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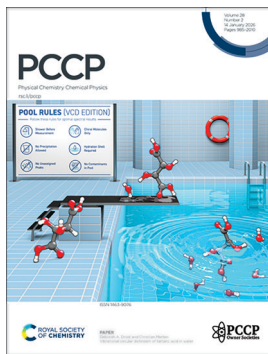
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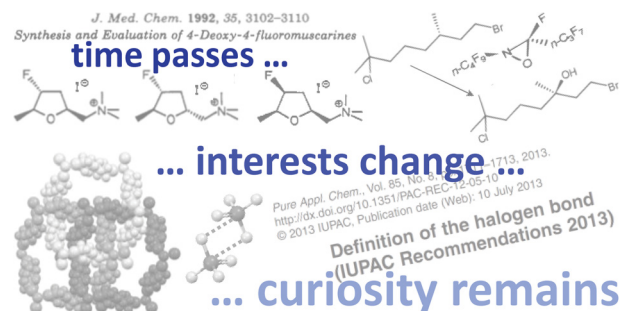
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From fluorine chemistry to noncovalent interactions: celebrating Prof. Giuseppe Resnati

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

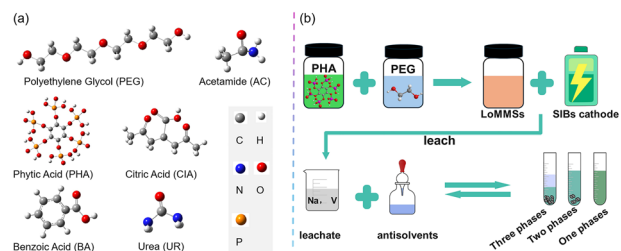


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Yu Chen,* Yaxue Shen, Zhuojia Shi, Zhenghui Liu, Yanlong Wang, Qi Liu and Zheng Li



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Fundamental questions
Elemental answers

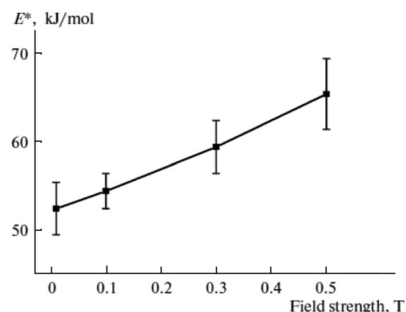


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Influence of an external magnetic field on gas–solid reactions

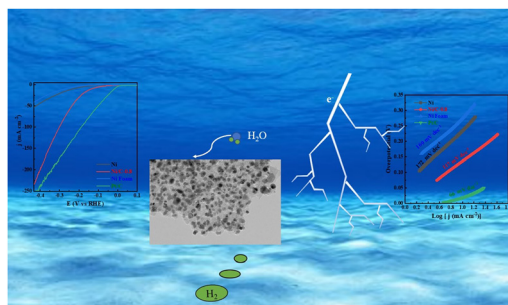
P. A. Chernavskii,* G. V. Pankina, B. S. Lunin and N. S. Perov*



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

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

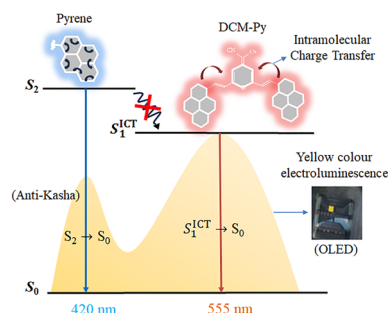


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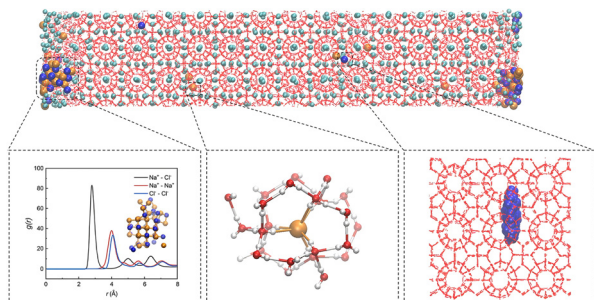
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Investigating unusual photoluminescence from the excited state in a DCM derivative and its application in lighting devices

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



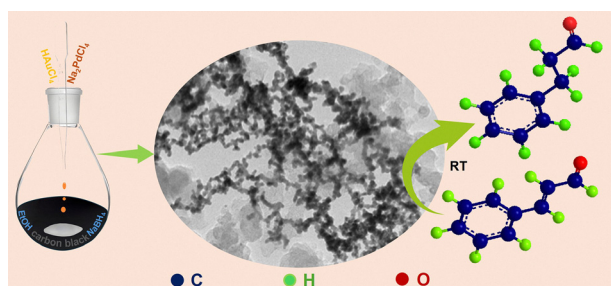
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Molecular dynamics simulation study on the growth of CO₂ hydrate from high-concentration NaCl solutions

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

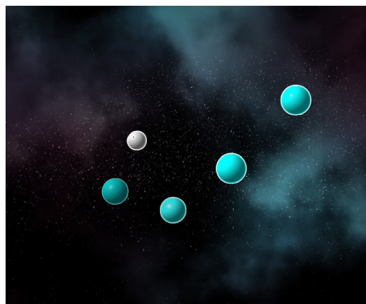
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Facile synthesis of carbon-supported PdAu nanonetworks for cinnamaldehyde hydrogenation

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

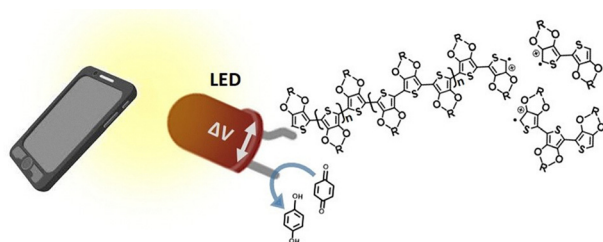
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Alvaro Muñoz-Castro

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

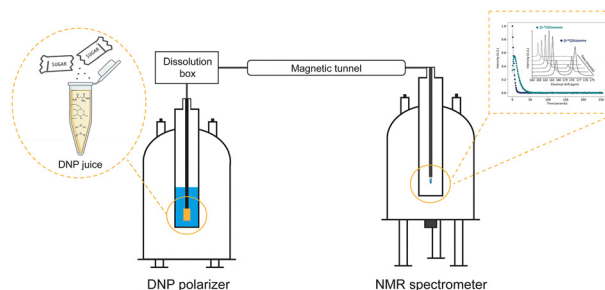


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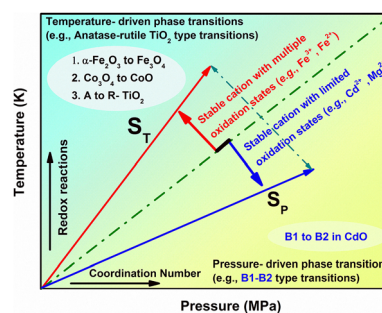
Léa Gutierrez, Karen Dos Santos, Mehdi Soussi-Therond, Aiky Razanahoera, Daniel Abergel, Nicolas Giraud* and Mathieu Baudin*



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

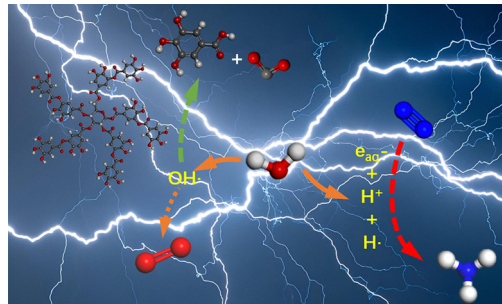
Sivakumar Aswathappa, Lidong Dai* and Sahaya Jude Dhas Sathiyadhas



