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IN THIS ISSUE

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Cover
See Deborah A. Drost and Christian Merten, pp. 1111–1117.
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Inside cover
See Kohei Tada *et al.*, pp. 1118–1131.
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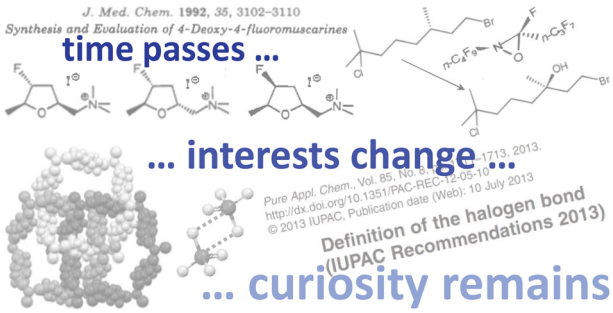
EDITORIAL

1013

From fluorine chemistry to noncovalent interactions: celebrating Prof. Giuseppe Resnati

Antonio Frontera,* Norio Shibata* and Kamran T. Mahmudov*

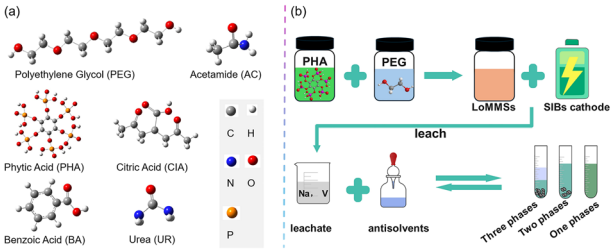


REVIEWS

1016

Capric acid-driven three-phase antisolvent precipitation strategy for recycling metal and lixiviant from the leachate of spent sodium-ion batteries cathode

Yu Chen,* Yaxue Shen, Zhuojia Shi, Zhenghui Liu, Yanlong Wang, Qi Liu and Zheng Li



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REVIEWS

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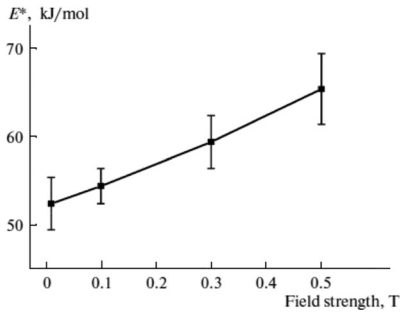
Influence of an external magnetic field on gas–solid reactions

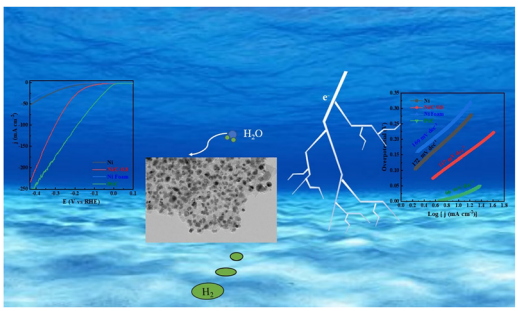
P. A. Chernavskii,* G. V. Pankina, B. S. Lunin and N. S. Perov*



1037

Nickel nanoparticles oriented on carbon materials as an efficient electrocatalyst for the hydrogen evolution reaction

Heng Ke,* Jixiang Zhang, Wenqi Luo, Yunshan Ding, Liangzhe Chen, Wentao Tang, Youbing Zhang, Jing Ding, Jun Wang* and Hong Wang*

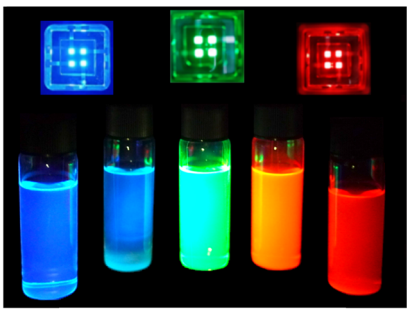


PERSPECTIVE

1046

Emerging ZnSeTe quantum dots as the sustainable solution for high-performance full-color QLEDs

Shiyang Ye, Keyi Pang, Yi Liang, Yuhe Bi, Zhengtuan Chen, Chenglin Lai, Yusheng Song, Jialong Zhao and Sheng Cao*

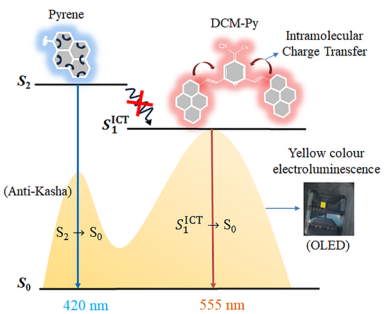


COMMUNICATIONS

1059

Investigating unusual photoluminescence from the excited state in a DCM derivative and its application in lighting devices

Abid Ali, Anastasiia S. Kozlenko, Ilya V. Ozhogin, Tomas Vincze, Martin Weis* and Farman Ali*



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COMMUNICATIONS

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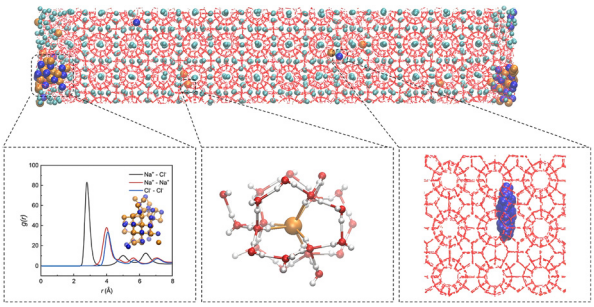
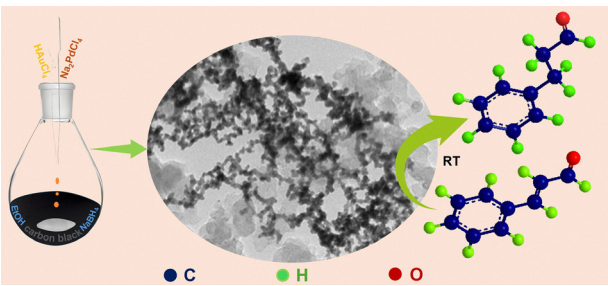


Molecular dynamics simulation study on the growth of CO_2 hydrate from high-concentration NaCl solutions

Ronghui Sun, Zhen Fan, Xin Zheng, Changyu Sun, Shouwei Zhou and Qingping Li*

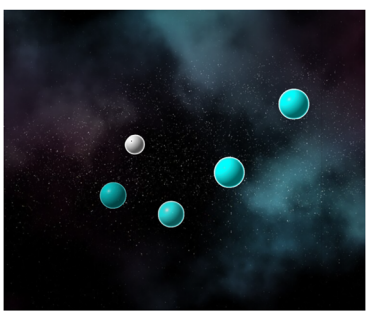
1079



Facile synthesis of carbon-supported PdAu nanonetworks for cinnamaldehyde hydrogenation

Ruigang Xie,* Xiaofang Ren, Wei Zhang, Lingli Zhou, Daixiang Chen and Shenghu Yan*

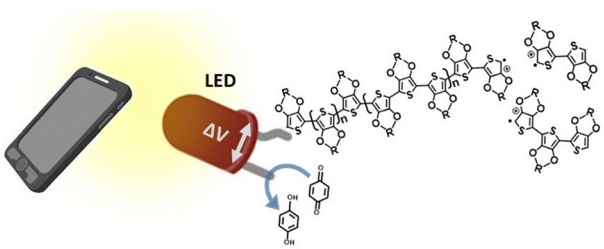
1085



Through-space magnetic response of noble gases

Alvaro Muñoz-Castro

1089



Smartphone light-driven electrocatalytic polymerization of thiophenes

Gerardo Salinas,* Rana Nakar, Getnet Kassahun, Jochen Lang, Matthieu Raoux, Damien Thuau, Mamatimin Abbas, Eric Cloutet and Alexander Kuhn*

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COMMUNICATIONS

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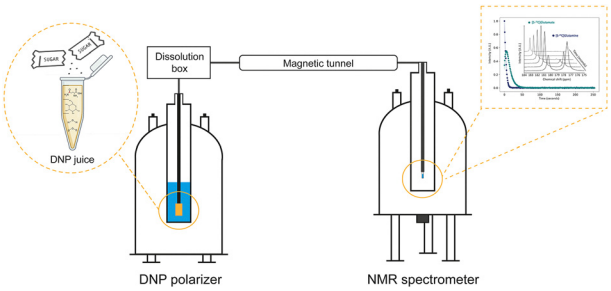
Sweet optimization: glucose-vitrified samples for hyperpolarizing glutamine in biological studies

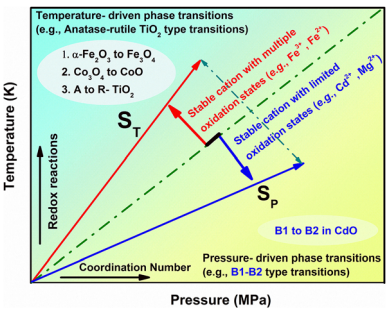
Léa Gutierrez, Karen Dos Santos, Mehdi Soussi-Therond, Aiky Razanahoera, Daniel Abergel, Nicolas Giraud* and Mathieu Baudin*



