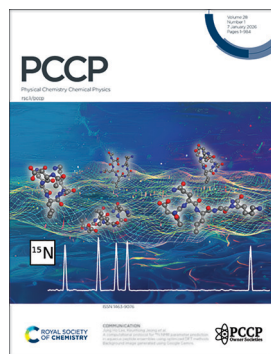


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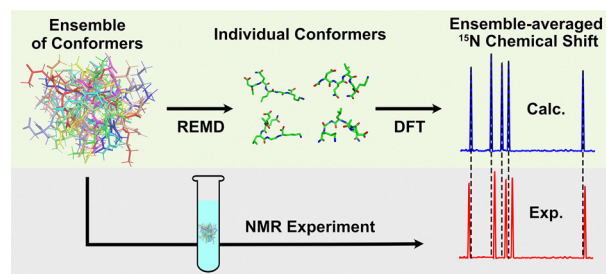
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COMMUNICATIONS

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Minji Kim, Jung Ho Lee* and Keunhong Jeong*

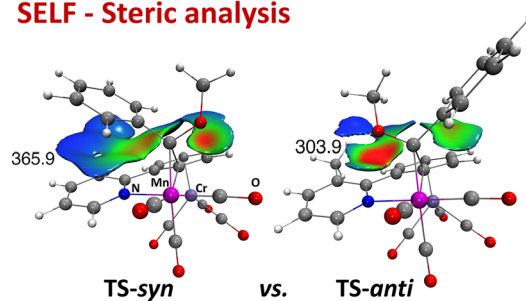


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Sara Figueirêdo de Alcântara Morais, Yann Cornaton, Eric Hénon* and Jean-Pierre Djukic*

SELF - Steric analysis



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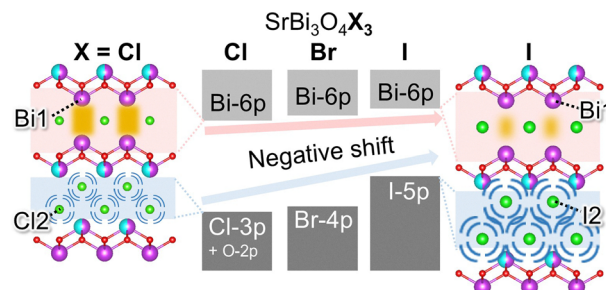
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COMMUNICATIONS

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Dual halogen layers diversify band engineering in Sillén oxyhalide photocatalysts: electronic structure control of $\text{SrBi}_3\text{O}_4\text{X}_3$ ($\text{X} = \text{Cl}, \text{Br}, \text{I}$) via halogen substitution

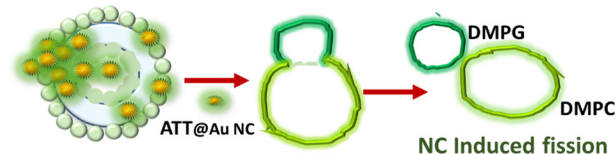
Yusuke Ishii, Hajime Suzuki,* Osamu Tomita, Akinobu Nakada and Ryu Abe*



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Impact of ligand-protected gold nanoclusters on liposomal morphology: fission to semi-gel formation in aqueous medium

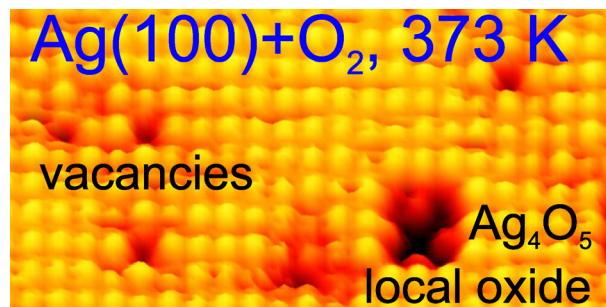
Mallika Mukherjee, Asmita Das and Pradipta Purkayastha*