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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*

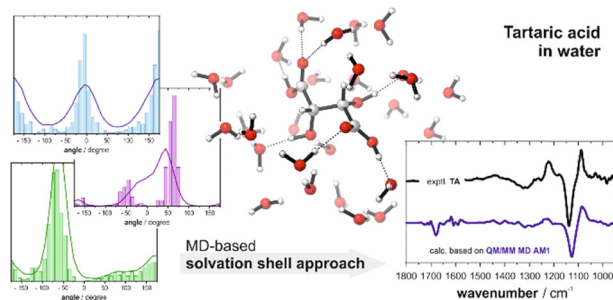


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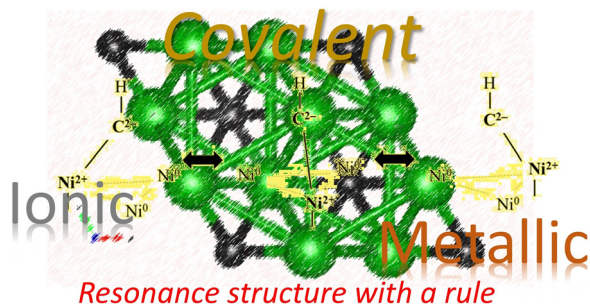
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Vibrational circular dichroism of tartaric acid in water

Deborah A. Drost and Christian Merten*



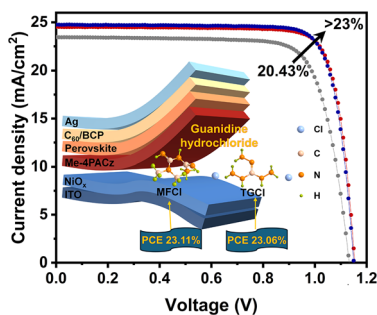
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Toward a deeper understanding of H–Ni₃C interactions: rule-based insights

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

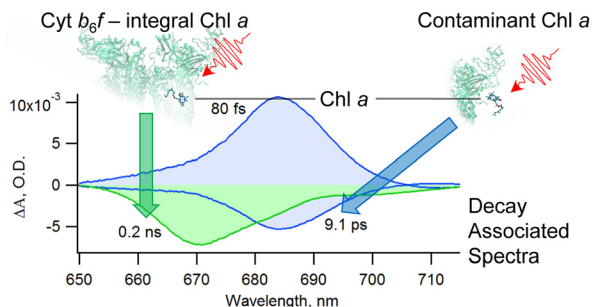
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Internal bridging engineering of NiO_x/Me-4PACz via selective guanidine-based hydrochlorides for efficient and stable inverted perovskite solar cells

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

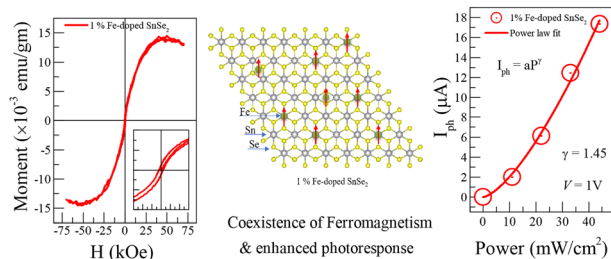
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Adrien A. P. Chauvet,* Rachna Agarwal and William A. Cramer

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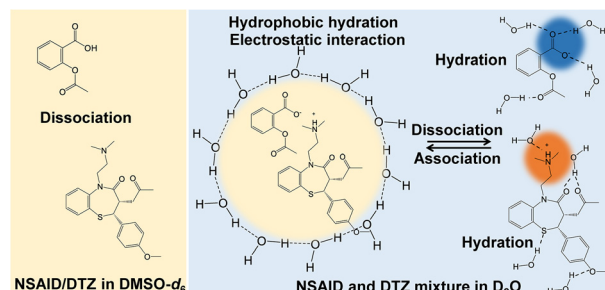
Aarti Lakhara and P. A. Bhohe*



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

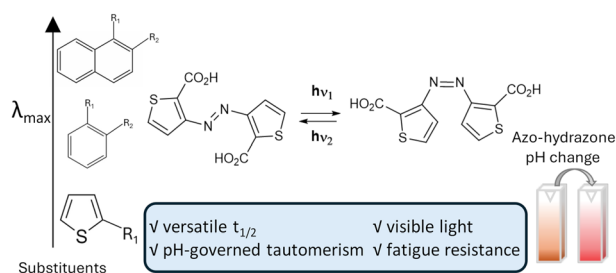
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Azothiophene-based molecular switches: influence of substituent position and solvent environment on photophysical behavior

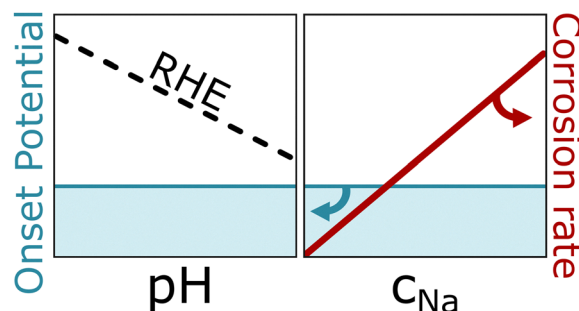
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Disentangling effects of pH, potential, and cation concentration in cathodic corrosion of platinum

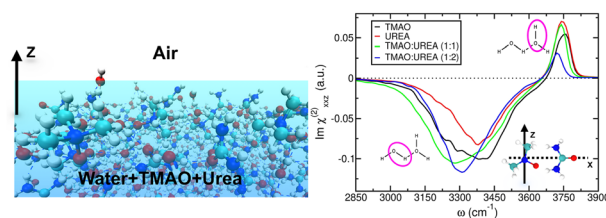
Mark Aarts,* Jamie A. Trindell and Marc T. M. Koper*



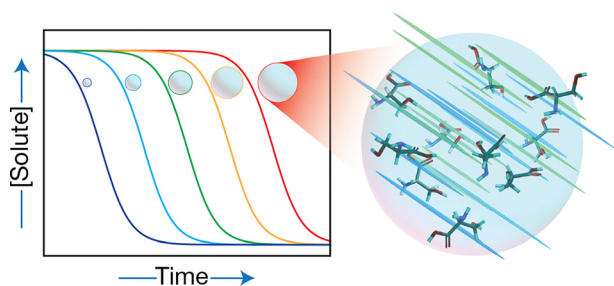
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Effects of trimethylamine N-oxide and urea on the structure of water at liquid–vapor interfaces studied through theoretical vibrational sum frequency generation spectroscopy

Anjali Negi, Ravi Malik* and Amalendu Chandra*



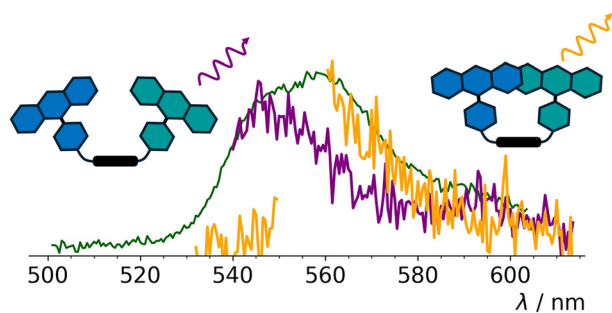
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Photochemical transformation of weakly absorbing organics by visible light in microdroplets

