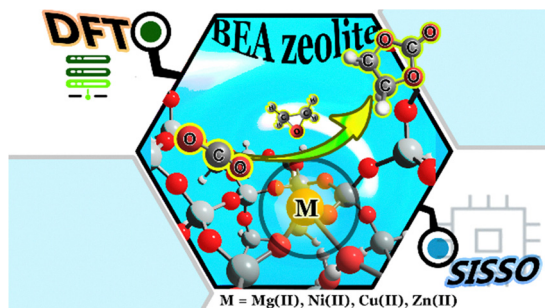
Complex active site structures influence absorption spectrum of Chrimson wild type and mutants

Katharina Spies,* Beatrix M. Bold and Marcus Elstner



RESEARCH PAPERS

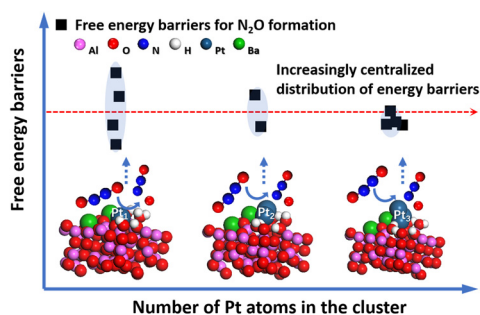
13371



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

Winyoo Sangthong and Jakkapan Sirijaraensre*

13382

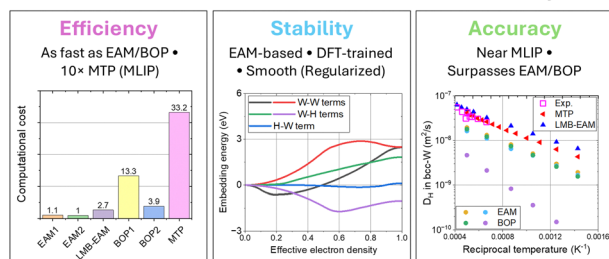


Mechanism of N₂O formation in catalytic after-treatment systems of ammonia/hydrogen-fuelled engines

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

13390

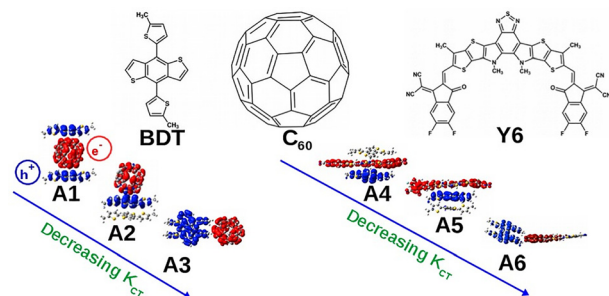
LMB-EAM: Fast, Stable, Near-MLIP Accuracy



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*

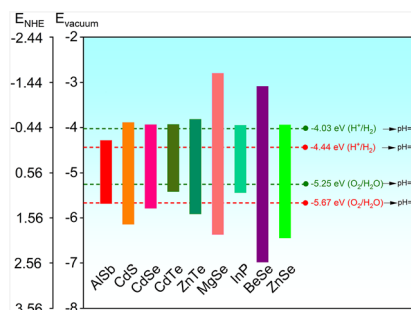


RESEARCH PAPERS

13415

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

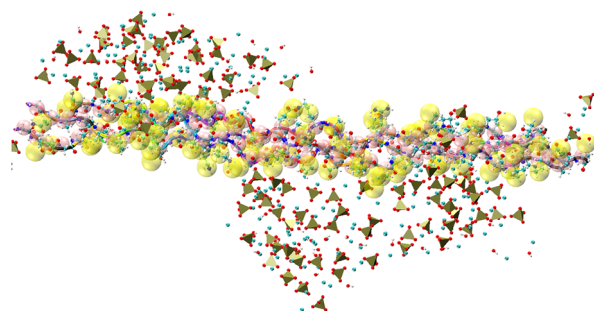
Ismail Shahid, Iqtidar Ahmad, Anwar Ali, Abid Raza, Xiaoliang Zhang,* Dawei Tang, Mohamed Kallel* and Shaimaa A. M. Abdelmohsen



