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IN THIS ISSUE

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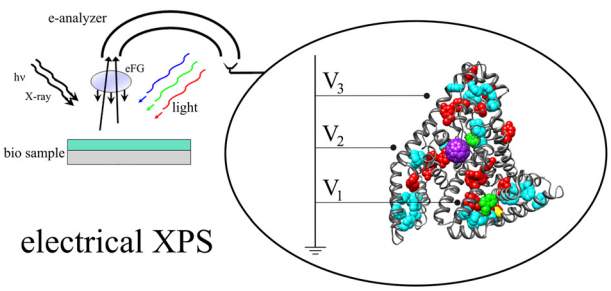
Cover
See Tomokazu Yoshimura *et al.*, pp. 19642–19650. Image reproduced by permission of Risa Kawai from *Phys. Chem. Chem. Phys.*, 2025, **27**, 19642.

TUTORIAL REVIEW

19591

Electrical XPS meets biology: *in situ* chemo-electrical sensing and activation of organic materials

Marco E. Miali, Ulyana Shimanovich and Hagai Cohen*

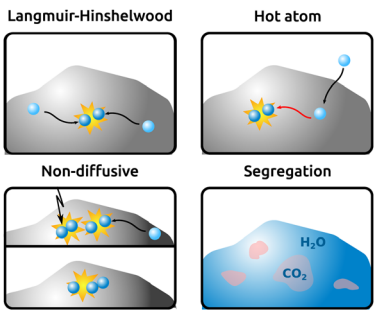


PERSPECTIVE

19630

Molecular mobility of extraterrestrial ices: surface diffusion in astrochemistry and planetary science

N. F. W. Ligterink, C. Walsh, H. M. Cuppen, M. N. Drozdovskaya, A. Ahmad, D. M. Benoit, J. T. Carder, A. Das, J. K. Díaz-Berríos, F. Dulieu, J. Heyl, A. Jardine, T. Lamberts, N. M. Mikkelsen and M. Tsuge



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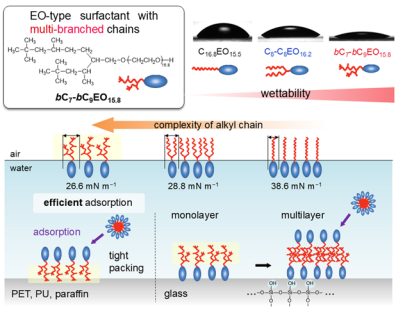
RESEARCH PAPERS

19642

Wetting behavior of polyoxyethylene-type nonionic surfactant with multi-branched chains on solid surfaces

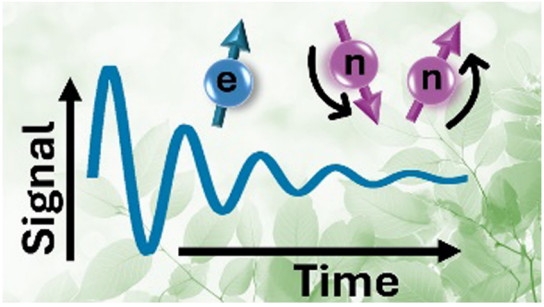
Risa Kawai, Nana Tsutsui, Kotoha Ueno, Shiho Yada, Masashi Ohno, Toshinari Koda and Tomokazu Yoshimura*



19651

Light-induced electron spin qubit coherences in the purple bacteria reaction center protein

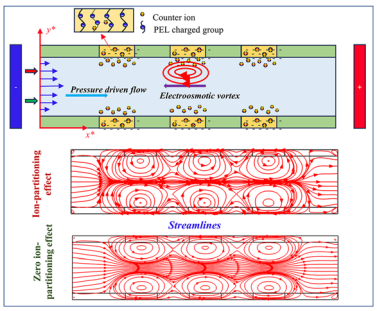
Jasleen K. Bindra, Jens Niklas, Yeonjun Jeong, Ahren W. Jasper, Lisa M. Utschig and Oleg G. Poluektov*



19662

Ion-partitioning effect promotes the electroosmotic mixing of non-Newtonian fluids in soft-patterned microchannels

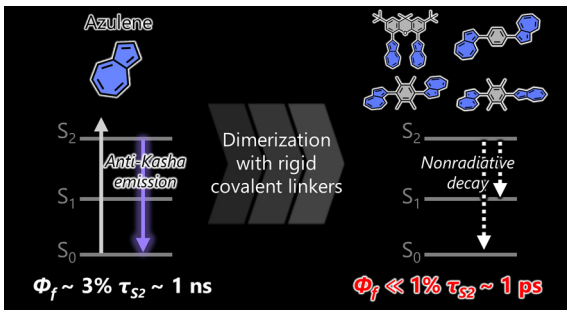
Sumit Kumar Mehta, Prateechee Padma Behera, Abhishek Dutta, Bhashkar Jyoti Sharma, Anubhab Gaurav Borah, Pragyan Bora, Subhrajit Borah, Somchai Wongwises and Pranab Kumar Mondal*



19677

Ultrafast nonradiative decay from higher-lying excited states in azulene-dimers

Yuta Sawada, Ami Takada, Ken Onda, Kiyoshi Miyata,* Yoichi Sasaki* and Nobuo Kimizuka*



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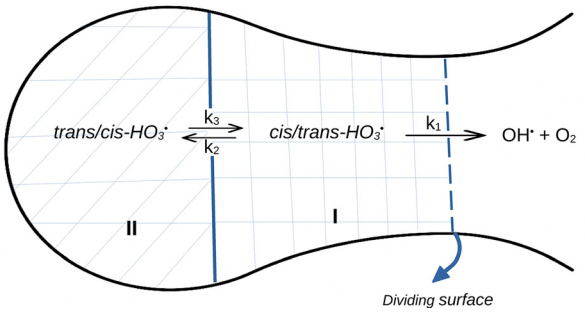
19684



The puzzle of high lifetime and low stabilization of $HO_3^{\bullet}$: rationalization and prediction