Alexander Logozzo and Thomas C. Preston*

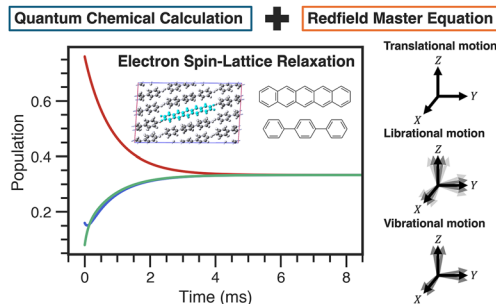
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Freezing out structural effects: strong dye–dye couplings in gaseous rhodamine dimers at cryogenic temperatures

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

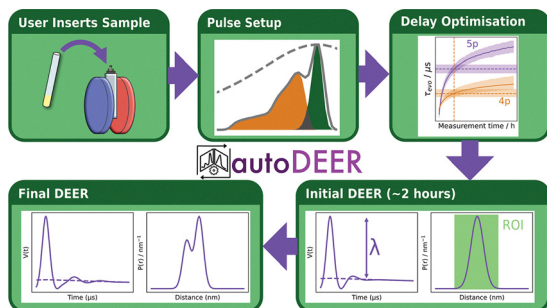
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Katsuki Miyokawa* and Yuki Kurashige*

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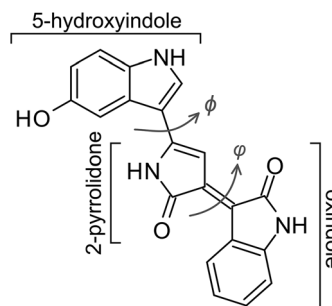
Hugo Karas, Sergei Kuzin, Stefan Stoll and Gunnar Jeschke*



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

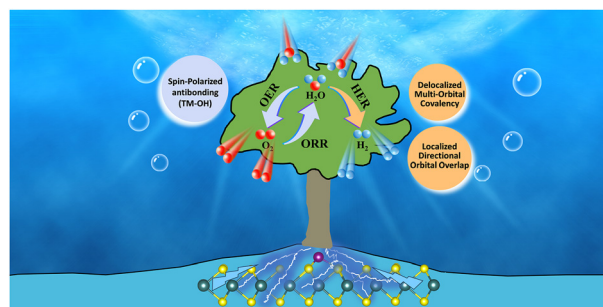
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Orbital-level insights into multifunctional electrocatalysis of transition-metal single atoms anchored on WS₂ monolayers

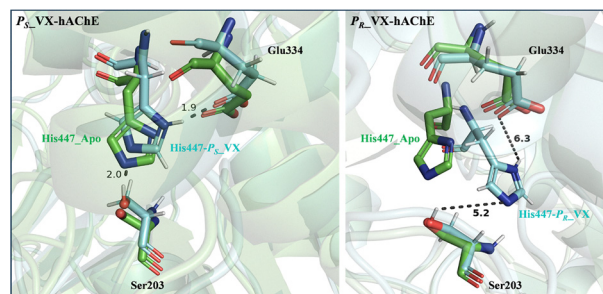
Bingling He, Mingyang Ren, Qianyi Bu, Liying Zhang, Song Ye, Mengyin Liu, Peng Lv,* Zhixue Tian* and Yu Jia*



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

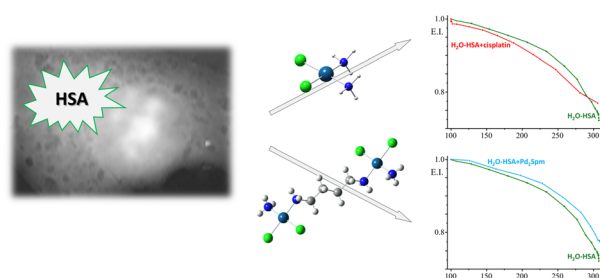
Dipankar Das, Shibaji Ghosh, Kalyanashis Jana and Bishwajit Ganguly*



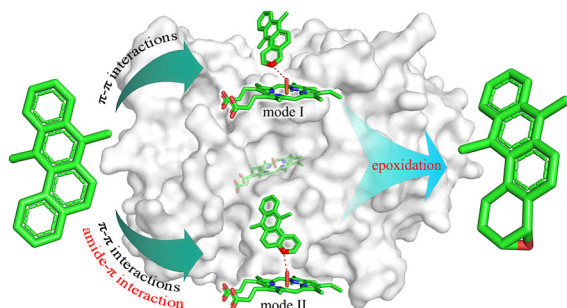
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Probing drug pharmacokinetics using neutron scattering techniques

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



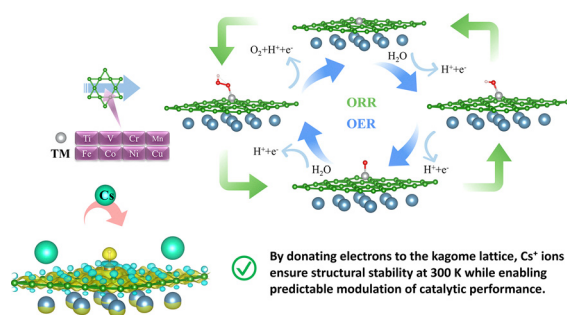
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Origin of the metabolic site selectivity of 7,12-dimethylbenz[a]anthracene catalysed by the P450 1B1 cytochrome: an *in silico* protocol

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

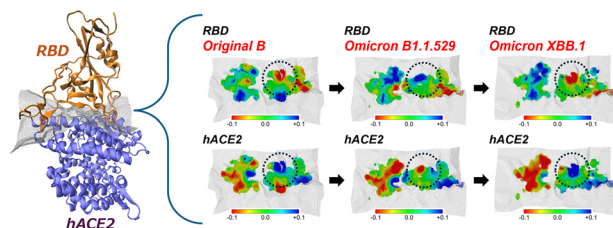
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Cesium-anchored MB₃ (M = Be, Ca, Sr) kagome monolayers: stabilizing active sites for bifunctional oxygen electrocatalysis

Yaowen Long and Hong Zhang*

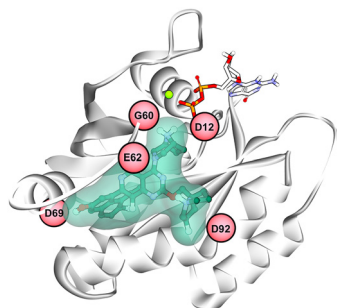
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Visualization of interfacial electrostatic complementarity reveals evolutionary changes in SARS-CoV-2 RBD–hACE2 interactions

Yosuke Muroya, Hiroki Ozono and Takeshi Ishikawa*

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

Donghwan Kim, Eunho Lee and Sangbae Lee*

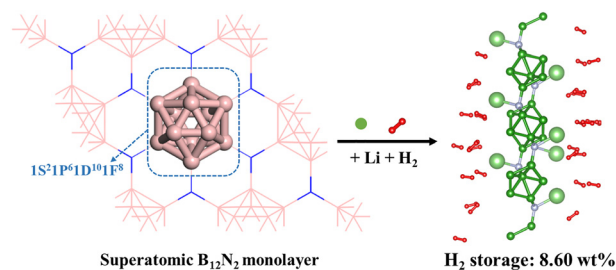


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A first-principles study of hydrogen storage on pristine and Li-decorated superatomic B₁₂N₂ monolayers

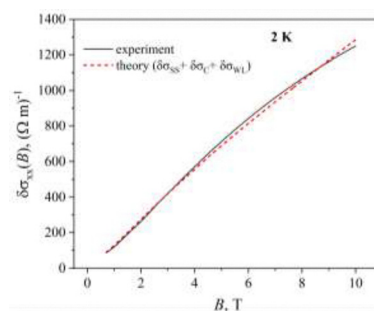
Qinqin Yuan, Zicheng Ling, Zaijun Gui, Lili Shi, Dan Li* and Longjiu Cheng*