13424

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

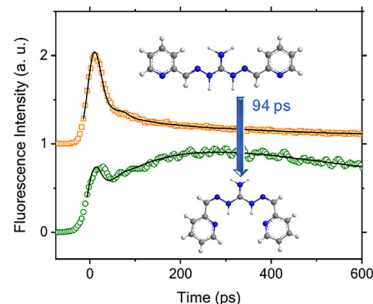
Zhiyu Xue, Xing Ye, Yao Cai, Xinyun Tan, XiaoMeng Wu, Fang Wu, Fei Li,* Dingguo Xu* and Bailing Zhou*



13434

Photoswitching dynamics of a guanidine anion receptor

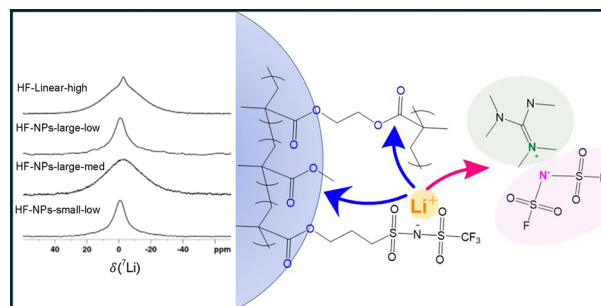
Ying-Zhong Ma,* Jeffrey D. Einkauf, Xinyou Ma, Duy-Khoi Dang, Paul M. Zimmerman, Radu Custelcean, Benjamin Doughty and Vyacheslav S. Bryantsev*



13447

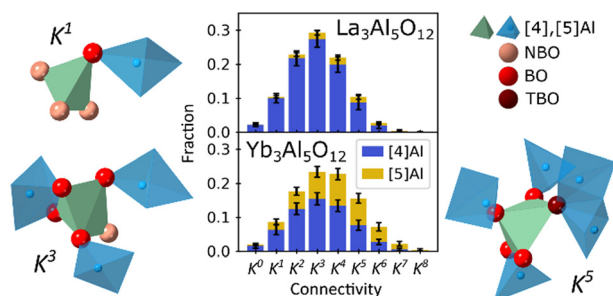
Effect of the polymer nature on the properties of composite solid electrolytes based on the organic ionic plastic crystal HMGFSI

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



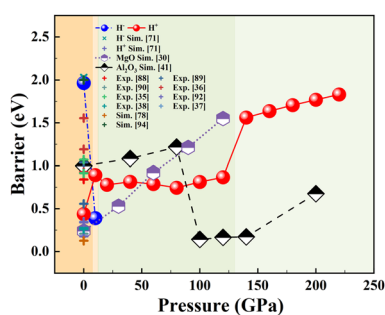
RESEARCH PAPERS

13464

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

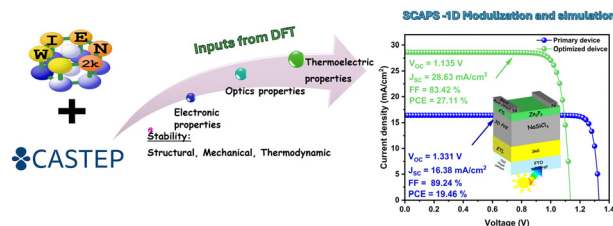
Stephen K. Wilke,* Chris J. Benmore,
Randall E. Youngman, Benjamin J. A. Moulton,
Abdulrahman Al-Rubkhi and Richard Weber