Philips Kumar Rai, Akash Gutal and Pradeep Kumar*

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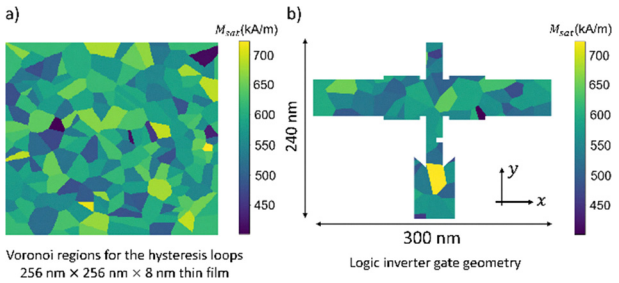
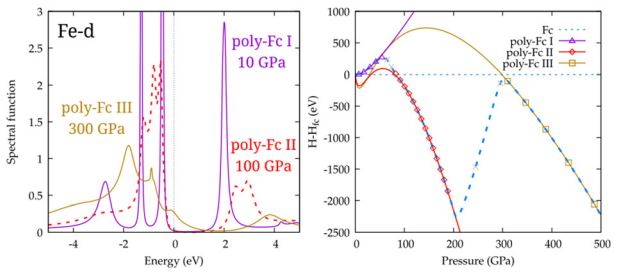


Quantifying polycrystallinity effects on skyrmion dynamics and device performance

Ahmet Bahadır Trabzon, Arash Mousavi Cheghabouri and Mehmet Cengiz Onbaşlı*

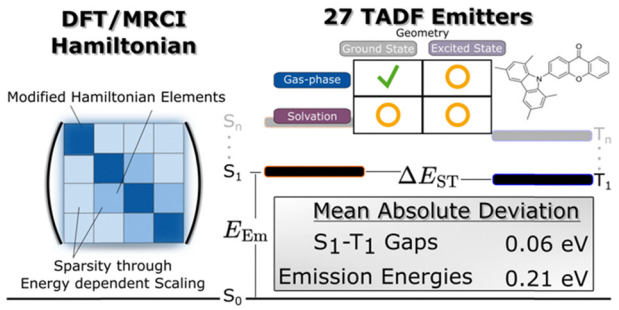
19703



The impact of electronic correlations on the structural stability and spectral properties of ferrocene and polyferrocene under pressure

Alexey A. Dyachenko,* Alexey V. Lukoyanov, Vladimir I. Anisimov and Artem R. Oganov

19710



On the performance of DFT/MRCI for singlet–triplet gaps and emission energies of thermally activated delayed fluorescence molecules

Mike Pauls, Thomas Froitzheim, Alexei Torgashov, Jan-Michael Mewes, Stefan Grimme and Christoph Bannwarth*

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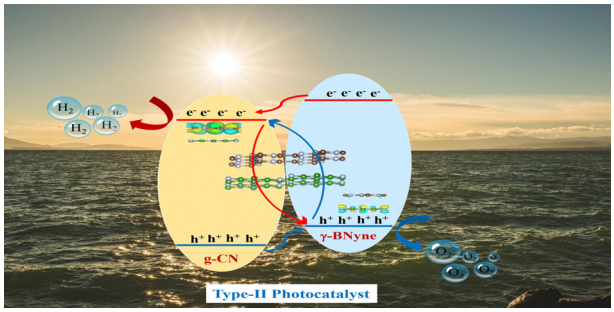
RESEARCH PAPERS

19724

Unveiling the photocatalytic water splitting over metal-free g-CN/γ-BNyne heterostructures using non-adiabatic molecular dynamics

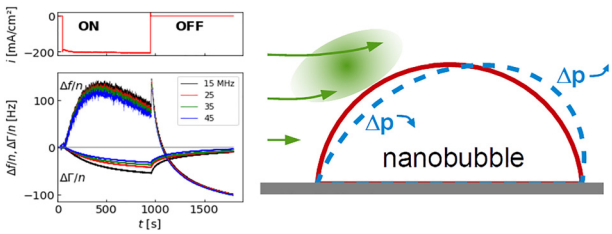
Subhash Kumar, Atish Ghosh and Pranab Sarkar*



19733

A fast electrochemical quartz crystal microbalance (EQCM) evidences the presence of nanobubbles in alkaline water splitting

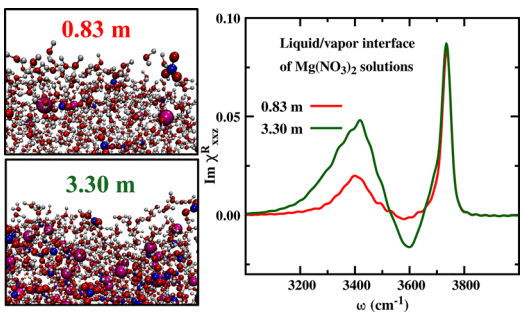
Christian Leppin, Arne Langhoff and Diethelm Johannsmann*



19748

Effects of salt concentration on the structure and vibrational sum frequency generation spectra of liquid/vapor interfaces of aqueous solutions of metal nitrates

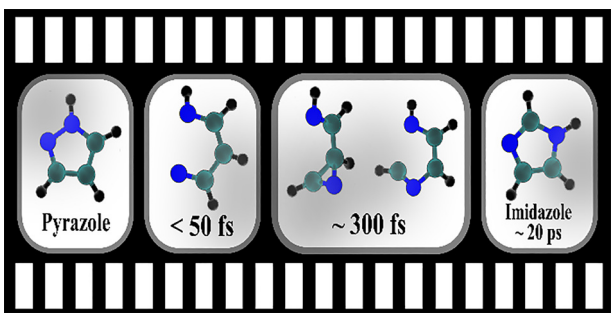
Abhilash Chandra and Amalendu Chandra*



19762

The Kick Inside: time-resolved mechanistic insights into the DUV-driven interconversion of pyrazole to imidazole

Derri J. Hughes, Wei Bo Ng, Richard T. Chapman, George Healing, Michael A. Parkes, Jennifer Rigden, Oliver J. Smith, Emma Springate, James O. F. Thompson, Tiffany Walmsley, Joanne L. Woodhouse and Russell S. Minns*



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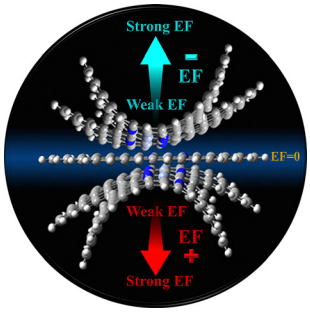
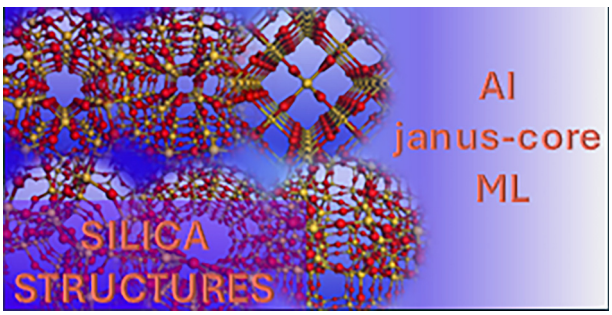