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Initial stage of O_2 adsorption on $\text{Ag}(100)$: vacancies and local oxide formation

B. V. Andryushechkin,* T. V. Pavlova, V. M. Shevlyuga, A. V. Nartova and V. I. Bukhtiyarov

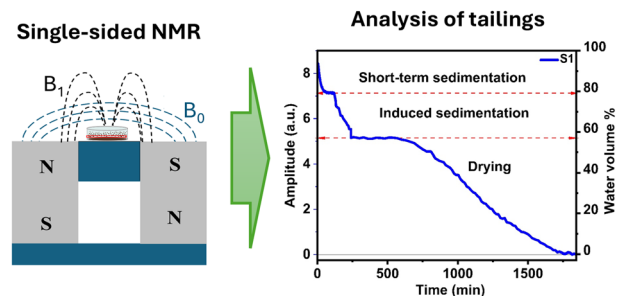


RESEARCH PAPERS

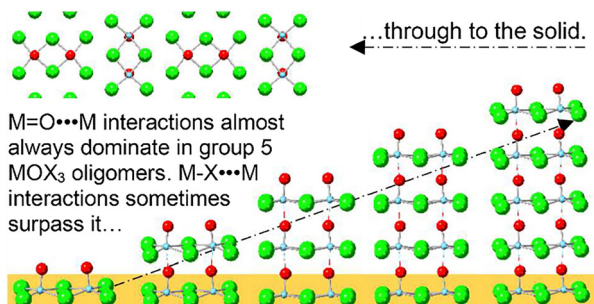
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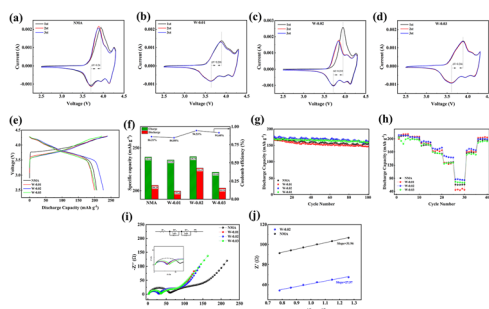
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Sigma-hole-supported interactions in complexes of group 5 oxyhalides (MOX₃) with insights for their extended solids

Donovan Hoilette Jr., Gabriel F. Stewart and Kelling J. Donald*

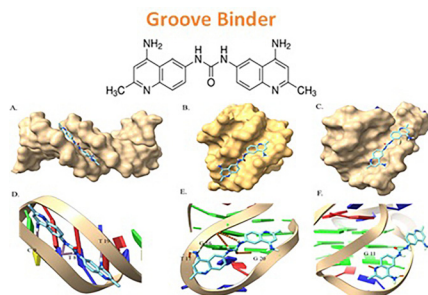
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W-incorporated high-performance layered cathode materials for advanced lithium-ion batteries

Xiaoyi Hou,* Haozhe Wu, Qirongxin Shen, Dengdeng Ai and Xi Wu

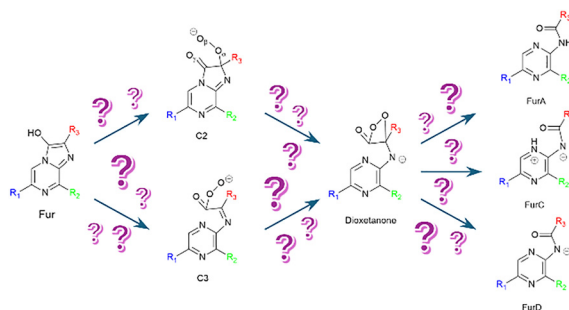
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Insights on the binding and selectivity of surfen towards different DNA topologies

Laxmi Kashyap, Kritika Varshney and Manoj Munde*

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Toward a mechanistic understanding of bioluminescence: a theoretical study of furimazine oxidation and luminescence