13476

**Investigation of hydrogen diffusion in zirconia under extreme conditions**

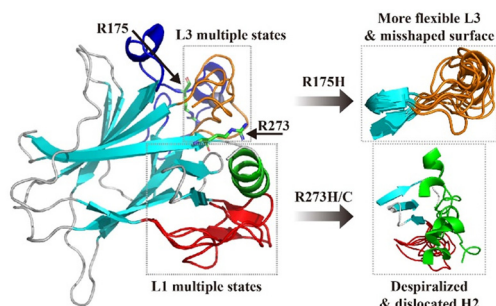
Fengqi Wang, Yuanqin Zhu and Xianlong Wang*

13490

**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

13508

**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*

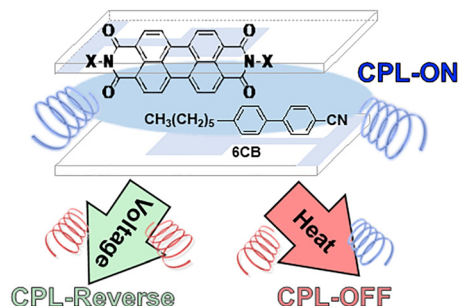


RESEARCH PAPERS

13519

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

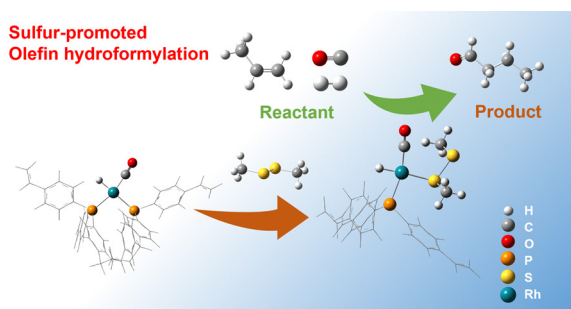
Daiya Suzuki, Seika Suzuki, Kosuke Kaneko, Tomonori Hanasaki, Motohiro Shizuma and Yoshitane Imai*



13527

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

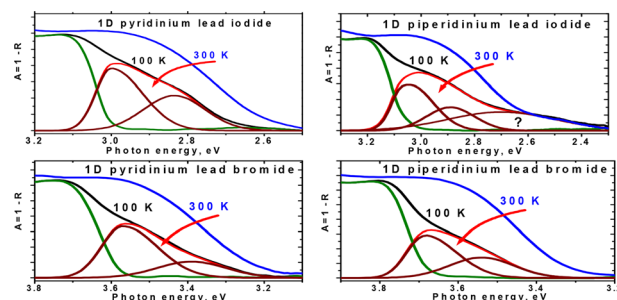
Yuxuan Zhou, Siquan Feng, Cunyao Li, Xiange Song, Li Yan, Yunjie Ding and Xue-Qing Gong*



13534

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

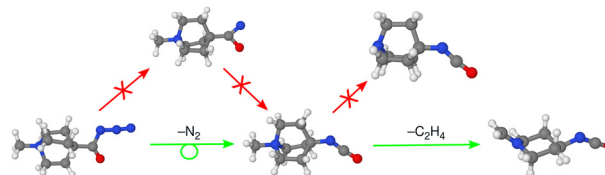
Vyacheslav N. Kuznetsov,* Yuri V. Chizhov, Nadezhda I. Glazkova, Ruslan V. Mikhaylov, Vladimir K. Ryabchuk, Alexei V. Emeline and Nick Serpone*



13543

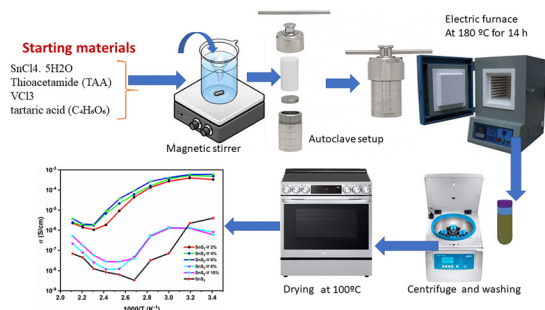
Gas-phase Curtius and Wolff rearrangement reactions investigated by tandem-MS, IR ion spectroscopy and theory