A DFT study on the curving of 4N-divacancy defected graphene quantum dots induced by an external electric field and the effects of metal-ion doping

Thanawit Kuamit, Wilasinee Santiwarodom, Pavee Apilardmongkol, Sirilak Kongkaew and Vudhichai Parasuk*

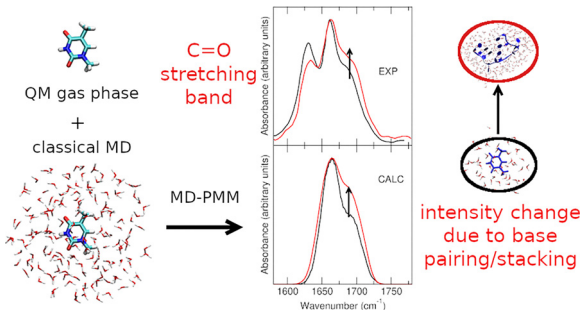
19784



Modelling silica using MACE-MP machine learnt interatomic potentials

Jamal Abdul Nasir, Jingcheng Guan, Woongkyu Jee, Scott M. Woodley, Alexey A. Sokol, C. Richard A. Catlow* and Alin-Marin Elena*

19797



Probing the environmental sensitivity of thymine C═O vibrations through infrared spectra simulations

Giovanni Parolin, Cedrix J. Dongmo Foumthuim, Stefano Corni and Laura Zanetti-Polzi*

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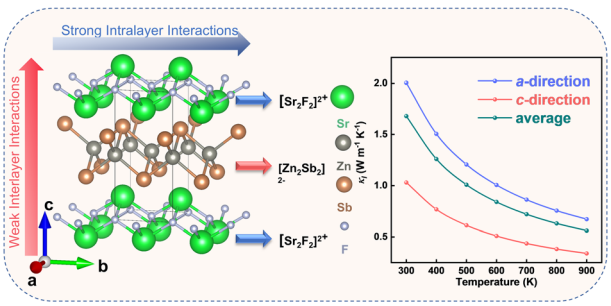

Low lattice thermal conductivity driven by weak interlayer interaction and acoustic–optical coupling in the SrZnSbF thermoelectric material

Yujie Bao, Shuwei Tang,* Pengfei Zhang, Shulin Bai, Da Wan, Peng Ai, Zhiwei Zhang and Yunzhuo Zhang

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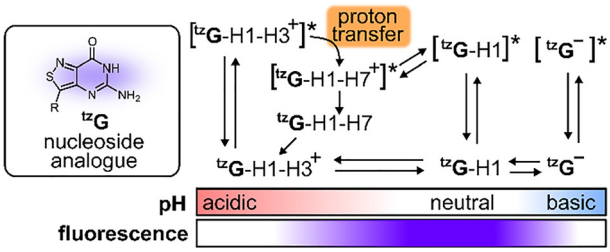
19820

Exploring excited-state proton transfer reactions in isothiazologuanosine, an isofunctional fluorescent analogue of guanosine

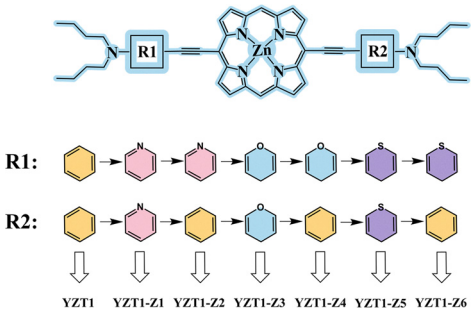
Olha Tkach, Lara Martinez-Fernandez, Atzin Esmeralda Ruiz-Lera, Nicolas Humbert, Ludovic Richert, Dmytro Dziuba, Elisa Bombarda, Aurélie Bourderioux, Fabien Hanser, Pascal Didier, Yitzhak Tor, Roberto Improta,* Jérémie Léonard* and Yves Mély*



19837

Effect of the donor unit heterocyclic substitution strategy on the performance of Zn^{II} porphyrin-based hole transport materials

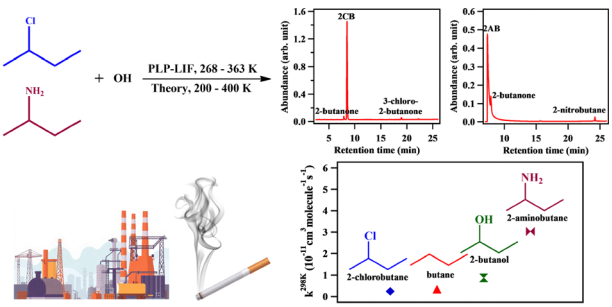
Xueling Zhang, Peng Song,* Fengcai Ma and Yuanzuo Li*



19852

Atmospheric reactions of substituted butanes with OH radicals: kinetics and atmospheric implications

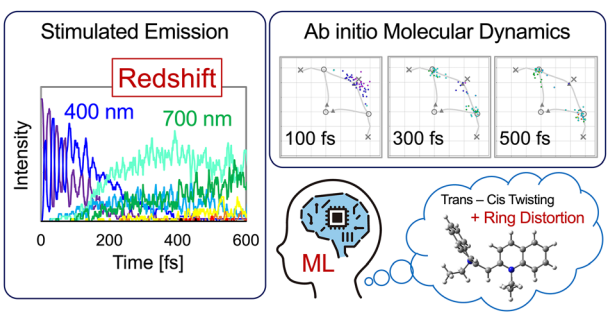
Bishnupriya Kar and Balla Rajakumar*



19868

Unraveling the structural origins of stimulated emission redshift in cyanine dye 1122C: a combined AIMD and machine learning study