1100

Thermodynamic origin of the structural transition pathway in metal oxide nanoparticles under acoustic shocked conditions

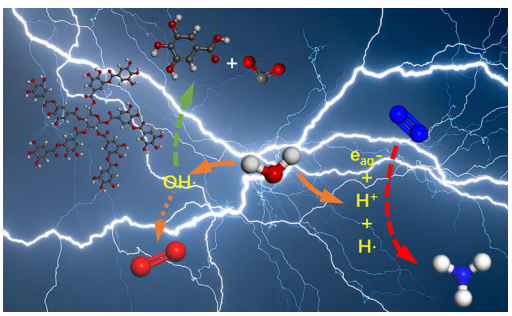
Sivakumar Aswathappa, Lidong Dai* and Sahaya Jude Dhas Sathiyadhas



1105

Catalyst-free efficient stoichiometric synthesis of ammonia and oxygen from nitrogen and water driven by γ-rays

Jian Liu, Xiao Sun,* Yang-Yang Zhang, Jun Li* and Weixin Huang*



RESEARCH PAPERS

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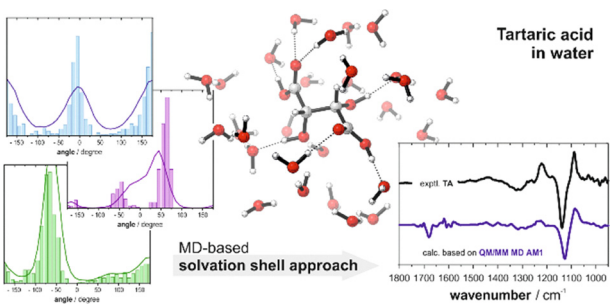
Vibrational circular dichroism of tartaric acid in water

Deborah A. Drost and Christian Merten*



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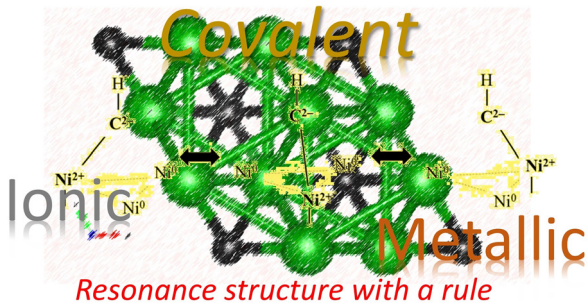
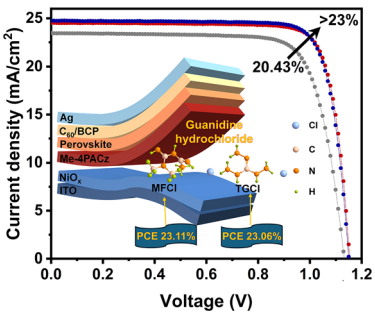


Toward a deeper understanding of H–Ni_3C interactions: rule-based insights

Kohei Tada,* Kai Matsuyama, Sho Yamaguchi, Ryohei Kishi, Tomoo Mizugaki and Yasutaka Kitagawa

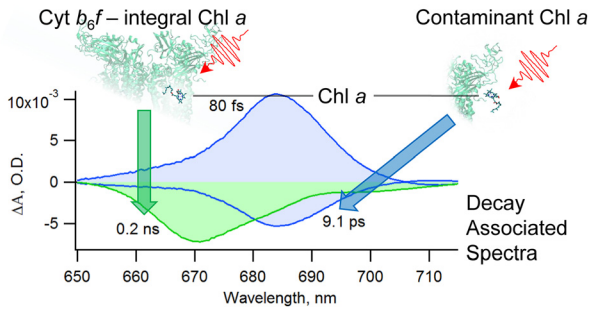
1132



Internal bridging engineering of NiO_x/Me-4PACz *via* selective guanidine-based hydrochlorides for efficient and stable inverted perovskite solar cells

Jiaqi Wang,* Zhirui Chen, Ye Song, Chang Li, Caixuan Wang, Jingjing Hui, Junyu Nie, Yi Wang, Zhihai Cheng, Qi Li and Cheng Mu*

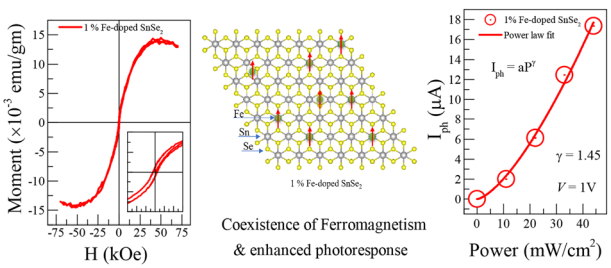
1142



Spectral and temporal differentiation between integral and contaminant chlorophyll *a* in the cytochrome b_6f complex

Adrien A. P. Chauvet,* Rachna Agarwal and William A. Cramer

1148



Coexistence of ferromagnetism and enhanced photo-response in Fe-doped $SnSe_2$ single crystals

Aarti Lakhara and P. A. Bhobe*

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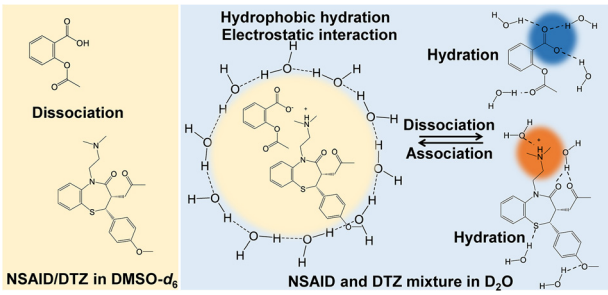
1159

Hydrophobic hydration of analgesics and diltiazem complexes explored by electrochemical impedance spectroscopy and diffusion-ordered spectroscopy

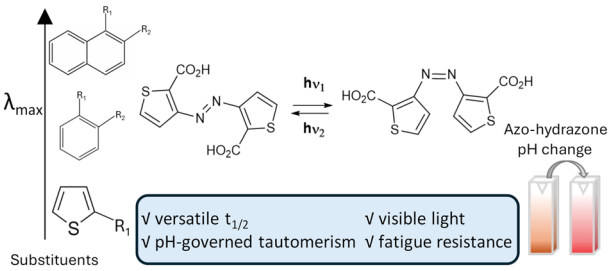
Ryotaro Koga, Takatoshi Kinoshita, Masahiro Ishiguro, Momoko Fujita, Hitoshi Chatani, Hikaru Kataoka, Hideshi Yokoyama, Takehisa Hanawa, Isao Shitanda and Satoru Goto*



1173

Azothiophene-based molecular switches: influence of substituent position and solvent environment on photophysical behavior

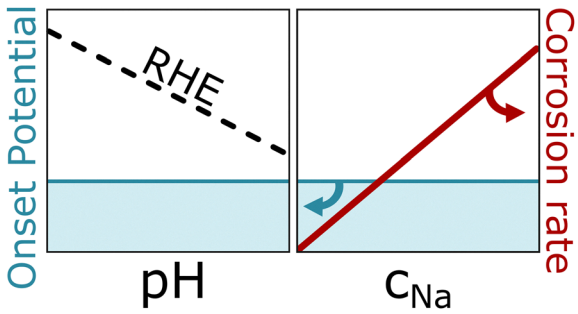
Xin Zhang, Konstantinos T. Kotoulas, P. M. Anuththara Bandaranayake, Dilani Chathumalee, Nuha Ehsan, Patrick R. Huddleston, John D. Wallis and Carole C. Perry*



1189

Disentangling effects of pH, potential, and cation concentration in cathodic corrosion of platinum

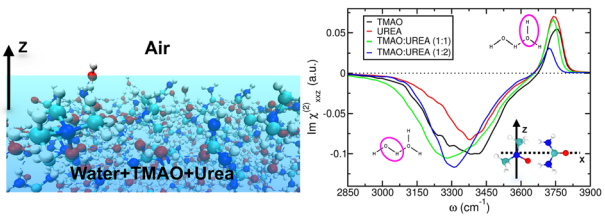
Mark Aarts,* Jamie A. Trindell and Marc T. M. Koper*



1196

Effects of trimethylamine *N*-oxide and urea on the structure of water at liquid–vapor interfaces studied through theoretical vibrational sum frequency generation spectroscopy

Anjali Negi, Ravi Malik* and Amalendu Chandra*



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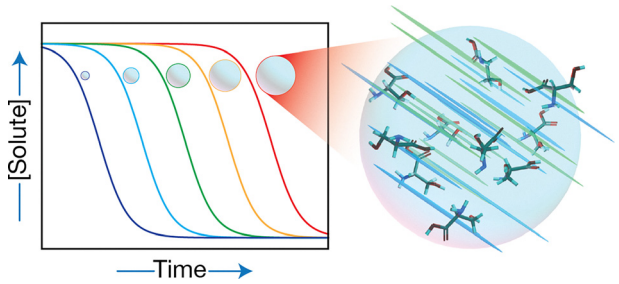
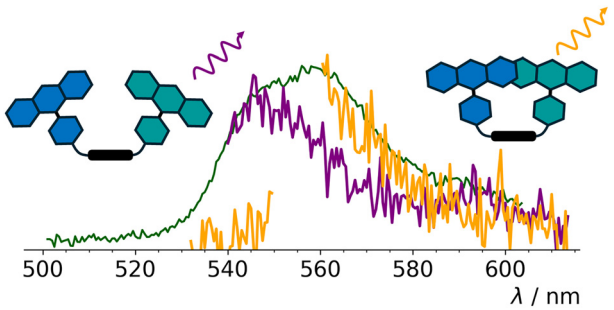