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

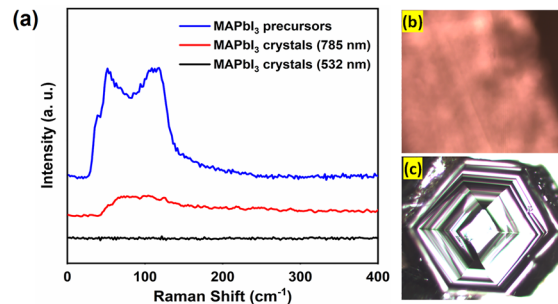
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Spectroscopic investigation of the solvated MAPbI₃ transition to perovskite crystals: a temperature-dependent Raman study

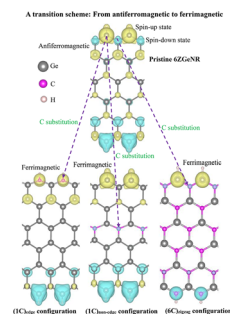
Abdul Zeeshan Khan, Muhammad Shafi, Tarek. A. Kandiel* and Abdulaziz A. Al-Saadi*



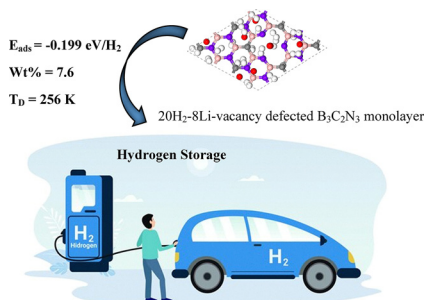
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Unlocking feature-rich properties of carbon-substituted germanene nanoribbons

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



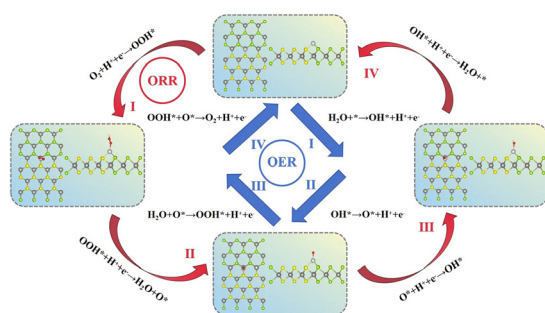
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B₃C₂N₃ monolayer with vacancy defects decorated with lithium as a potential hydrogen storage system: a DFT study

Rezvan Rahimi,* Mohammad Solimannejad* and Yafei Zhang

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Single transition metal atoms anchored on WSe₂/WS₂ 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*

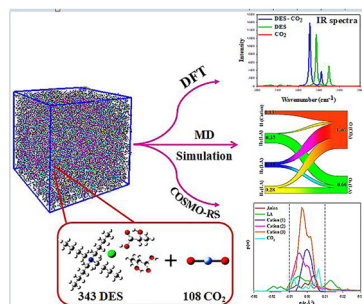
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A new step in understanding the process of the lithium battery manufacturing process: analysis of the CH₃CN-PF₅ species in matrices at cryogenic temperatures

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

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Ammonium-based deep eutectic solvents for sustainable CO₂ capture: insights from DFT, COSMO-RS, and MD simulations

Zahra Ostadsharif Memar and Majid Moosavi*

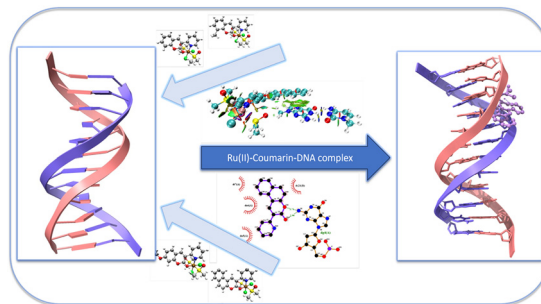


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Computational insights into Ru(II)–coumarin complexes as potential anticancer agents: a DFT, QTAIM, NCI-RDG, molecular docking and molecular dynamics approach

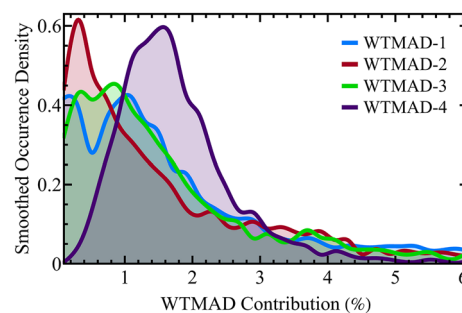
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WTMAD-4: a fair weighting scheme for GMTKN55

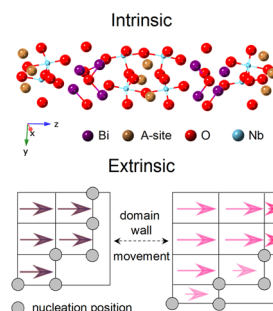
Kyle R. Bryenton and Erin R. Johnson*



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Deciphering the potential piezoelectricity optimization mechanism in Aurivillius compounds

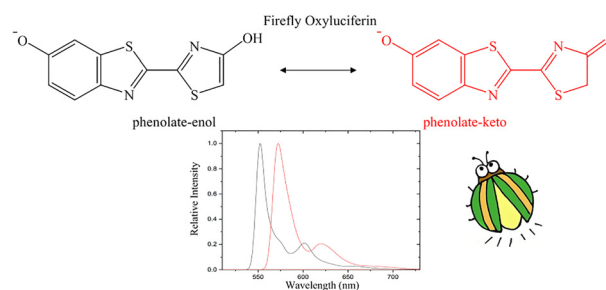
Shangyi Guan, Xiaojun Wu, Lanji Wen, Liang Kong, Zhi Tan,* Hiroko Yokota* and Qiang Chen*



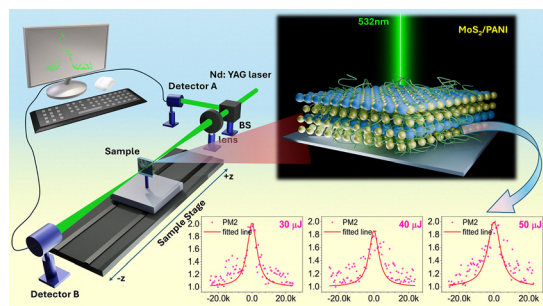
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Combined influence of the QM methods, active space size, Franck–Condon approximation, Herzberg–Teller effect and Duschinsky effect on vibrationally resolved electronic spectra: insights from firefly oxyluciferin

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



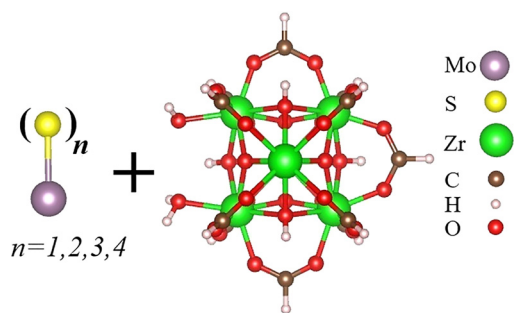
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Polarons and Pauli-blocking enhanced saturable absorption in MoS₂ nanorod/PANI nanocomposite films