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



RESEARCH PAPERS

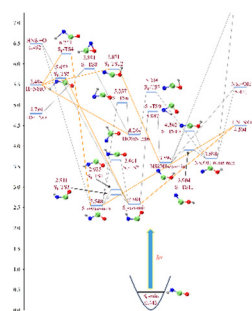
13557



Ionic conductivity of vanadium-doped tin disulfide for photovoltaic applications

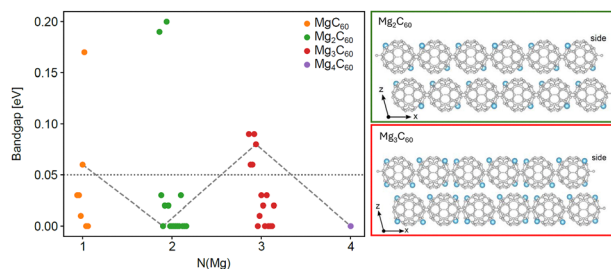
Shafi Ullah, Hanif Ullah, Abel García-Bernabé, Andreu Andrio, Bernabe Mari Soucase and Vicente Compañ*

13567

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

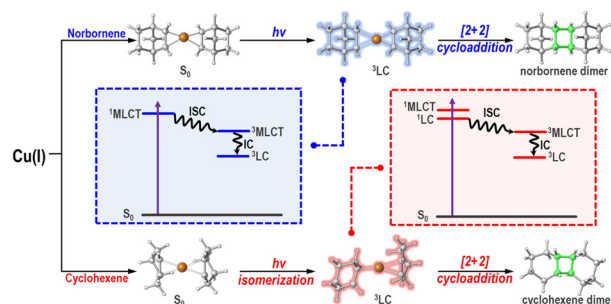
Tingchuan Shang, Siting Hou, Huixian Han* and Changjian Xie*

13578

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

Alexander E. Barnes, Stephanie Lambie and Nicola Gaston*

13588



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*

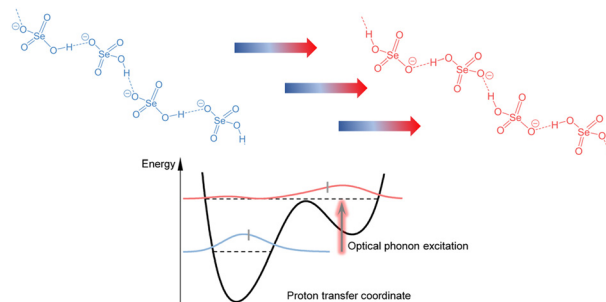


RESEARCH PAPERS

13601

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

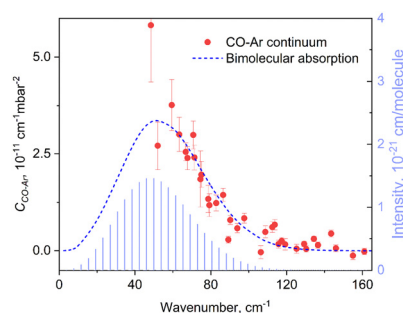
Roberta Beccaria, Andrea Pizzi, Edem Chakalov, Giuseppe Resnati* and Peter Tolstoy*



13618

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

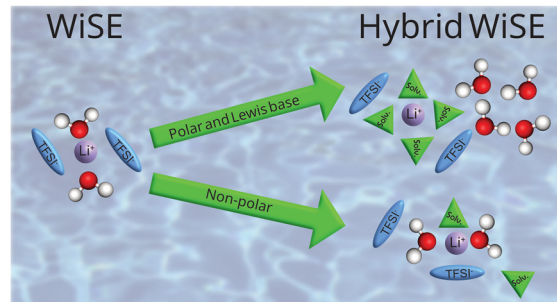
Aleksandra O. Koroleva,* Tatyana A. Galanina, Maksim A. Koshelev and Mikhail Yu. Tretyakov