Yusuke Minegishi, Kenichiro Saita, Takuro Tsutsumi and Tetsuya Taketsugu*



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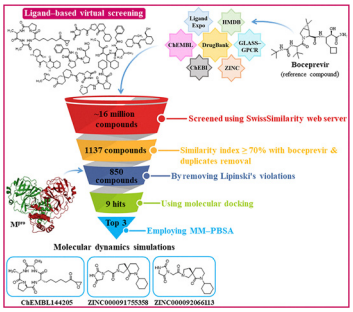
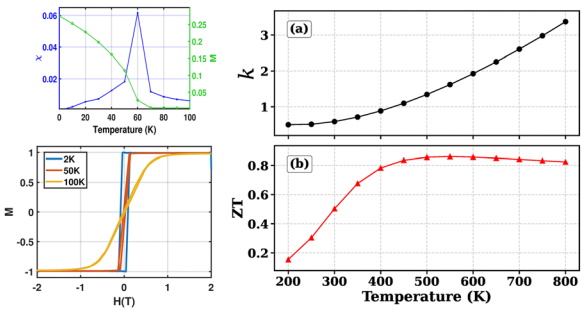


Ligand-based virtual screening to discover potential inhibitors of SARS-CoV-2 main protease

Gurmeet Kaur and Bhupesh Goyal*

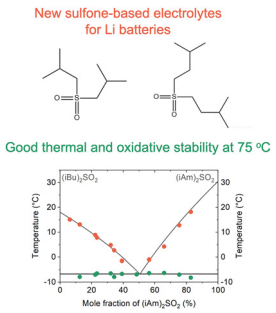
19898



Observation of competing magnetic phases, mechanical stability, electronic structure, magnetism, and remarkable thermoelectric aspects of Ba_2GdRuO_6

Usman Saeed, Shehla Yasmeen, A. Ibrahim and S. Nazir*

19911



Aliphatic saturated sulfones C8–C10 as new electrolyte solvents for Li batteries

E. V. Belova, J. D. Shakirova, Z. V. Bobyleva,*
D. S. Lutsenko, A. A. Kurashkina, R. R. Samigullin,
M. A. Solovieva, D. A. Aksyonov, O. A. Drozhzhin and
E. V. Antipov

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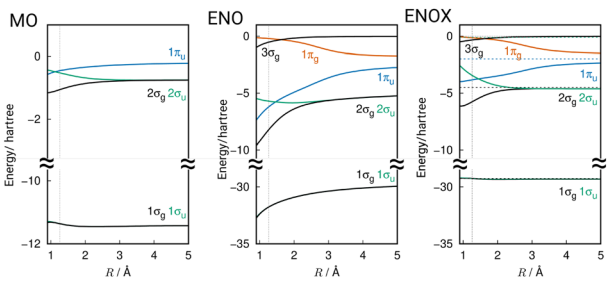

Orbital perspective of the nature of chemical bonds and potential energy surfaces: 55 years after Wahl's molecular orbital representation of homopolar diatomic molecules

Yasuki Arasaki and Kazuo Takatsuka*

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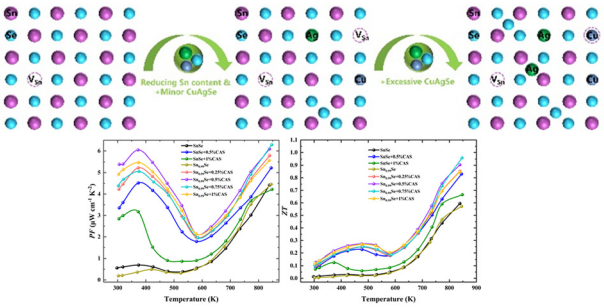
19939

Optimized thermoelectric properties of SnSe through the joint strategies of Sn-content fine-tuning and CuAgSe alloying

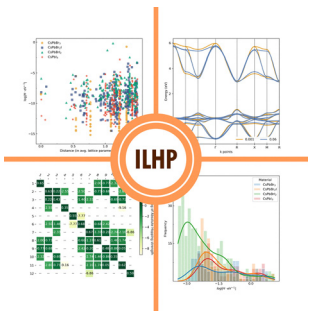
Zhangheng Lai, Xiangbin Chen, Qixian Zheng, Zhengmao Luo, Zhongshuo Li, Ning Qi and Zhiquan Chen*



19950

Hopscotching perovskites: DFT leveraged tight-binding insights into inorganic lead halide perovskites

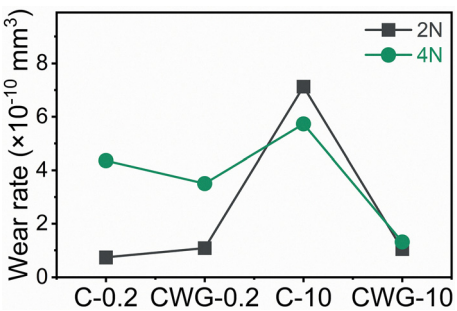
Misbah Shaheen and Sheharyar Pervez*



19960

Arriving at ultralow wear using cellulose/two-material composites

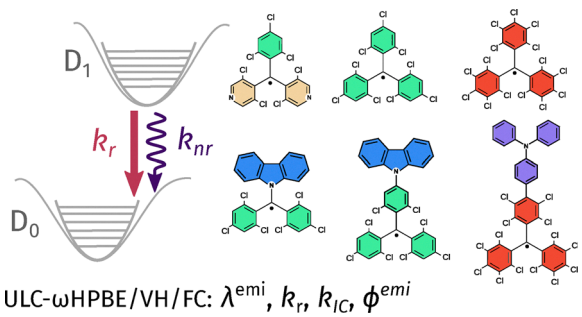
Xuan Yin,* Dingyao Zhang and Bing Zhang



19970

Modeling the emission spectra and radiative decay rates in polychlorinated organic radicals

Carmelo Naim* and Denis Jacquemin*



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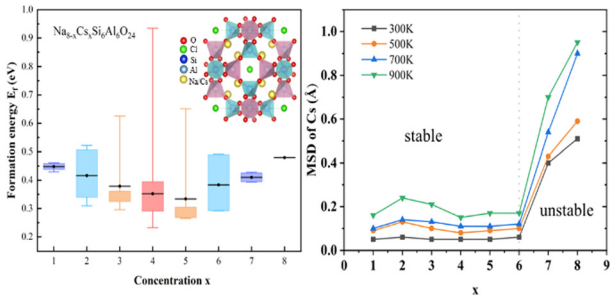
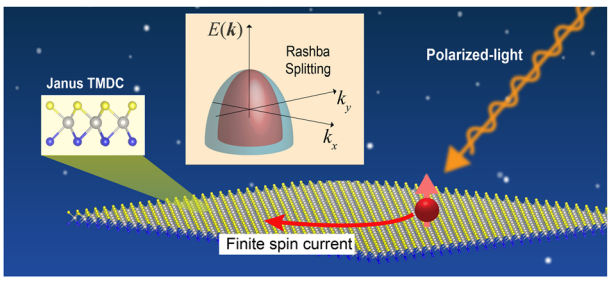