Anjali Sharma and B. Karthikeyan*

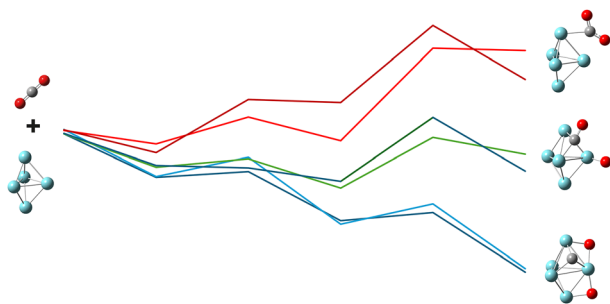
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Hydrogenation of ethylene over molybdenum-sulfur complexes supported on UiO-66

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

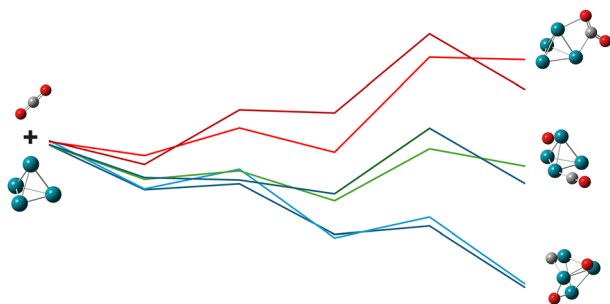
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Associative vs. dissociative binding of CO₂ on M₅ transition metal clusters

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 CO₂ on M₄ transition metal clusters

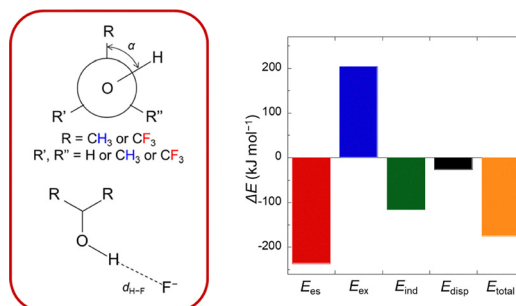
Sherfi Sherif, Bala Aakash Velmurugan, Naeem Abbas, Muskanbanu Shaikh and Matthew A. Addicoat*



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

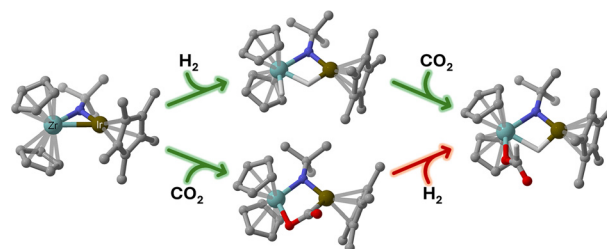
Nozomi Yoneda, Kohei Tada, Seiji Tsuzuki and Kazuhiko Matsumoto*



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Mechanism, selectivity, and what prevents closure of the catalytic cycle for H₂ reduction of CO₂ promoted by a heterodinuclear zirconium–iridium complex

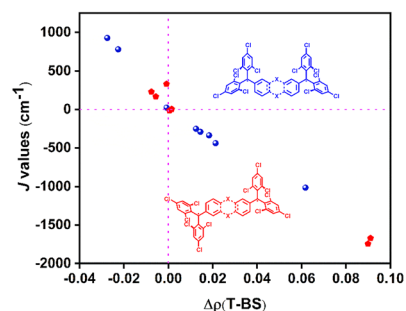
Kevin P. Quirion and Daniel H. Ess*



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

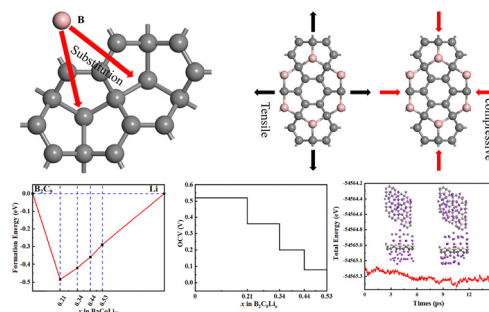
Li Shen,* Rui Dong, Jia-nan Lang, Yihan Li, Yue Li, Jitao Lu, Qian Wu and Qingguo Meng*



1565

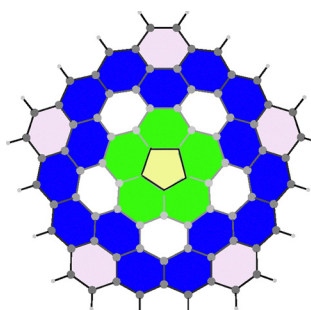
B₂C₉ as a high-performance Li-ion battery anode: effects of boron-incorporation and strain-engineering on the adsorption and diffusion of lithium

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



RESEARCH PAPERS

1573

Carboncane[1,3] ($C_{80}H_{20}$)

25 Clar structures with 9 sextets each

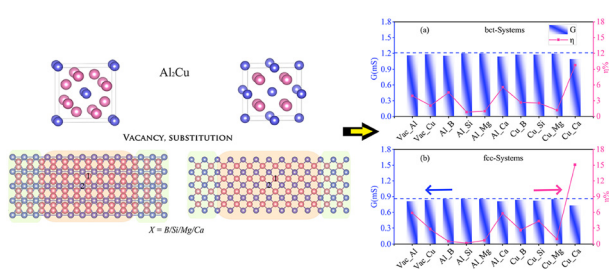
Sextets can be located only in green (6 times) and blue (7 times) rings

A sextet is never found in empty rings

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

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

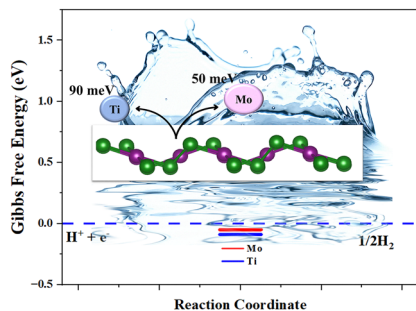
1586



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

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

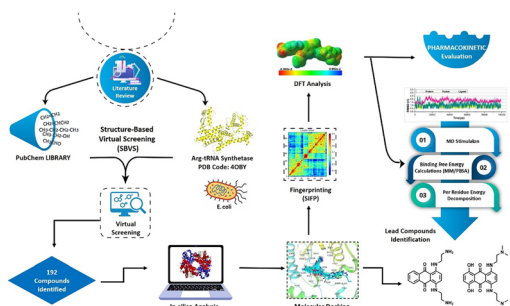
1594



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*

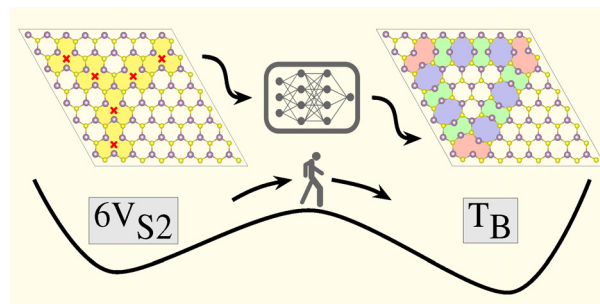


RESEARCH PAPERS

1626

Completing the hierarchy of rotational defects in monolayer MoS₂ through symmetry-aware evolutionary search

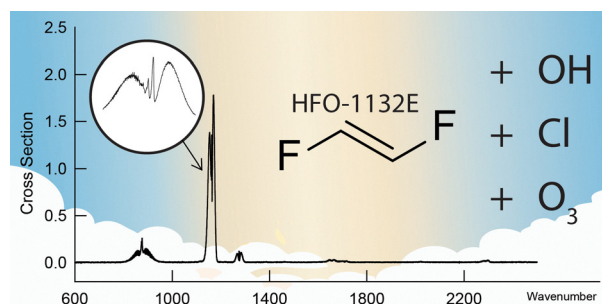
Alexander Adel, Ralf Wanzenböck and Georg K. H. Madsen*