Photochemical transformation of weakly absorbing organics by visible light in microdroplets

Alexander Logozzo and Thomas C. Preston*

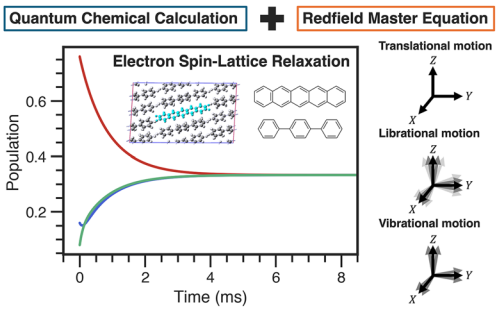
1222



Freezing out structural effects: strong dye–dye couplings in gaseous rhodamine dimers at cryogenic temperatures

Iden Djavani-Tabrizi,* Thomas Toft Lindkvist, Kaja Bangsgaard Johansen and Steen Brøndsted Nielsen

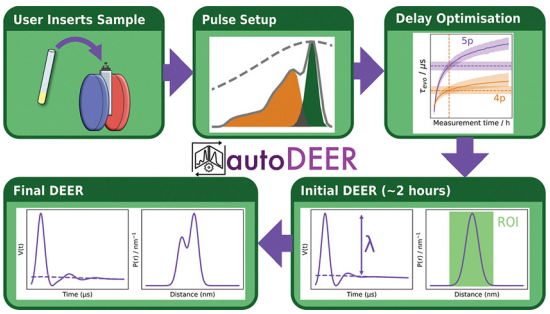
1230



Electron spin–lattice relaxation in triplet-state oligoacenes: a first-principles-based approach

Katsuki Miyokawa* and Yuki Kurashige*

1241



Towards full optimisation of automated double electron–electron resonance spectroscopy

Hugo Karas, Sergei Kuzin, Stefan Stoll and Gunnar Jeschke*

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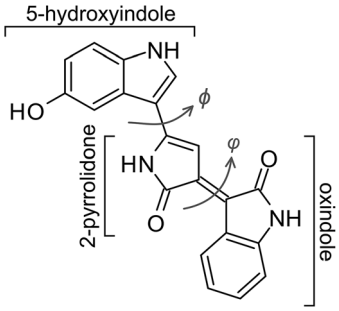
Photomolecular rotor dynamics of the oxindole-based photoprotective bacterial pigment violacein

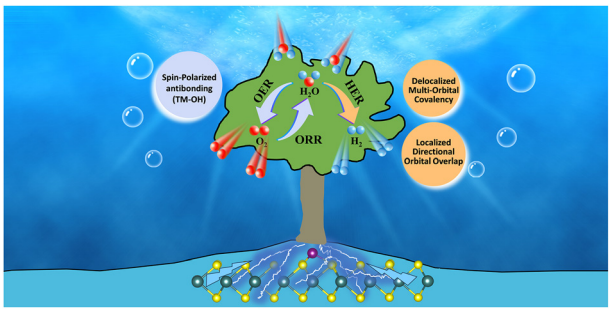
Giovanni Bressan, Khalid M. Siddiqui, Eleanor K. Ashworth, Pratip Chakraborty, Dipanjan Banerjee, Erico M. Braun, Stephen R. Meech and James N. Bull*



1269

Orbital-level insights into multifunctional electrocatalysis of transition-metal single atoms anchored on WS_2 monolayers

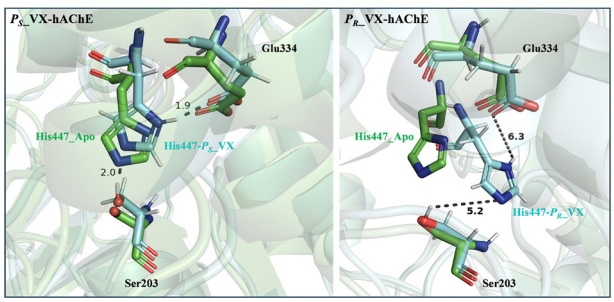
Bingling He, Mingyang Ren, Qianyi Bu, Liying Zhang, Song Ye, Mengyin Liu, Peng Lv,* Zhixue Tian* and Yu Jia*



1281

Unraveling the stereoisomeric toxicity of V-series nerve agent VX on human acetylcholinesterase: a well-tempered metadynamics study

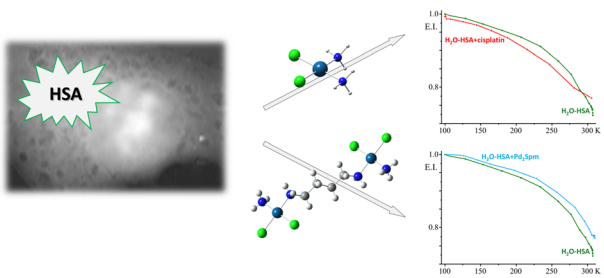
Dipankar Das, Shibaji Ghosh, Kalyanashis Jana and Bishwajit Ganguly*



1293

Probing drug pharmacokinetics using neutron scattering techniques

Clara B. Martins, Mona Sarter, Ana L. M. Batista de Carvalho, Victoria García-Sakai, Tilo Seydel, Jacques Ollivier, Luís A. E. Batista de Carvalho and Maria P. M. Marques*



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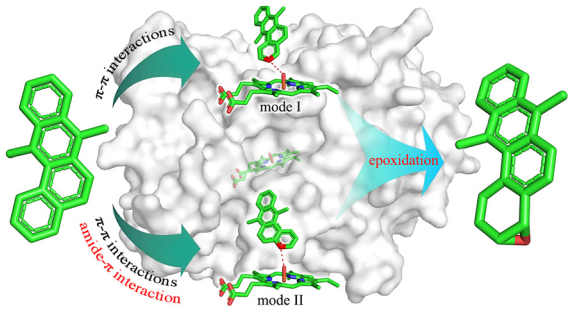
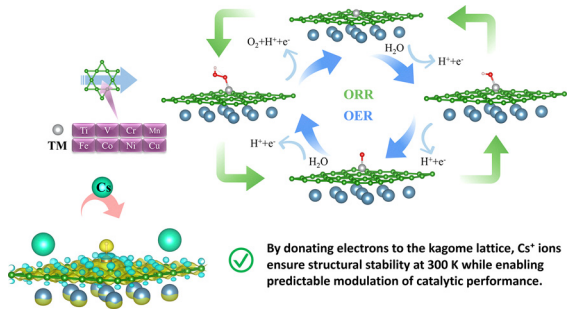


Origin of the metabolic site selectivity of 7,12-dimethylbenz[*a*]anthracene catalysed by the P450 1B1 cytochrome: an *in silico* protocol

Chong Liu, Yan Zhao, Shi Feng and Qingchuan Zheng*

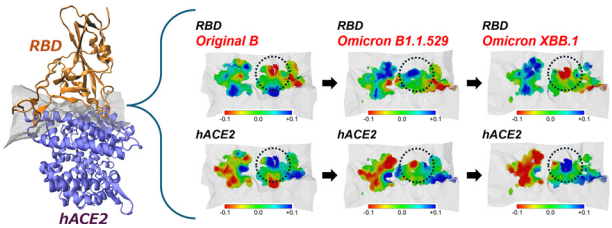
1316



Cesium-anchored MB_3 (M = Be, Ca, Sr) kagome monolayers: stabilizing active sites for bifunctional oxygen electrocatalysis

Yaowen Long and Hong Zhang*

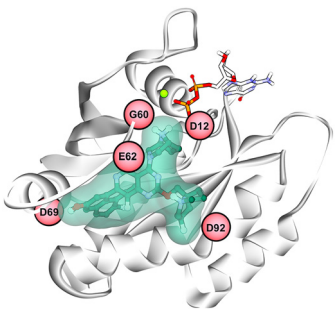
1325



Visualization of interfacial electrostatic complementarity reveals evolutionary changes in SARS-CoV-2 RBD–hACE2 interactions

Yosuke Muroya, Hiroki Ozono and Takeshi Ishikawa*

1336



Mechanistic insights into $KRAS^{G12D}$ inhibitor binding revealed by molecular dynamics simulations of multiple crystal structures

Donghwan Kim, Eunho Lee and Sangbae Lee*

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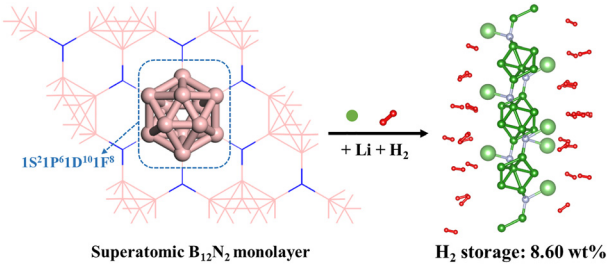
RESEARCH PAPERS

1347

A first-principles study of hydrogen storage on pristine and Li-decorated superatomic $B_{12}N_2$ monolayers