13629

On the structure of hybrid water-in-salt electrolytes

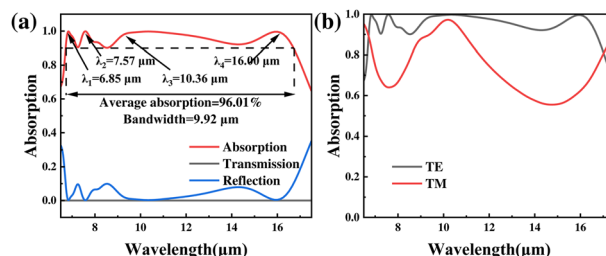
Raúl Lois-Cuns, Antía Santiago-Alonso, Martín Otero-Lema, Juan J. Parajó, Josefa Salgado, Hadrián Montes-Campos,* Trinidad Méndez-Morales* and Luis M. Varela



13645

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

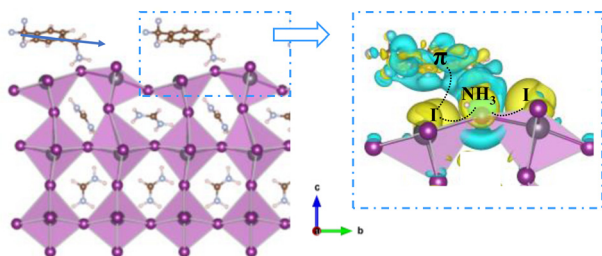
Jiao Wang, Qianju Song, Hua Yang, Chaojun Tang, Zao Yi* and Jianguo Zhang*



RESEARCH PAPERS

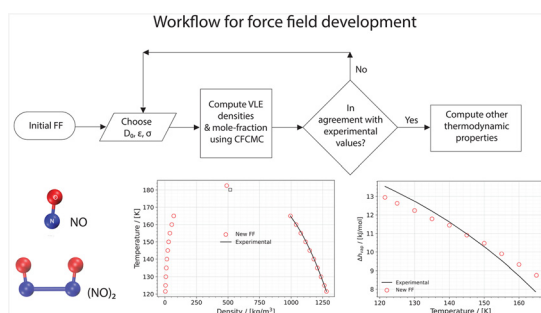
13653

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*

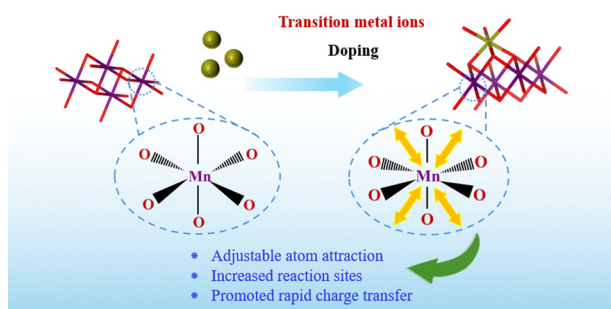
13662



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

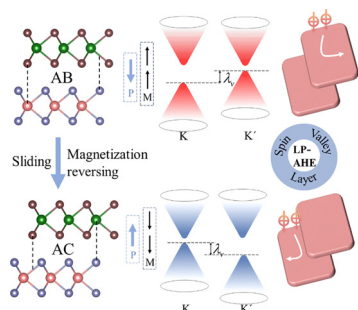
Tijin H. G. Saji, Thijs J. H. Vlugt, Sofia Calero and Behnaz Bagheri*