1634

Atmospheric chemistry of (*E*)-1,2-difluoroethene: kinetics and mechanisms of the reactions with Cl atoms, OH radicals and O₃

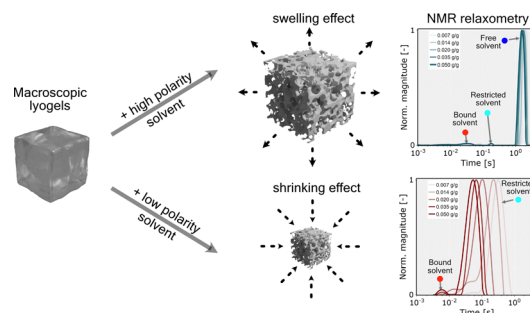
Mads. P. Sulbaek Andersen,* Ellen R. Kjaergaard, Connor Blair and Ole J. Nielsen



1645

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

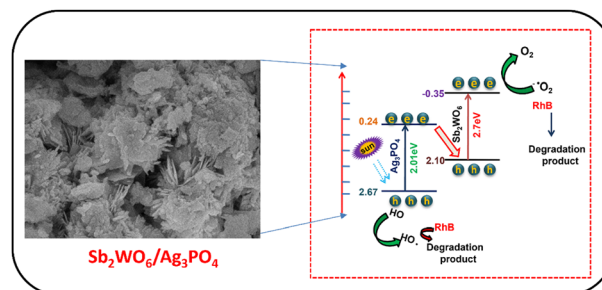
Muhammad Adrian,* Kathrin Marina Eckert, M. Raquel Serial, Artyom Tsanda, Lukas Rennpferdt, Stefan Benders, Hoc Khiem Trieu, Tobias Knopp, Irina Smirnova and Alexander Penn



1655

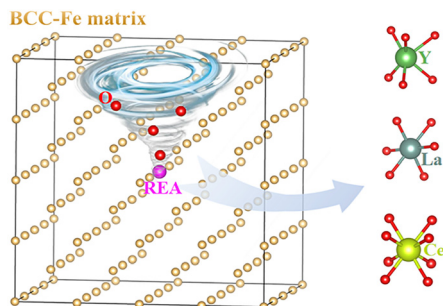
Development of a novel direct Z-scheme Sb₂WO₆/Ag₃PO₄ nanocomposite with sustainable design for simultaneous electrochemical detection of Pb²⁺ and photocatalytic degradation of RhB dye

Nadi Mlihan Alresheedi



RESEARCH PAPERS

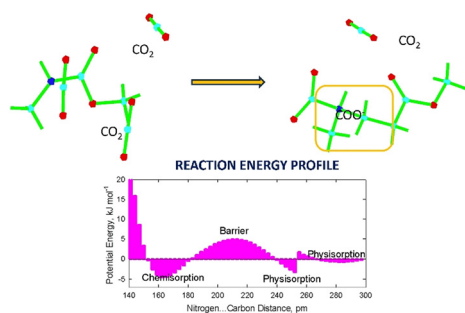
1671



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*

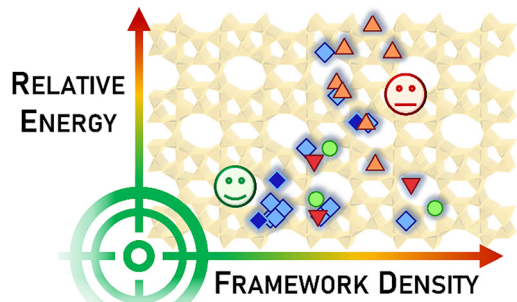
1681



Investigation of a novel urethane-inspired CO₂ chemisorbent: structure modifications and activation barriers

Vitaly V. Chaban

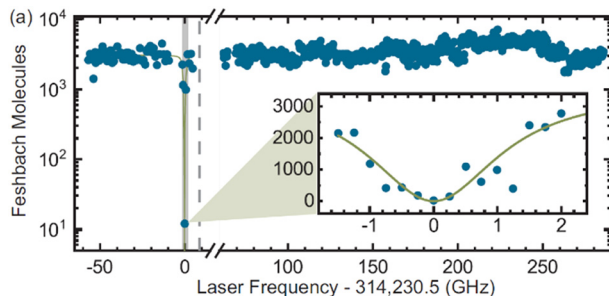
1692



Balancing accuracy and efficiency in density functional theory studies of SiO₂ polymorphs

Michael Fischer

1705



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

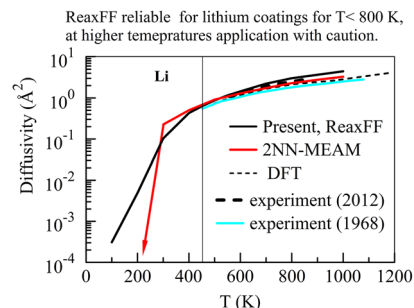
Anbang Yang, Xiaoyu Nie, Hao Lin Yu, Yiming Liu, Victor Avalos, Canming He, Jacek Kłos, Svetlana Kotochigova and Kai Dieckmann*



1712

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

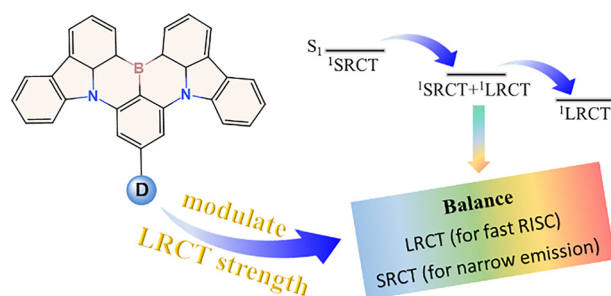
P. S. Krstic,* S. Dwivedi, A. C. T. van Duin and B. E. Koel



1720

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

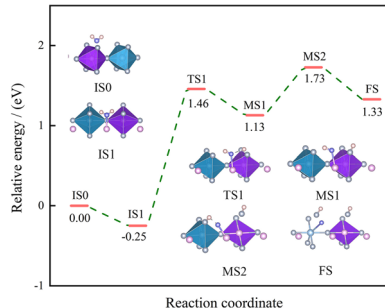
Zhu Chang, Rajat Walia, Dandan Zhang, Xian-Kai Chen and Jiaqi Li*