Mechanisms of cesium incorporation and thermal stability in sodalite

Mingfeng Shao, Zeao Wang, Guoqiang Qin, Zhi Wang, Shengjian Qin,* Linyan Li,* Yi Liu and Shengdong Zhang

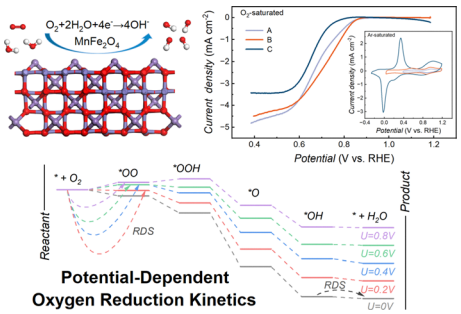
19997



Optically induced spin Hall current in monolayer Janus NbSSe: a first-principles study

Souren Adhikary, Tomoaki Kameda and Katsunori Wakabayashi*

20005



Deciphering potential-dependent oxygen reduction kinetics in spinel manganese ferrite

Junxiang Wang, Zhaoyi Jiang, Jingwen Wei and Ye Zhou*

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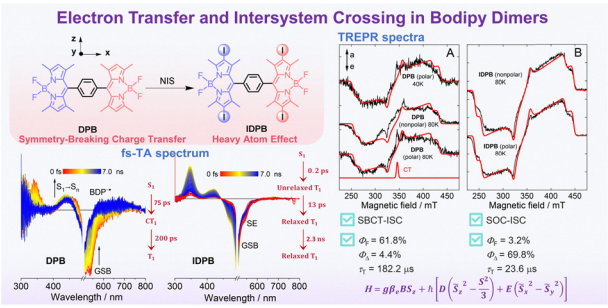

Electron transfer and intersystem crossing in Bodipy dimers: a study of their photophysical properties using steady state and transient optical and electron paramagnetic resonance spectroscopic methods

Yanran Wu, Marcel M. Bakirov, Andrei A. Sukhanov, Huaiman Cao, Jiayu Li, Sheng Liao, Jianzhang Zhao,* Yuri E. Kandrashkin,* Violeta K. Voronkova* and Ming-De Li*

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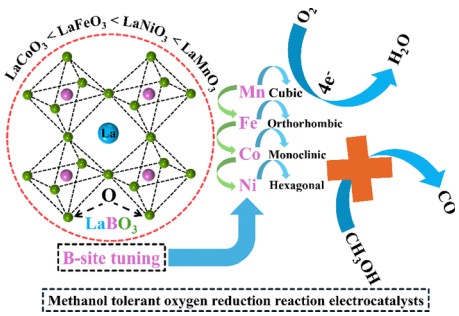
20023

Tailoring $LaBO_3$ (B = Mn, Fe, Co, Ni) perovskite oxides for methanol-tolerant oxygen reduction reaction electrocatalysts

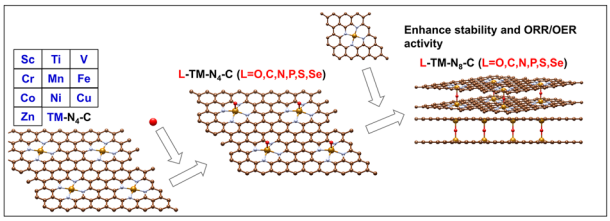
Shaikh Parwaiz, Fazlurrahman Khan, James Robert Jennings, Mohammad Hilni Harunsani, Young-Mog Kim and Mohammad Mansoob Khan*



20039

Axial engineering of bilayer single-atom catalysts for enhanced bifunctional oxygen electrocatalysis

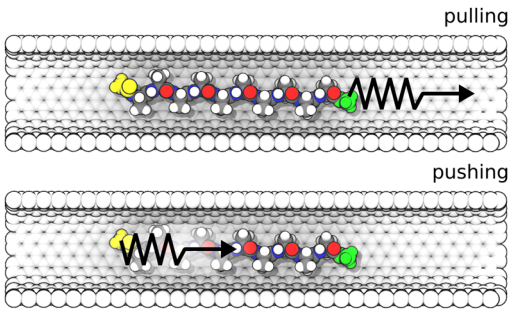
Xinge Wu, Wenzhu Tan, Zhaoying Yang, Chao Li, Shuai Shao and XiangYing Meng*



20050

Sensitivity of peptide conformational dynamics in carbon nanotubes to directional mechanical forces

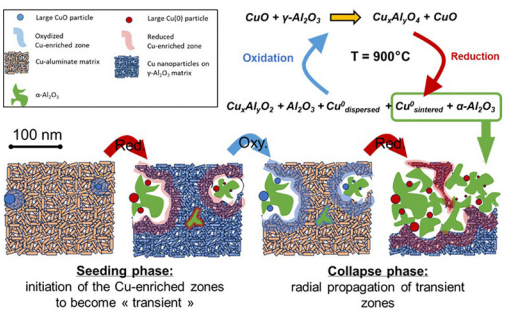
Felipe C. Nepomuceno and Michal H. Kolář*



20063

High-temperature phase evolution in CuO/Al_2O_3 oxygen carriers: insights from *in situ* quick XAS

Sharmin Sharna,* Virgile Rouchon,* Arnold Lambert, Valerie Briois, David Chiche, Anne-Sophie Gay, Christèle Legens and Ovidiu Ersen



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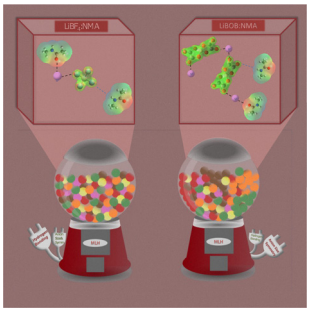
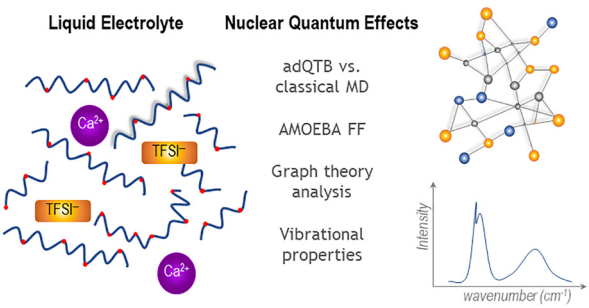