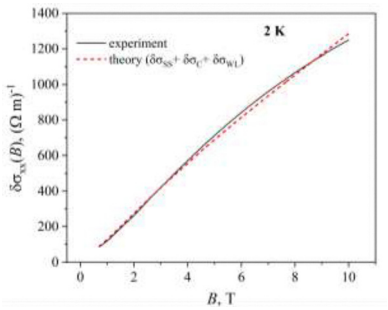
Qinqin Yuan, Zicheng Ling, Zaijun Gui, Lili Shi, Dan Li* and Longjiu Cheng*



1357

Role of quantum contributions in the magnetoconductance behavior of iridate films at low temperatures

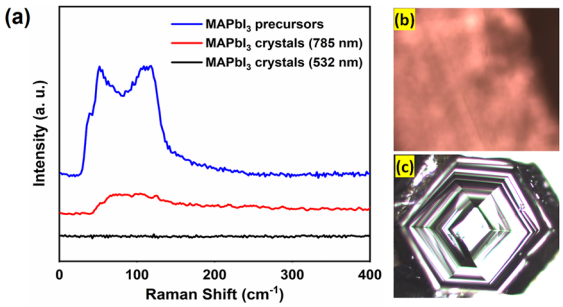
A. L. Danilyuk, D. A. Podryabinkin, A. B. Filonov, G. A. Ovsyannikov, G. D. Ulev, K. Y. Constantinian and D. B. Migas*



1368

Spectroscopic investigation of the solvated $MAPbI_3$ transition to perovskite crystals: a temperature-dependent Raman study

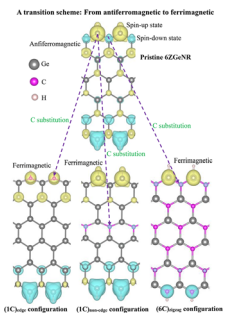
Abdul Zeeshan Khan, Muhammad Shafi, Tarek. A. Kandiel* and Abdulaziz A. Al-Saadi*



1377

Unlocking feature-rich properties of carbon-substituted germanene nanoribbons

D. M. Hoat, Ngoc Thanh Thuy Tran, Quoc-Duy Ho, Duc-Quang Hoang, Minh Triet Dang and Duy Khanh Nguyen*



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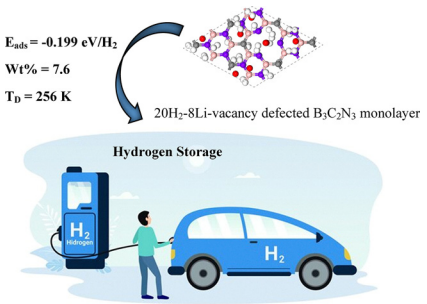
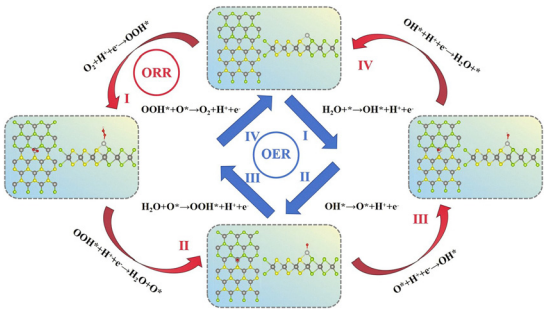


$B_3C_2N_3$ monolayer with vacancy defects decorated with lithium as a potential hydrogen storage system: a DFT study

Rezvan Rahimi,* Mohammad Solimannejad* and Yafei Zhang

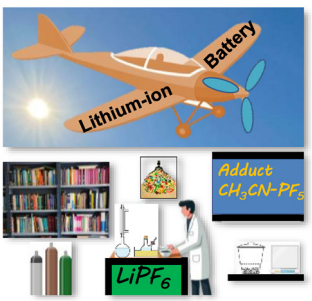
1410



Single transition metal atoms anchored on WSe_2/WS_2 heterostructures as efficient bifunctional electrocatalysts for the OER/ORR

Kai Zhang, Jianjun Fang, Chenkun Li, Tongmeng Xing, Qiuyan Xiang, Xianfang Yue, Breno R. L. Galvão* and Jing Li*

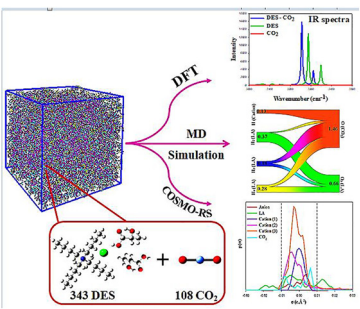
1420



A new step in understanding the process of the lithium battery manufacturing process: analysis of the CH_3CN-PF_5 species in matrices at cryogenic temperatures

Agustín Spaltro, Marcos I. Leone, Carlos O. Della Védova, Rosana M. Romano,* Mei Wen, Holger Pernice and Sebastian Riedel

1429



Ammonium-based deep eutectic solvents for sustainable CO_2 capture: insights from DFT, COSMO-RS, and MD simulations

Zahra Ostadsharif Memar and Majid Moosavi*

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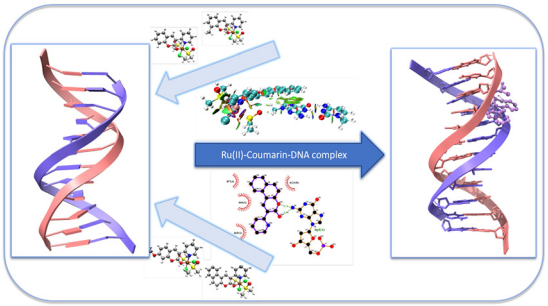
Computational insights into Ru(II)–coumarin complexes as potential anticancer agents: a DFT, QTAIM, NCI-RDG, molecular docking and molecular dynamics approach

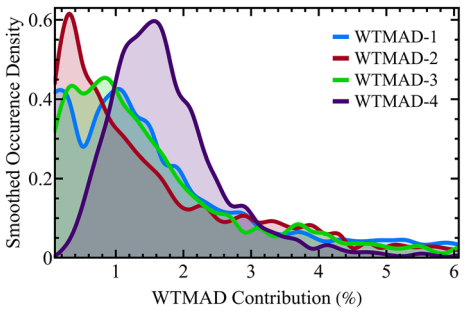
Pratyashee Barukial, Rajib Nandi, Manazira Ahmed, Rituraj Barman, Tamal Banerjee* and Bipul Bezbaruah*



1463

WTMAD-4: a fair weighting scheme for GMTKN55

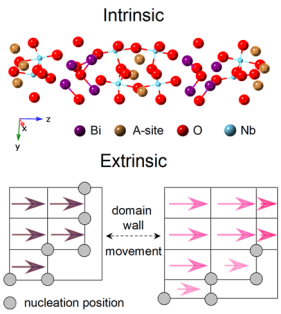
Kyle R. Bryenton and Erin R. Johnson*



1470

Deciphering the potential piezoelectricity optimization mechanism in Aurivillius compounds

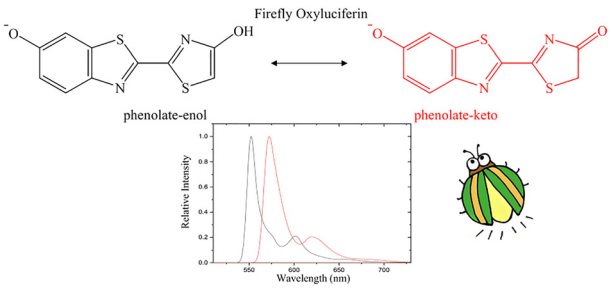
Shangyi Guan, Xiaojun Wu, Lanji Wen, Liang Kong, Zhi Tan,* Hiroko Yokota* and Qiang Chen*



1477

Combined influence of the QM methods, active space size, Franck–Condon approximation, Herzberg–Teller effect and Duschinsky effect on vibrationally resolved electronic spectra: insights from firefly oxyluciferin

Shuangqi Pi, Cheng Peng, Haibo Ma* and Ya-Jun Liu*



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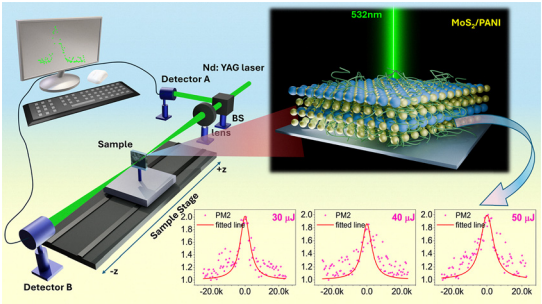
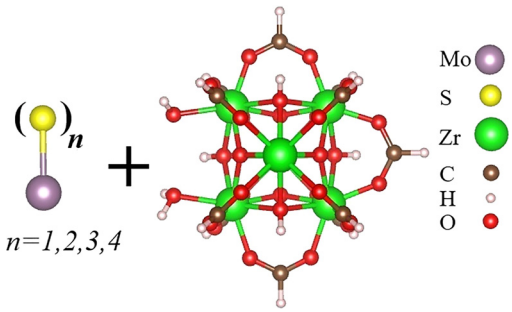


Polarons and Pauli-blocking enhanced saturable absorption in MoS_2 nanorod/PANI nanocomposite films