1730

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

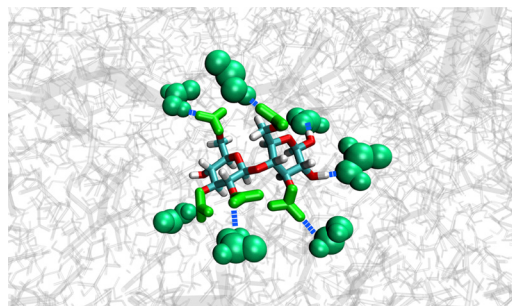
Jian Zhang* and Shuangtao Pan



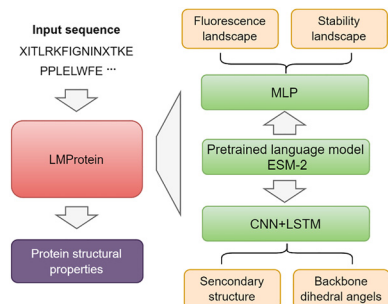
1739

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*



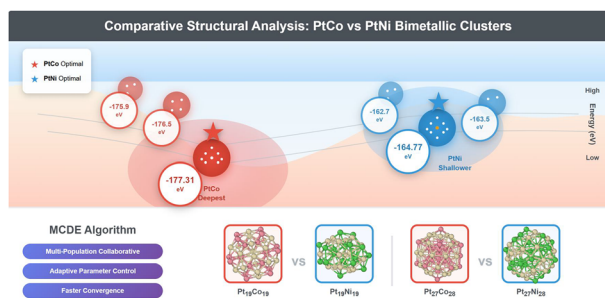
1747



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

Yongna Yuan,* Hui Luo and Yaojie Tian

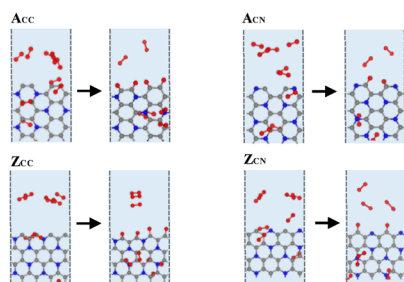
1759



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

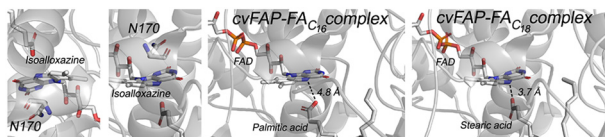
1770

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

Phase diagram and dynamics of the edge oxidation of C₃N monolayers in O₂ 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

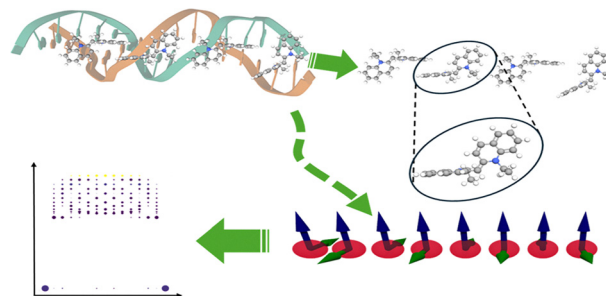
Min-Shih Su and Ya-Ting Kao*



1792

Enhancing energy transport utilising permanent molecular dipoles

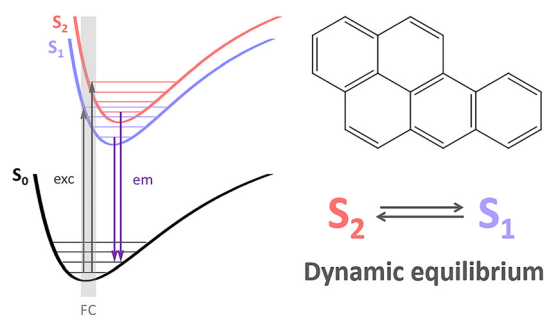
Adam Burgess* and Erik M. Gauger



1806

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

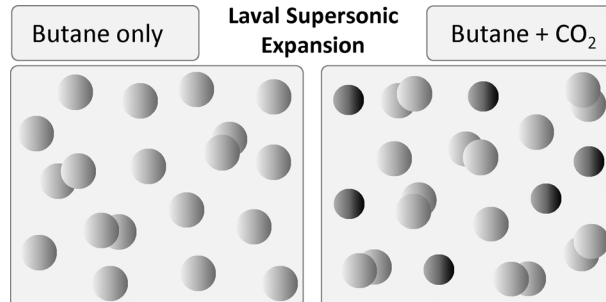
Nikita A. Shekhovtsov* and Mark B. Bushuev*



1820

Acceleration of butane vapor nucleation by carbon dioxide gas

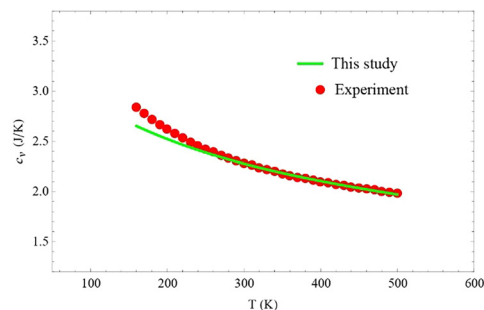
Arnab Choudhury, Felix Graber, Stefan Feusi, Jan Krohn, Jai Khatri, Fernando Torres Hernandez, Chenxi Li and Ruth Signorell*



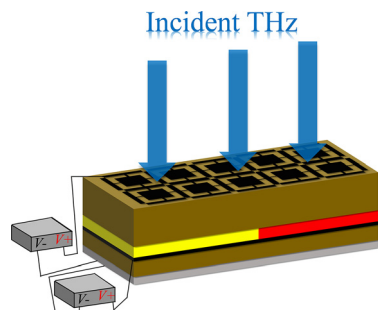
1829

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



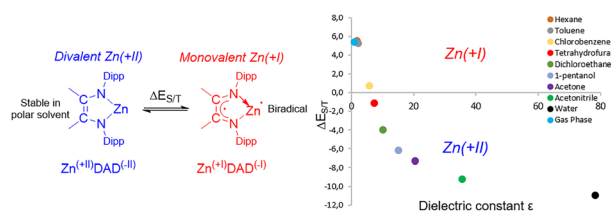
1835



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*

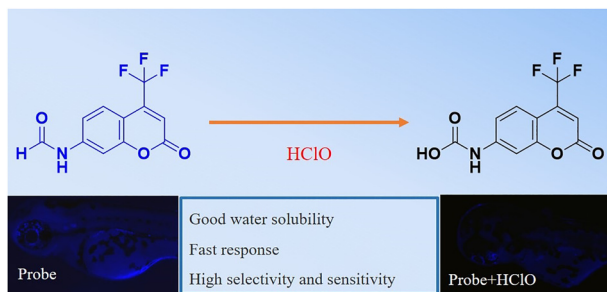
1845



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, H  l  ne G  rard, Fabrice Chemla and St  phanie Halbert*

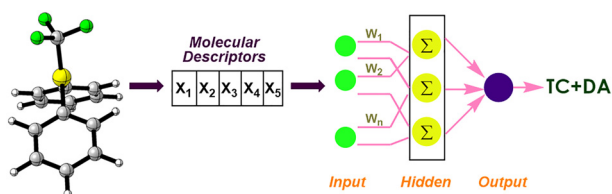
1853



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

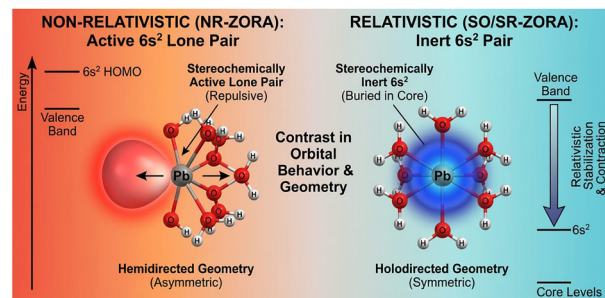
Vaneet Saini* and Shivansh Kanwar



1877

Coordination of lead(II) in solvated clusters with water $[\text{Pb}(\text{H}_2\text{O})_{1-8}]^{2+}$: insights from relativistic effects, energy analysis, molecular orbitals, and electron density

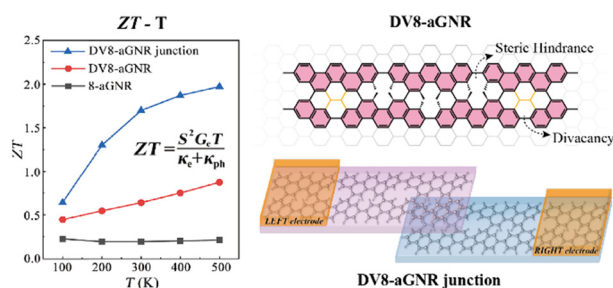
Andy D. Zapata-Escobar,* Franklin Ferraro, Edison Flórez and Alejandro F. Maldonado*