Molecular-level heterogeneity in deep eutectic electrolytes

Mirna Alhanash, Carolina Cruz and Patrik Johansson*

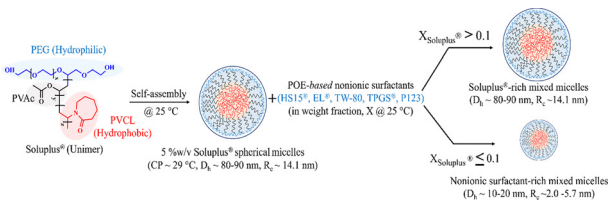
20084



Improved modeling of battery electrolytes: betting on model fitting or quantum effects?

Defne Saraç, Diego Moreno Martinez, Marie-Liesse Doublet* and Christophe Raynaud*

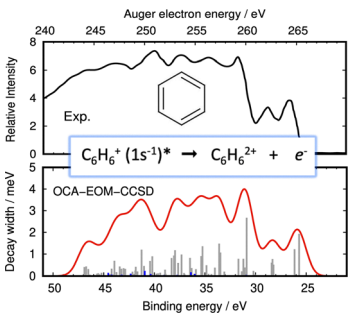
20092



Physicochemical characterization of polyoxyethylene (POE)-based nonionic surfactants in single and mixed micellar environments for anticancer drug solubilization enhancement

Virendra Prajapati, Yashika Tomar, Gautam Singhvi, Debes Ray, Vinod Aswal, Ketan Kuperkar* and Pratap Bahadur

20117



An equation-of-motion coupled cluster singles and doubles approach to Auger–Meitner spectra based on the one-center approximation

Wojciech Skomorowski,* Bruno Nunes Cabral Tenorio and Sonia Coriani*

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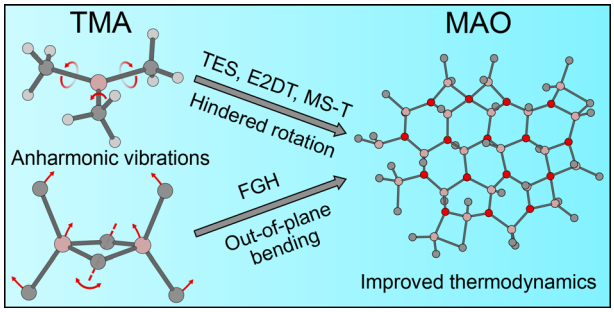
20131

Hindered rotation and bending anharmonicity in aluminum alkyls: implications for methylaluminoxane thermodynamics

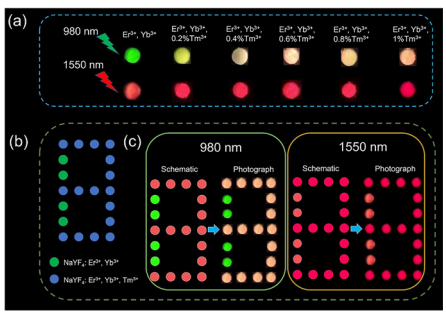
Perttu Hanhisalo and Mikko Linnolahti*



20143

Controlling Er^{3+} multiphoton upconversion by synergistically regulating energy transfer and cross-relaxation for optical anti-counterfeiting

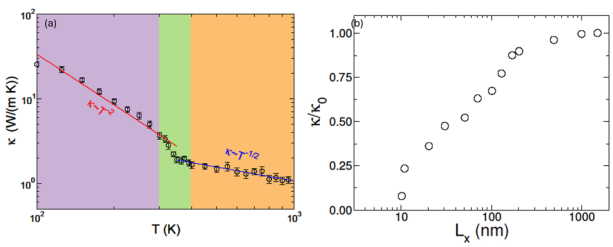
Yangyang Zhang, Zhengce An, Liping Lu* and Xiaoyun Mi



20154

Anomalous temperature induced transition and convergence of thermal conductivity in germanene monolayer

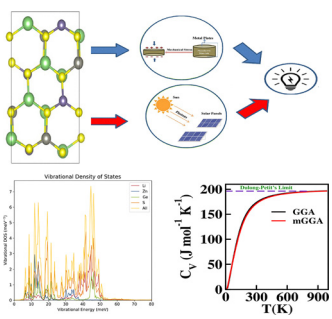
Sapta Sindhu Paul Chowdhury, Sourav Thapliyal and Santosh Mogurampelly*



20163

Exploring the functional properties of the diamond-like quaternary compound Li_2ZnGeS_4 for potential energy applications: a theoretical approach

Lalengmawia Celestine, Michael T. Nunsanga, Saurav Suman, Renthlei Zosiamliana, Lalruat Sanga, Hani Laltlanmawii, Lalhriat Zuala, Shivraj Gurung, A. Laref and D. P. Rai*



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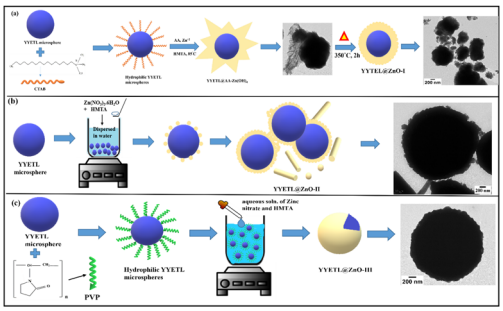
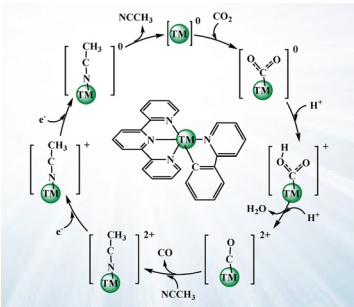
20177



Systematic growth of non-epitaxial ZnO shell over Ln^{3+}–Li^{+} co-doped Y_2O_3 phosphor core