Anjali Sharma and B. Karthikeyan*

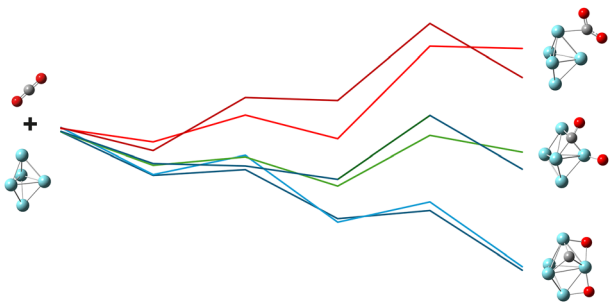
1504



Hydrogenation of ethylene over molybdenum–sulfur complexes supported on UiO-66

Maryam Mansoori Kermani, Matthew Neurock and Donald G. Truhlar*

1515



Associative *vs.* dissociative binding of CO_2 on M_5 transition metal clusters

Nguyen T. T. Le, Alireza Nazari, Yash Rele, Mighila Rixon, Ishudeep Singh Narula and Matthew A. Addicoat*

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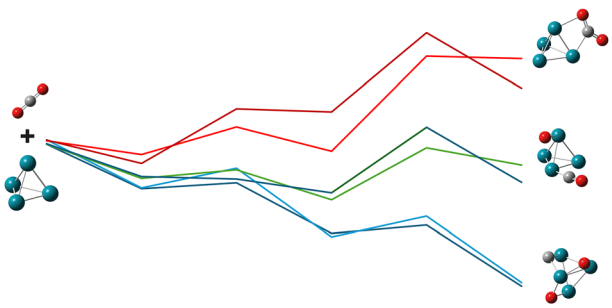

Associative *vs.* dissociative binding of CO_2 on M_4 transition metal clusters

Sherfi Sherif, Bala Aakash Velmurugan, Naeem Abbas, Muskanbanu Shaikh and Matthew A. Addicoat*

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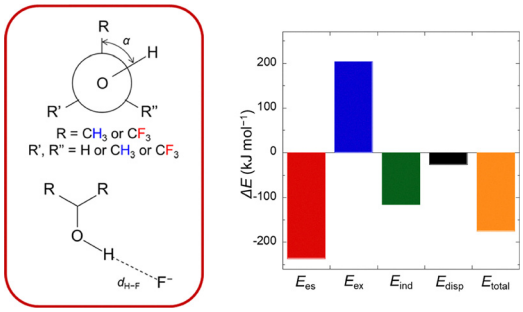
Effects of the fluorination degree in alcohols on the interaction with fluoride ions

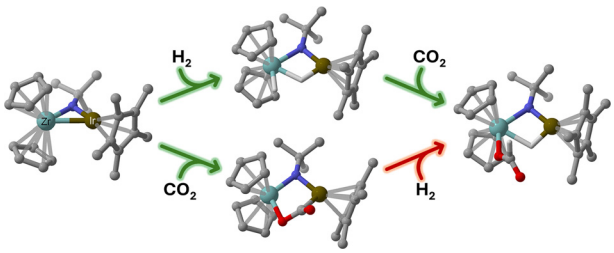
Nozomi Yoneda, Kohei Tada, Seiji Tsuzuki and Kazuhiko Matsumoto*



1549

Mechanism, selectivity, and what prevents closure of the catalytic cycle for H_2 reduction of CO_2 promoted by a heterodinuclear zirconium–iridium complex

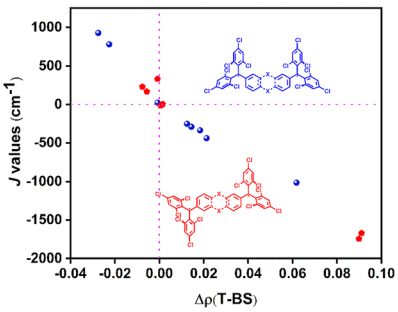
Kevin P. Quirion and Daniel H. Ess*



1556

Heteroatom effects on the magnetic exchange interactions in bis(2,4,6-trichlorophenyl)methyl-based diradicals

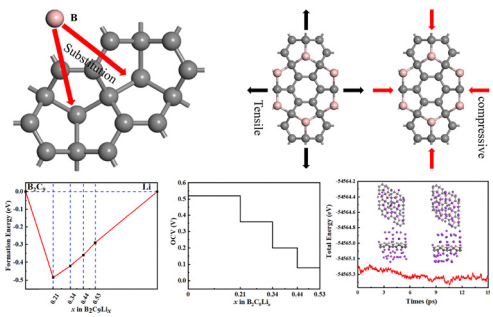
Li Shen,* Rui Dong, Jia-nan Lang, Yihan Li, Yue Li, Jitao Lu, Qian Wu and Qingguo Meng*



1565

B_2C_9 as a high-performance Li-ion battery anode: effects of boron-incorporation and strain-engineering on the adsorption and diffusion of lithium

Rui Shen, Hao Cheng, Guo-Xiang Gao, Xin-Yue Li, Chun-Sheng Liu* and Xiao-Juan Ye*



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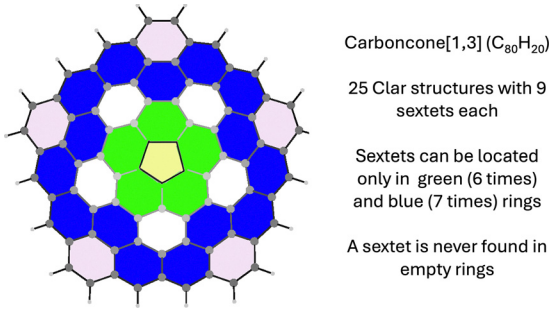
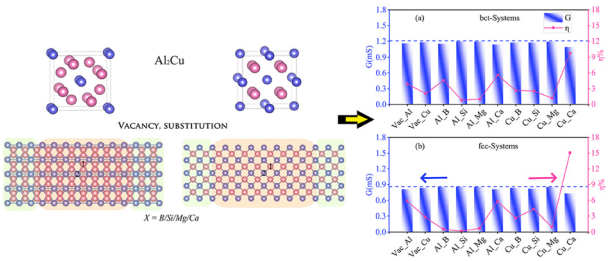


Paratropic ring currents discovered in six-membered rings of conical nanographenes: carboncones

Francesco F. Summa, Lawrence T. Scott, Riccardo Zanasi* and Guglielmo Monaco

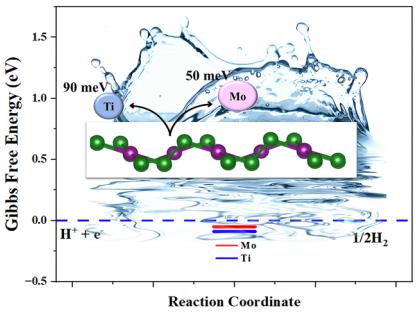
1586



Impacts of vacancy defects and element substitution on the electrical transport properties of θ-Al_2Cu and : A NEGF-DFT study

Shumin Yan, Mingyan Chen, Yibin Hu and Yin Wang*

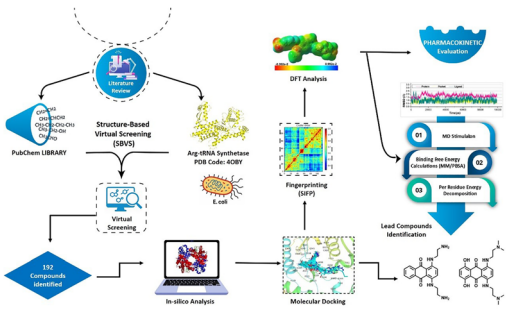
1594



Unveiling the HER potential of TM-substituted $PdTe_2$ monolayers: a first-principles study

Poonam Parkar, Ajay Chaudhari* and Brahmananda Chakraborty*

1608



Structure-based virtual screening and MD refinement reveal novel inhibitors of *Escherichia coli* arginyl-tRNA synthetase

M. Bilal Tayyab and Jianshu Dong*

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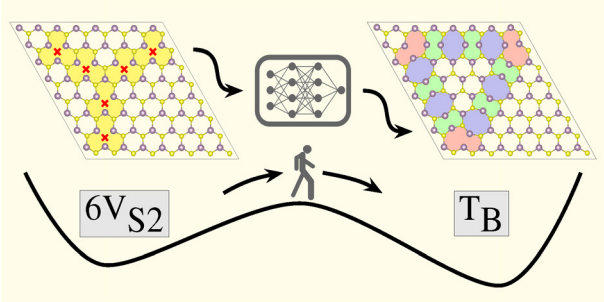
1626

Completing the hierarchy of rotational defects in monolayer MoS_2 through symmetry-aware evolutionary search

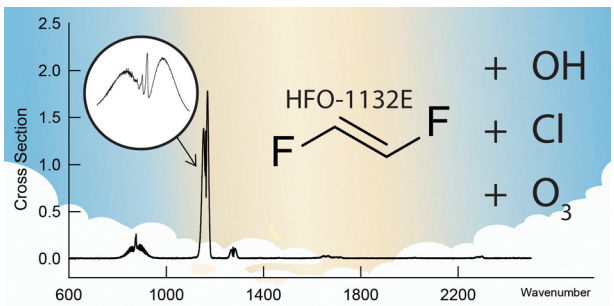
Alexander Adel, Ralf Wanzenböck and Georg K. H. Madsen*