1892

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

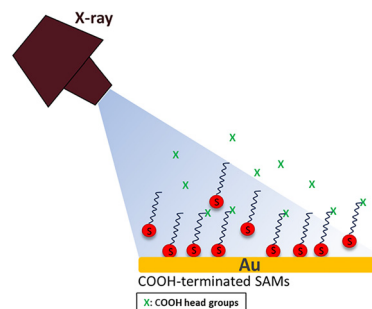
Jianing Wang, Jie Meng, Weiyi Wang* and Qunxiang Li*



1901

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

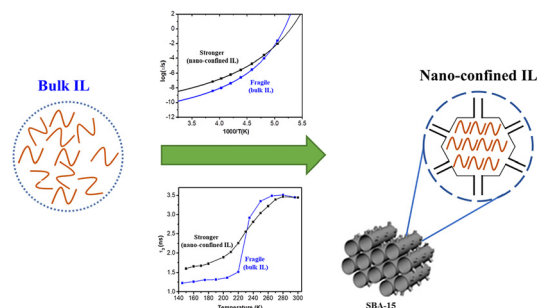
Ahlam R. M. Alharbi, Ingo Köper and Gunther G. Andersson*



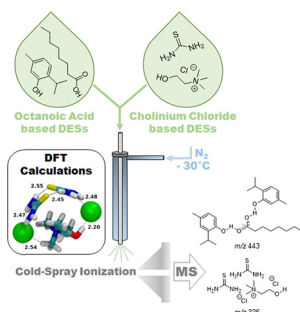
1911

Reduction in liquid fragility and enhancement in ionic conductivity in the glassy phase of $[\text{Bmlm}][\text{NTf}_2]$ ionic liquid under nano-confinement: PALS and BDS investigations

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



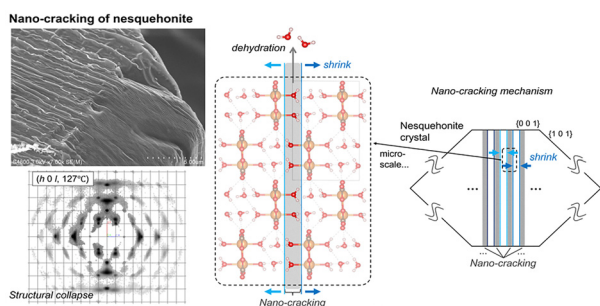
1924



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 Delhay, Rachel Schurhammer, Alain Chaumont, Emmanuelle Limanton, Béatrice Legouin, Ludovic Paquin, Xavier Castel, Mohammed Himdi and David Rondeau*

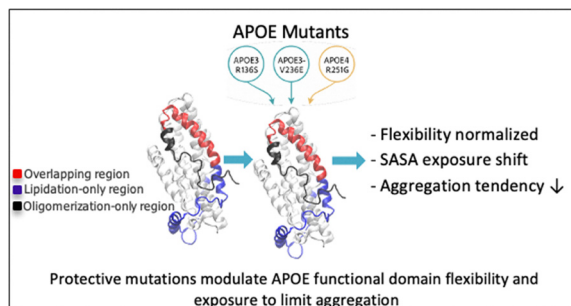
1939



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

Ryo Yamane,* Hiroshi Sakuma and Kenji Tamura

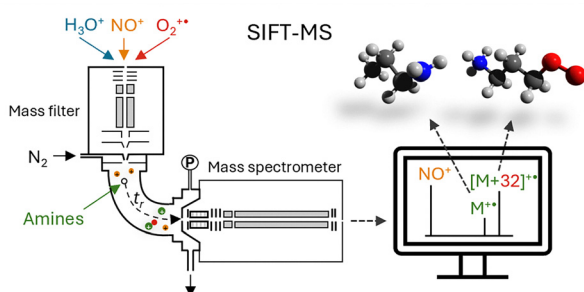
1947



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

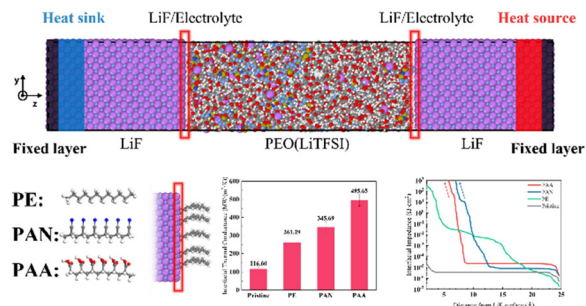


RESEARCH PAPERS

1976

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

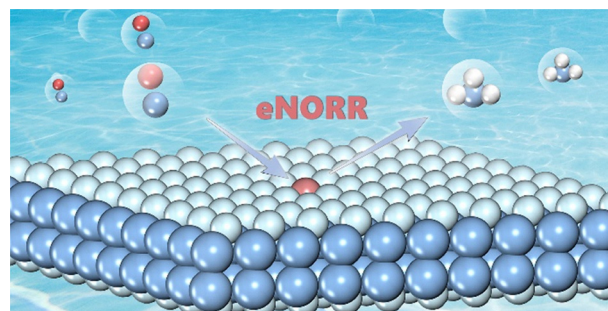
Kang Yi and Dongwei Xu*



1985

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

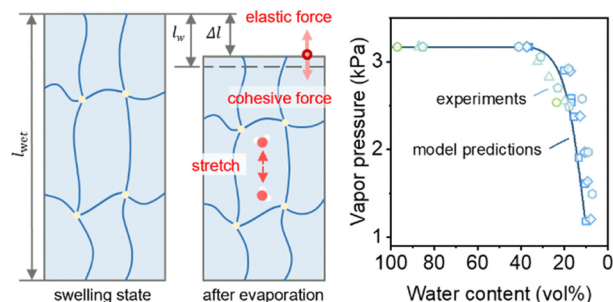
Yongxu Fu, Hu Li, Qingbo Kang, Jiangke Li, Minghui Wu, Lei Liu, Xiaobing Yan, Weichao Wang and Linxia Wang*



1994

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

Zehua Yu, Yongshun Ren and Kang Liu*

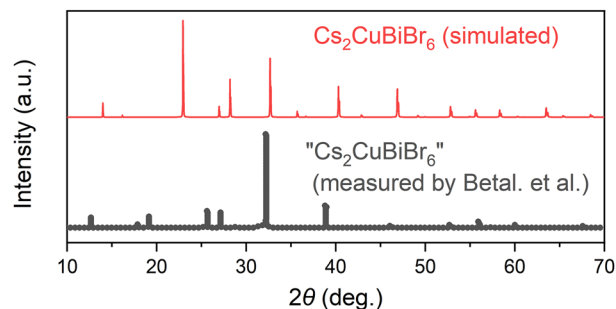


COMMENTS

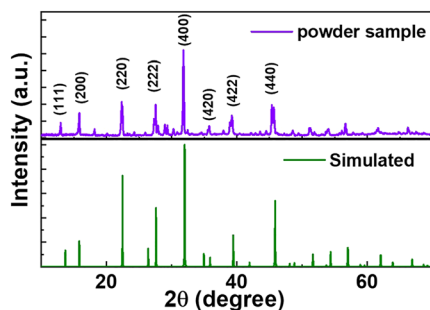
2003

Comment on "Air-stable double halide perovskite $\text{Cs}_2\text{CuBiBr}_6$: 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 Cs₂CuBiBr₆: 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*