13675

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*

13686

Interlayer coupling of valley and layer in the homostructure bilayer Scl₂

Xiao-Jing Dong and Chang-Wen Zhang*

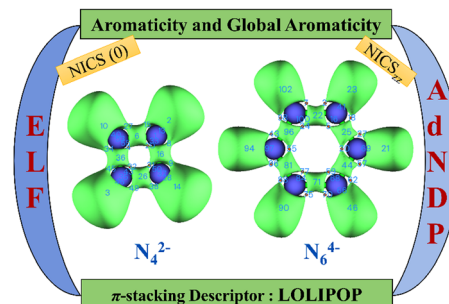


RESEARCH PAPERS

13694

A careful scrutiny of the aromaticity in anionic polynitrogen clusters

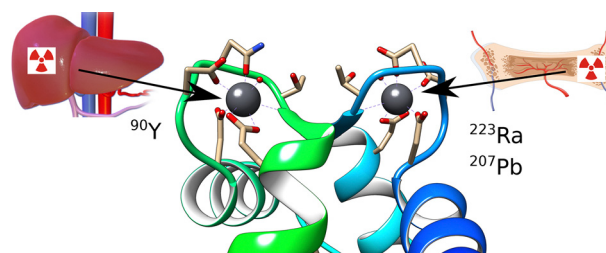
Gourhari Jana* and Pratim K. Chattaraj*



13705

Estimating protein binding upon treatment with radionuclide ions

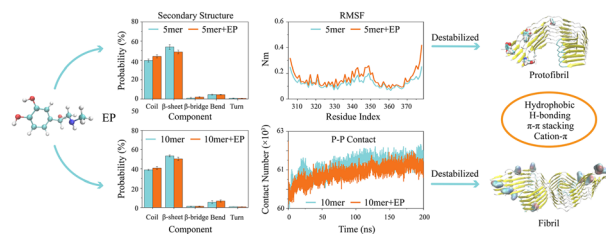
Ran Friedman



13714

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

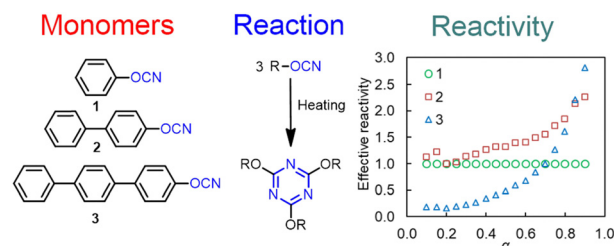
Jiaxing Tang, Dushuo Feng, Feng Wang, Lulu Guan, Zhengdong Xu and Yu Zou*



13727

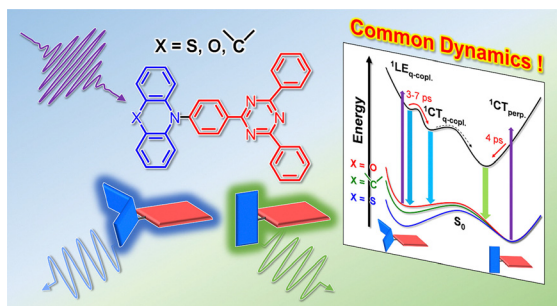
Assessing the reactivity of cyanate esters in [2+2+2] cyclotrimerization: meeting the challenge by augmenting differential scanning calorimetry with kinetic computations

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



RESEARCH PAPERS

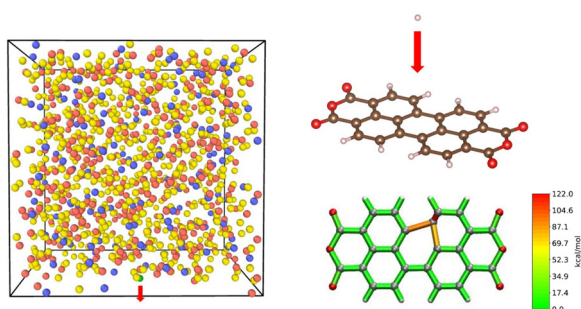
13735



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*

13745



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

Chieh-Min Hsieh, Alexander Dellwisch and Tim Neudecker*