1634

Atmospheric chemistry of (*E*)-1,2-difluoroethene: kinetics and mechanisms of the reactions with Cl atoms, OH radicals and O_3

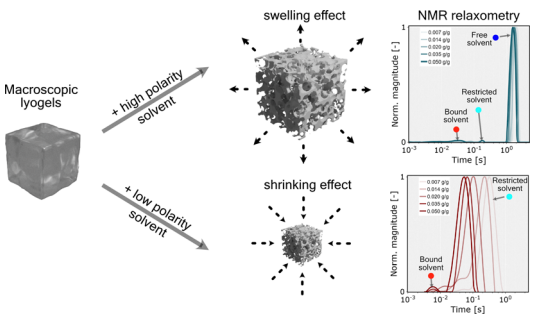
Mads. P. Sulbaek Andersen,* Ellen R. Kjaergaard, Connor Blair and Ole J. Nielsen



1645

NMR relaxometry probes solvent-polarity-dependent molecular interactions in stimuli-responsive lyogels

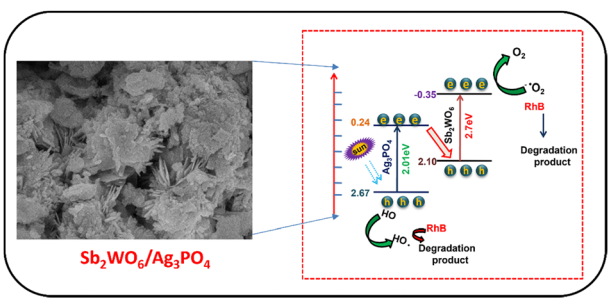
Muhammad Adrian,* Kathrin Marina Eckert, M. Raquel Serial, Artyom Tsanda, Lukas Rennpferdt, Stefan Benders, Hoc Khiem Trieu, Tobias Knopp, Irina Smirnova and Alexander Penn



1655

Development of a novel direct Z-scheme Sb_2WO_6/Ag_3PO_4 nanocomposite with sustainable design for simultaneous electrochemical detection of Pb^{2+} and photocatalytic degradation of RhB dye

Nadi Mlihan Alresheedi



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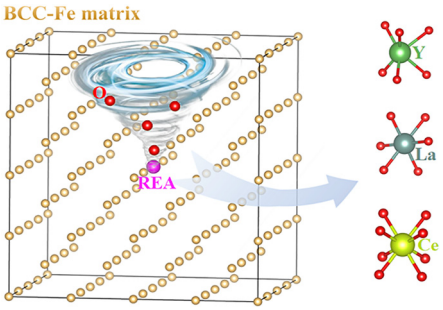
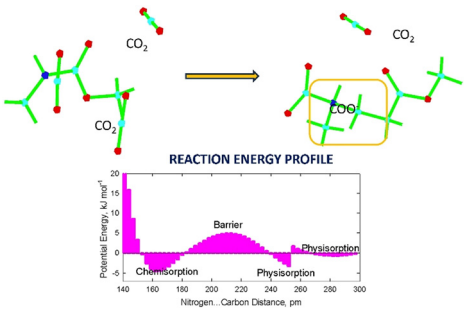


First-principles investigation of oxygen interstitial solubility, site preference, and nucleation behavior in BCC-Fe doped with rare earth elements (Y, La, Ce)

Liangfu Zhou, Zeyu Wang, Kaiqi Li, Xiaoyang Fu, Rui Ma, Ruixue Tian, Jun Cheng and Lei Ren*

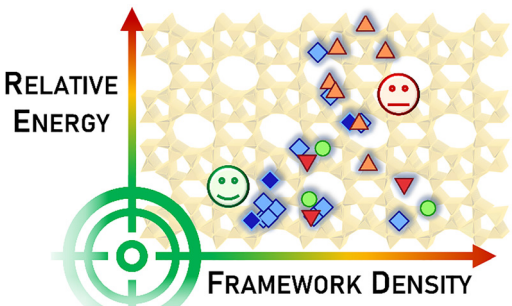
1681



Investigation of a novel urethane-inspired CO_2 chemisorbent: structure modifications and activation barriers

Vitaly V. Chaban

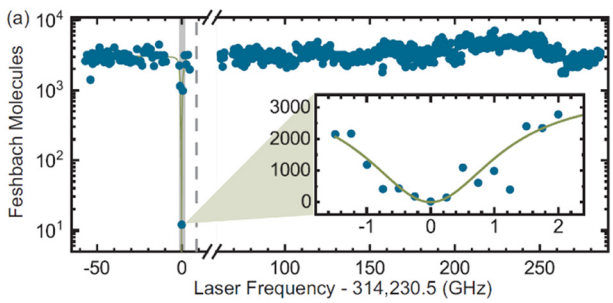
1692



Balancing accuracy and efficiency in density functional theory studies of SiO_2 polymorphs

Michael Fischer

1705



Perturbation-assisted observation of the lowest vibrational level of the $b^3\Pi_0$ state of ultracold LiK molecules

Anbang Yang, Xiaoyu Nie, Hao Lin Yu, Yiming Liu, Victor Avalos, Canming He, Jacek Kłos, Svetlana Kotochigova and Kai Dieckmann*

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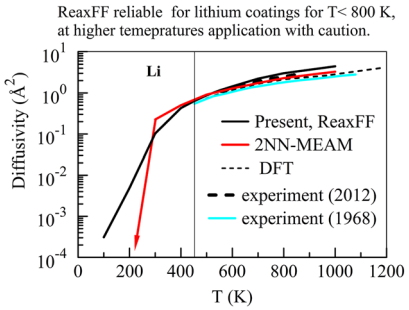
Suitability of the ReaxFF potential for MD modeling of lithium across low and high temperatures

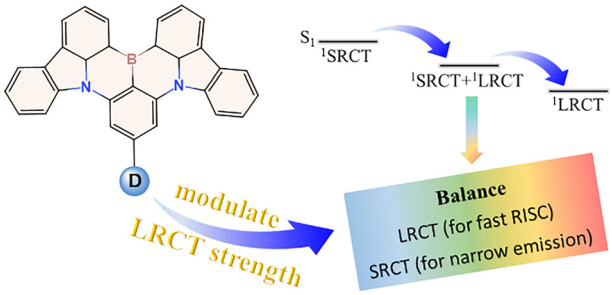
P. S. Krstic,* S. Dwivedi, A. C. T. van Duin and B. E. Koel



1720

Modulating excited state *via* diversified electron-donating units in MR-TADF emitters: a theoretical exploration of structure–property relationships

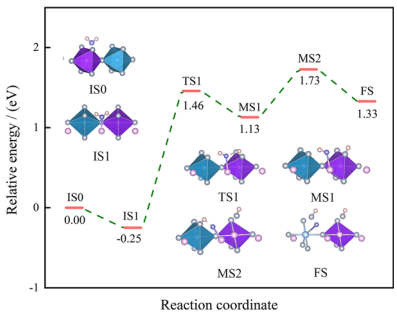
Zhu Chang, Rajat Walia, Dandan Zhang, Xian-Kai Chen and Jiaqi Li*



1730

Thermodynamic and kinetic studies of the hydrolysis mechanism of halide solid state electrolytes Li_3MCl_6 (M = In, Y)

Jian Zhang* and Shuangtao Pan



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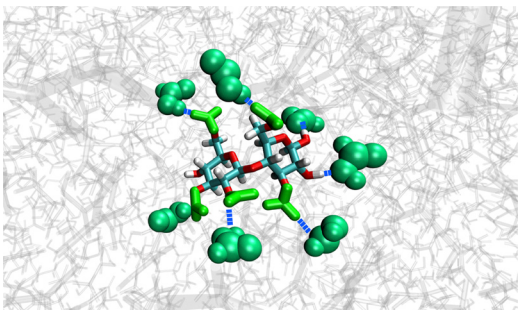
Molecular origin of high-concentration cellulose dissolution in organic acid media: a combined experimental and computational study

Kanta Hayashi, Tomoya Tashiro, Tomohiro Hashizume, Takashi Watanabe and Kenta Fujii*



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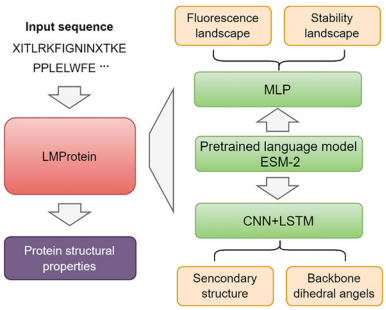
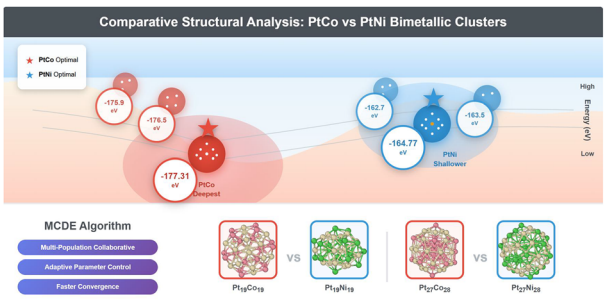


LMProtein: a protein language model based framework for protein structural property prediction

Yongna Yuan,* Hui Luo and Yaojie Tian

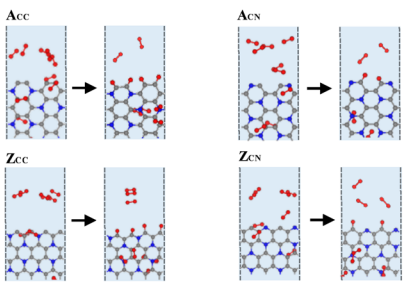
1759



Comparative structural analysis of PtCo and PtNi bimetallic clusters: a systematic study using the MCDE algorithm

Miao He, Xiaomin Wu,* Ruoyu Gan, Lin Tao and Yuheng Chen

1770

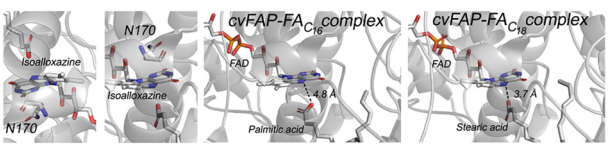


Four types of C3N edges can be easily oxidized at O2 atmospheres.