Shefali Jayswal* and Rakesh S. Moirangthem

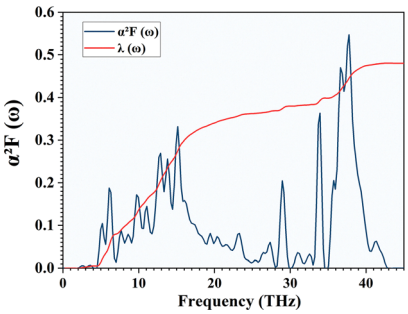
20185



Photocatalytic CO_2 reduction reaction on $[TM(tpy)(ppy)]^0$ (TM = Re and Rh) species with a square pyramidal nitrogen-coordinated structure: a computational study

Chengxu Hu,* Donghua Zhang, Yunjie Chu, Xinyu Zuo and Min Zhang*

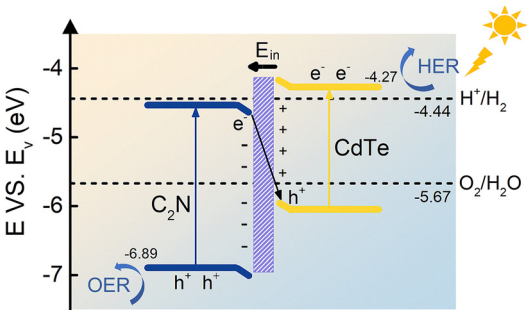
20193



Ideal strength and emergent superconductivity in a three-dimensional sp^2-carbon network cT16

Hao Chen, Shan Jiang, Jing Wang, Ying Xu and Dan Zhou*

20199



Boosted photocatalytic water splitting over a direct Z-scheme CdTe/C_2N van der Waals heterojunction: a first-principles insight into photocatalytic activity

Yi Li, Cheng Gong,* Tong Chen, Dong-Lan Zhang, Ling-Ling Wang, Kejun Dong and Liang Xu*

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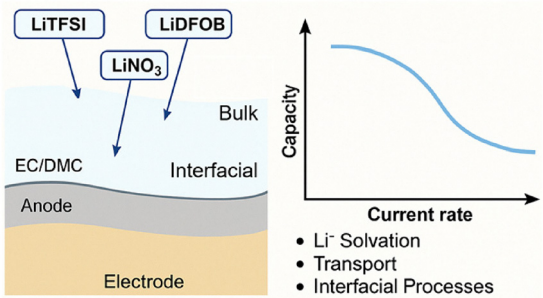
20209

Toward a bottom-up understanding of the impact of high-entropy electrolyte components on the charge storage performance of lithium ion batteries

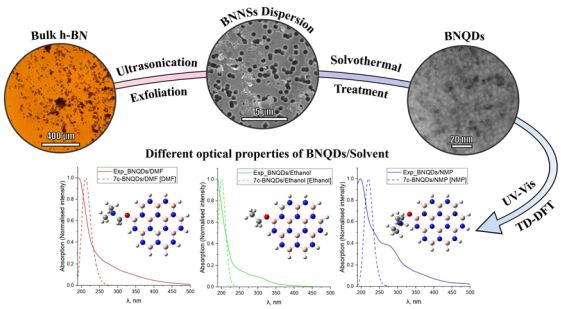
Zihao Zeng, Tengxiang Qi, Bing-Ang Mei,* Zhengxing Zuo, Huihua Feng and Rui Xiong



20226

Absorption properties of boron nitride quantum dots: effects of solvents

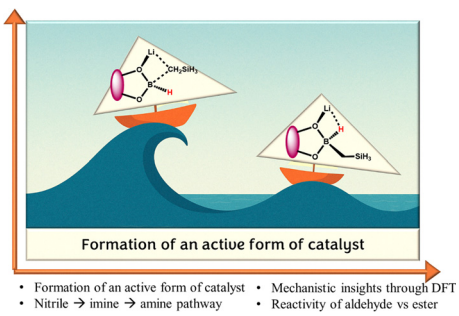
E. A. Sidorov, I. O. Simonenko, N. M. Chtchelkatchev, E. D. Gribova, I. N. Fadeykina, P. P. Gladyshev and R. G. Nazmitdinov*



20237

Mechanistic insights into neosilyllithium-catalyzed hydroboration of nitriles, aldehydes, and esters: a DLPNO-CCSD(T) study

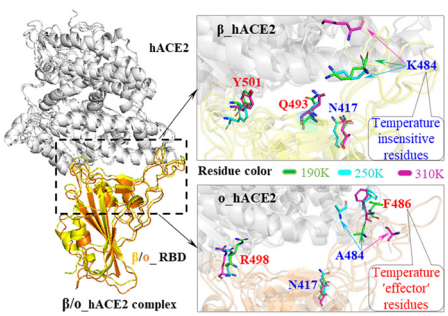
Mridula Choudhary, Tarun K. Panda* and Saurabh Kumar Singh*



20250

Identification of temperature-insensitive residues in regulating SARS-CoV-2 variants-human ACE2 interaction—a study of molecular dynamics simulation

Chuanbo Wang, Zijian Liu, Jinfei Mei, Mengke Jia, Sajjad Ahmad and Hongqi Ai*



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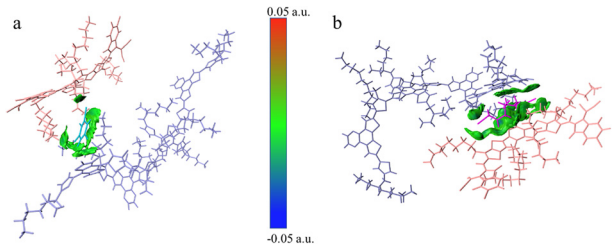
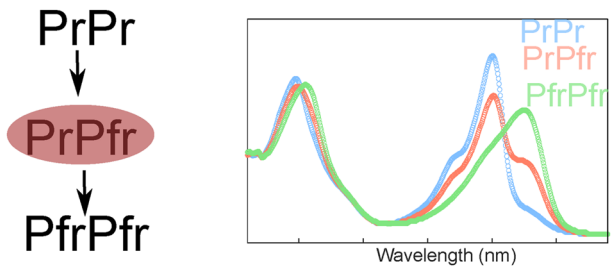
20266



Unveiling additive effects on molecular packing and charge transfer in organic solar cells: an AIMD and DFT study

Xiang Li, Qingxing Wu, Qiuhua Liu,* Zaichun Zhou,* Guangjun Zhang* and Wanqiang Liu*