Phase diagram and dynamics of the edge oxidation of C_3N monolayers in O_2 atmosphere from first-principles calculations

Zhongyue Li, Nan Zhao, Haitao Chen* and Liang Zhao*

1781



Effects of substrate length and active-site residue on catalytic function of fatty acid photodecarboxylase

Min-Shih Su and Ya-Ting Kao*

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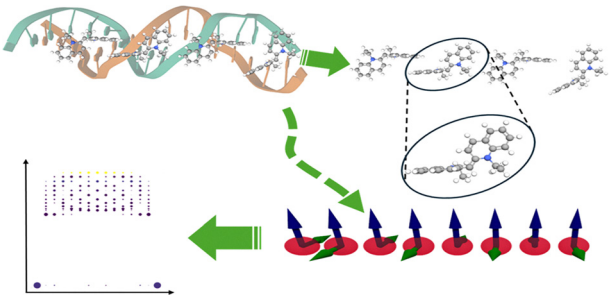
RESEARCH PAPERS

1792

Enhancing energy transport utilising permanent molecular dipoles

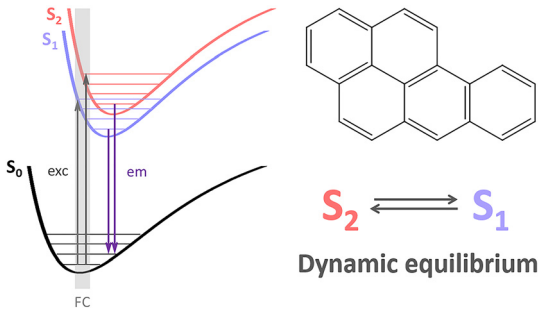
Adam Burgess* and Erik M. Gauger



1806

Non-adiabatic quantum dynamics of polycyclic aromatic hydrocarbons exhibiting anti-Kasha emission from the S_2 state

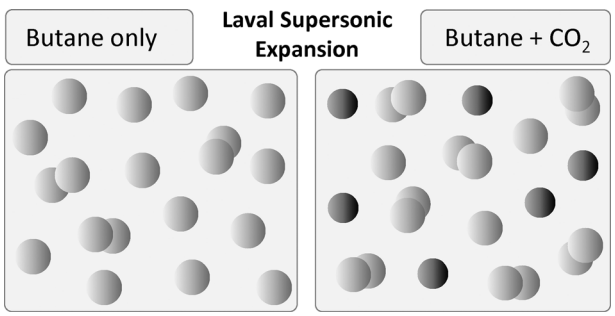
Nikita A. Shekhovtsov* and Mark B. Bushuev*



1820

Acceleration of butane vapor nucleation by carbon dioxide gas

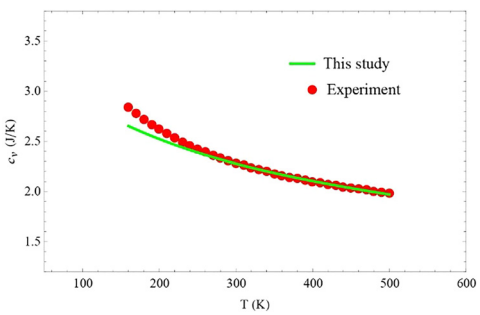
Arnab Choudhury, Felix Graber, Stefan Feusi, Jan Krohn, Jai Khatri, Fernando Torres Hernandez, Chenxi Li and Ruth Signorell*



1829

A study of Frenkel frequency and heat capacity as a function of pressure and temperature using a new approach to the phonon theory of liquids

M. Y. Esmer* and Bahtiyar A. Mamedov



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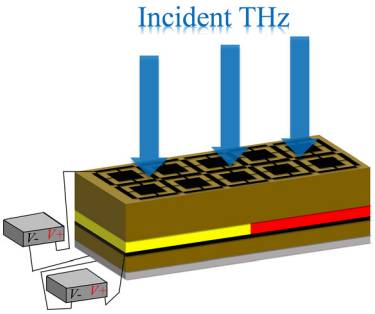
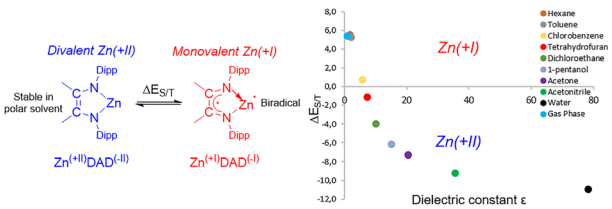
1835



A switchable and tunable THz metasurface absorber with broadband and dual-band absorption features

Usama Arif, Amna Inayat, Muhammad Mohsin, Muhammad Fasih, Jiang Yue and Wei Su*

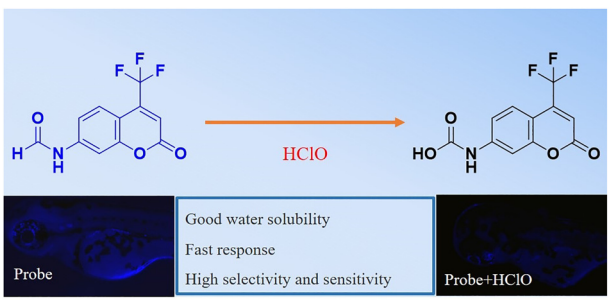
1845



Solvent-dependent electronic dichotomy in zinc complexes with non-innocent ligands: divalent $Zn^{(+II)}$ *vs.* monovalent $Zn^{(+I)}$ forms

Mikaël Le Roch, Alejandro Perez-Luna, Hélène Gérard, Fabrice Chemla and Stéphanie Halbert*

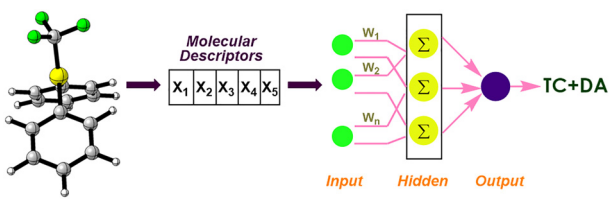
1853



Development of a novel fluorescent probe for highly sensitive detection and visualization of HClO in environmental and biological systems

Mingshuo Ma, Bingxin Zhu, Shihua Yu, Xiaodan Zeng* and Zhigang Liu*

1864



Interpretable machine learning framework for predicting the reactivity of trifluoromethylating reagents

Vaneet Saini* and Shivansh Kanwar

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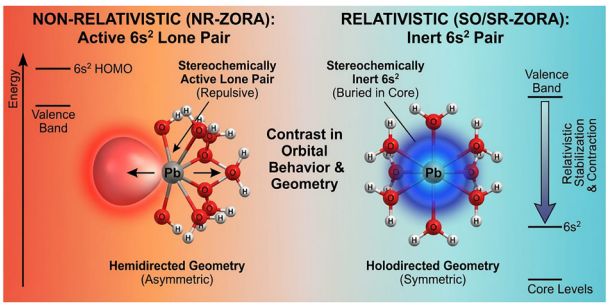
1877

Coordination of lead(II) in solvated clusters with water $[Pb(H_2O)_{1-8}]^{2+}$: insights from relativistic effects, energy analysis, molecular orbitals, and electron density

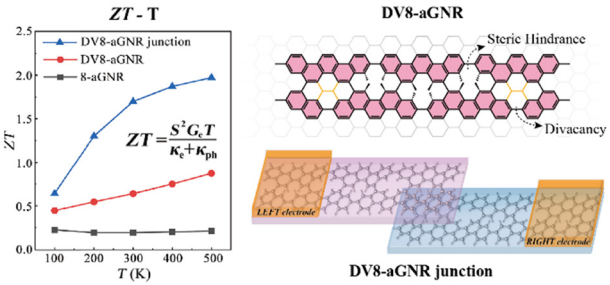
Andy D. Zapata-Escobar,* Franklin Ferraro, Edison Flórez and Alejandro F. Maldonado*



1892

High thermoelectric figure of merit in nonplanar graphene nanoribbons with periodic divacancies

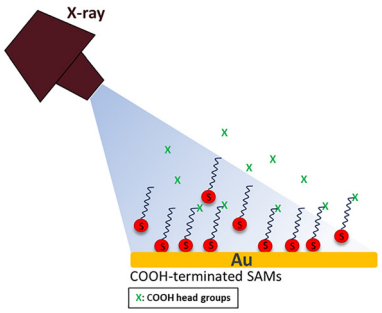
Jianing Wang, Jie Meng, Weiyi Wang* and Qunxiang Li*



1901

X-ray exposure effects on carboxylic-terminated self-assembled monolayers and change in the interface electronic structure

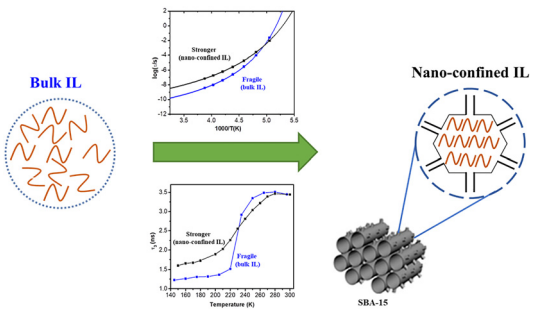
Ahlam R. M. Alharbi, Ingo Köper and Gunther G. Andersson*



1911

Reduction in liquid fragility and enhancement in ionic conductivity in the glassy phase of [BmIm][NTf_2] ionic liquid under nano-confinement: PALS and BDS investigations

Shapath Bhandari, Jaideep Mor, Debasis Sen, Jitendra Bahadur, Kanaklata Pandey and Dhanadeep Dutta*



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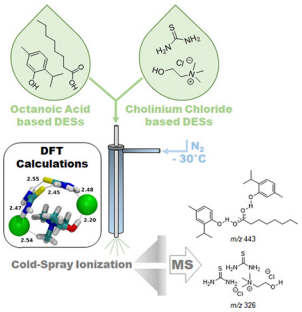
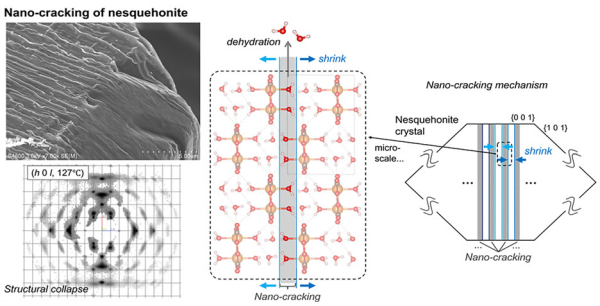
1924



Evaluating the strength of molecular interactions in a deep eutectic solvent (DES) by means of ionization mechanisms involved in cold-spray ionization mass spectrometry and by DFT calculations

Emilie Bertrand, Camille Cousseau, Swaroop V. S. Kunapuli, Thomas Delhaye, Rachel Schurhammer, Alain Chaumont, Emmanuelle Limanton, Béatrice Legouin, Ludovic Paquin, Xavier Castel, Mohammed Himdi and David Rondeau*

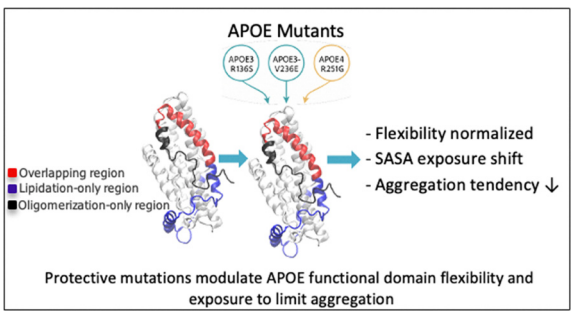
1939



Origin of the nano-cracking of dehydrated nesquehonite ($MgCO_3{\cdot}3H_2O$)

Ryo Yamane,* Hiroshi Sakuma and Kenji Tamura

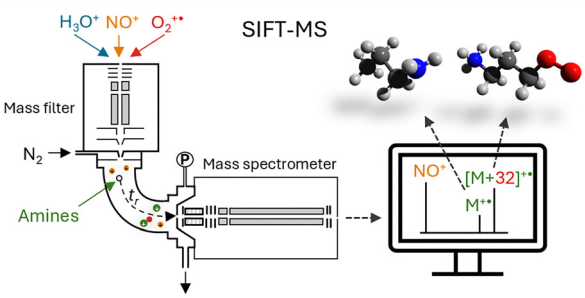
1947



Effect of protective mutation on structure and dynamics of APOE: a molecular dynamics simulation study

Newton A. Ihoeghian, Usman L. Abass, Ibrahim Imam and Qing Shao*

1963



SIFT-MS analysis of amines: unusually efficient O_2 addition to the radical cation product

Christoph Schaefer,* Kseniya Dryahina, Patrik Španěl, Mark J. Perkins and Vaughan S. Langford

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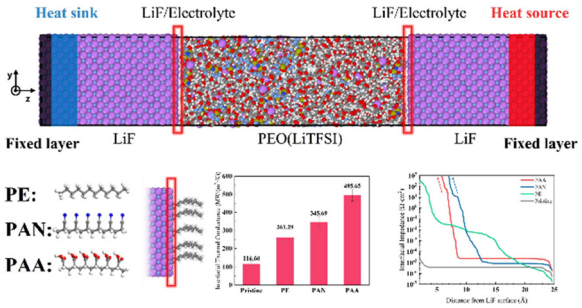
1976

Effects of self-assembled monolayers on thermal and lithium-ion transport at the SEI/PEO-based polymer electrolyte interface: a molecular dynamics study

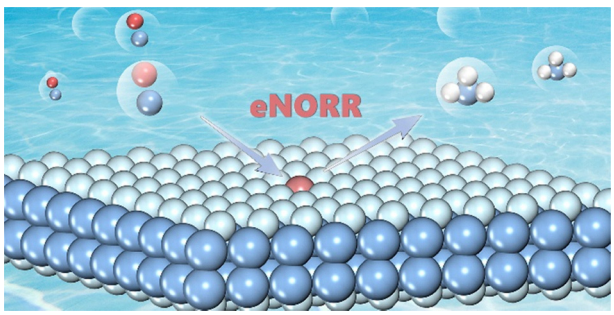
Kang Yi and Dongwei Xu*



1985

A silicon single atom anchored on an α-BS monolayer for efficient electrocatalytic nitric oxide reduction to ammonia

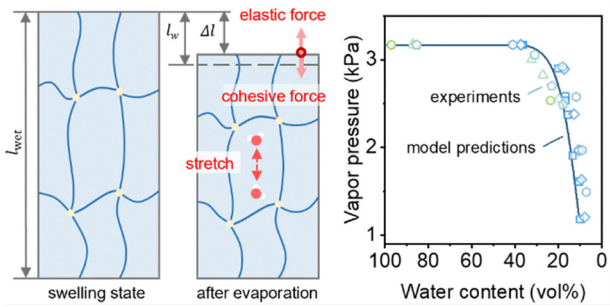
Yongxu Fu, Hu Li, Qingbo Kang, Jiangke Li, Minghui Wu, Lei Liu, Xiaobing Yan, Weichao Wang and Linxia Wang*



1994

Modelling of water evaporation in hydrogels considering the state of water in tension

Zehua Yu, Yongshun Ren and Kang Liu*

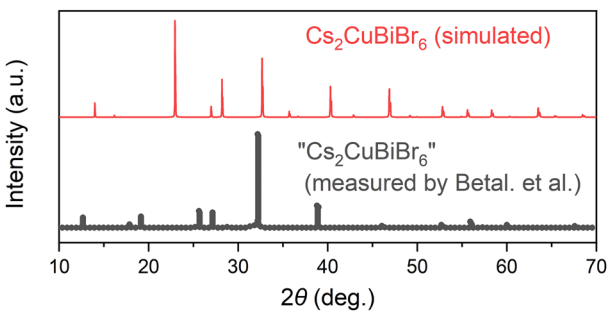


COMMENTS

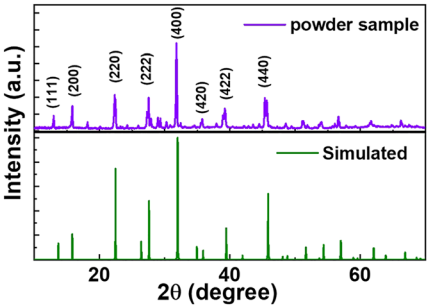
2003

Comment on "Air-stable double halide perovskite $Cs_2CuBiBr_6$: synthesis and memristor application" by A. Betal, A. Chetia, D. Saikia, K. Karmakar, G. Bera, N. V. Dambhare, A. K. Rath and S. Sahu, *Phys. Chem. Chem. Phys.*, 2025, 27, 3150

Lixia Xiao, Junwei Guo, Gang Tang and Zewen Xiao*



2006



Reply to the 'Comment on "Air-stable double halide perovskite $Cs_2CuBiBr_6$: synthesis and memristor application"' by L. Xiao, J. Guo, G. Tang and Z. Xiao, *Phys. Chem. Chem. Phys.*, 2025, 27, DOI: 10.1039/D5CP00194C

Atanu Betal, Anupam Chetia, Dibyajyoti Saikia, Krishnendu Karmakar and Satyajit Sahu*

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