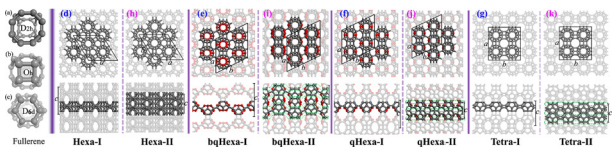
20279



Detection of a hybrid PrPfr state in the dark reversion of a bathy phytochrome indicates inter-dimer allostery

Sayan Prodhan, Petra Mészáros, Szabolcs Bódizs, Yalin Zhou, Michał Maj and Sebastian Westenhoff*

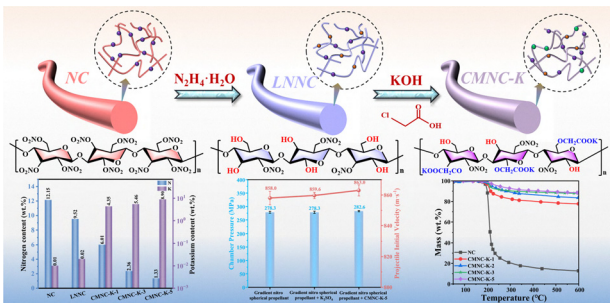
20288



Integrating intrinsic lightweight, superhard, and magnetic properties in 3D covalent fullerene C_{24} networks: a first-principles study

Haoyu Liu, Adili Kuerban, Saierjiang Bieerdemulati, Haiping Wu,* Erjun Kan and Yan Qian*

20299



Synthesis and performance study of potassium-based flame-retardant groups grafted onto nitrocellulose

Changle Qu, Shiying Li,* Chenzhao Gao, Zhongliang Xiao and Qingbo Ma

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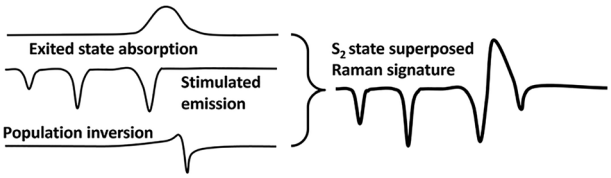
20313

Vibrational signature of $1^1B_u^+$ and hot $2^1A_g^-$ excited states of carotenoids revisited by femtosecond stimulated Raman spectroscopy

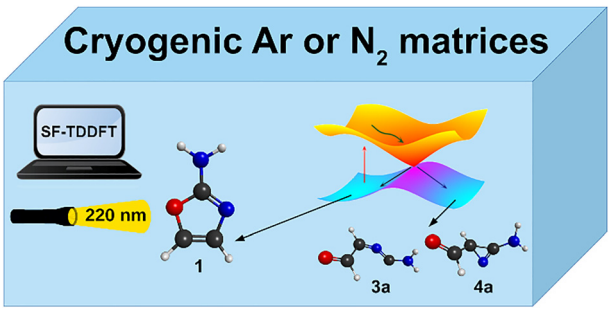
Petra Chrupková, Andrej Hovan, Michal Koblížek, Alastair T. Gardiner, Tomáš Polívka and Miroslav Kloz*



20326

Photochemistry of 2-aminooxazole: a matrix-isolation and computational study of a putative key prebiotic molecule

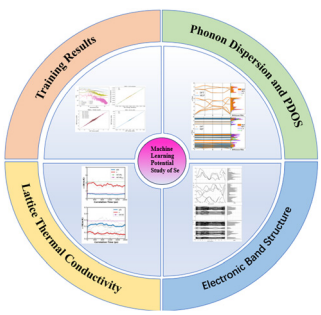
Cláudio M. Nunes,* Luís P. Viegas,* Anuj Tripathi, Sofia Braz and Rui Fausto



20334

Thermal conductivity of selenium crystals based on machine learning potentials

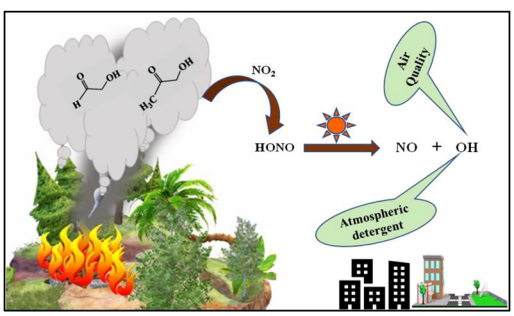
Xiao Tang, Liangcai Wu,* Ziang Xu, Lei Liu, Zhitang Song and Wenxiong Song*



20344

NO_2 reduction to HONO by small α-hydroxycarbonyls: a laboratory investigation relevant to nighttime production of atmospheric HONO

Subhasis Mandal, Rinjini Saha and Tapas Chakraborty*



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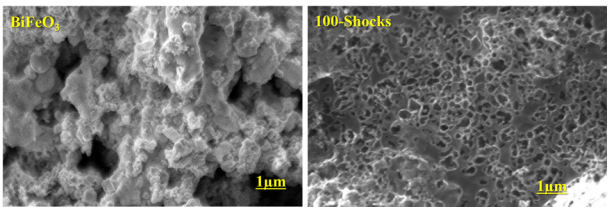
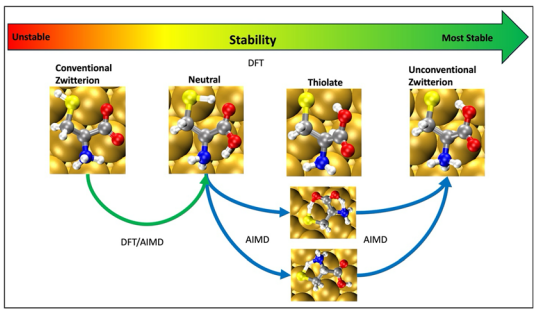


Acoustic shock wave-induced phase transition from an *R*3*c*-distorted rhombohedral to an *R*3*m*-rhombohedral perovskite structure: bandgap tunability and morphological evolution of porous $BiFeO_3$ microparticles

F. Irine Maria Bincy, S. Oviya, D. Rajkumar* and S. A. Martin Britto Dhas*

20368



Adsorption modes of cysteine on gold: from neutral molecules to unconventional zwitterions

Clayton B. Smith, Aishat Idris, Elvis C. M. Ting and Irina Paci*

CORRECTION

20377

Correction: Harnessing the polymer-particle duality of ultra-soft nanogels to stabilise smart emulsions

Alexander V. Petrunin, Steffen Bochenek, Walter Richtering and Andrea Scotti*

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