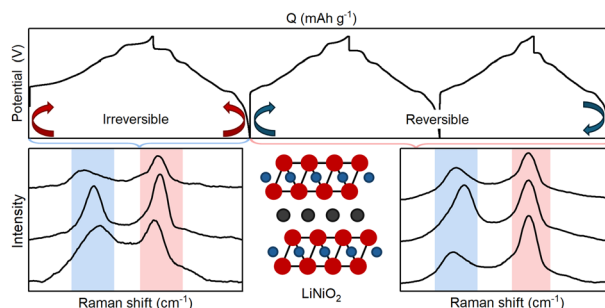
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Multicycle *operando* Raman spectroscopy reveals reversible and irreversible transitions in LiNiO₂ electrodes

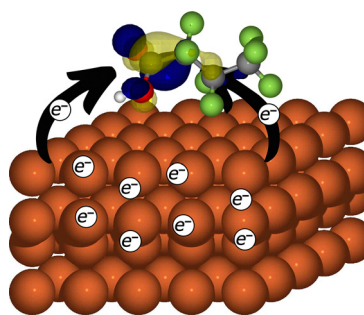
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Exploring the initial bond activations of PFAS on zero-valent iron

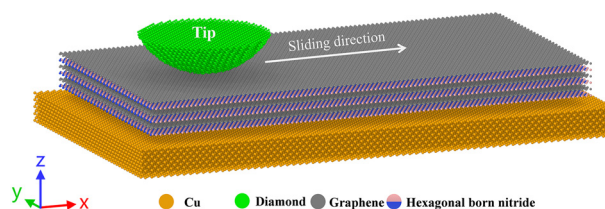
Glen R. Jenness,* Elizabeth R. Zengel and Manoj K. Shukla*



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Layer-dependent friction on the surface of alternately stacked graphene and h-BN

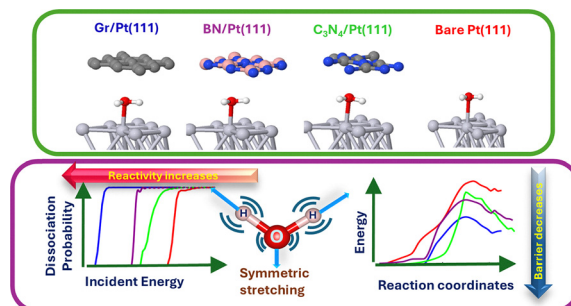
Hao Wang, Lu Chen, Yunxiao Wang, Yongteng Wei, Junqin Shi, Tengfei Cao and Xiaoli Fan*



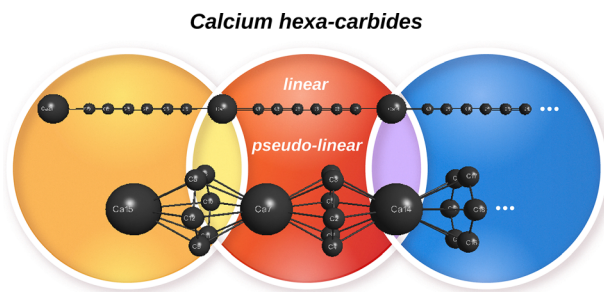
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Mode-selective H₂O dissociation on Pt(111) under two-dimensional confinement

Nidhi Tiwari, Sandip Ghosh and Ashwani K. Tiwari*



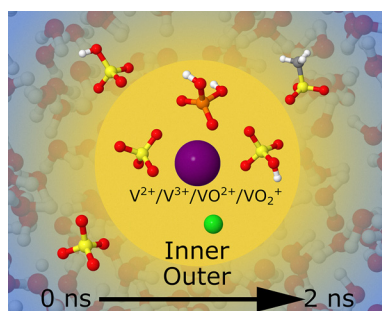
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Calcium carbides: can hexa-carbides grow unlimitedly? Theoretical perspectives and issues that oppose a definite answer

A. J. C. Varandas

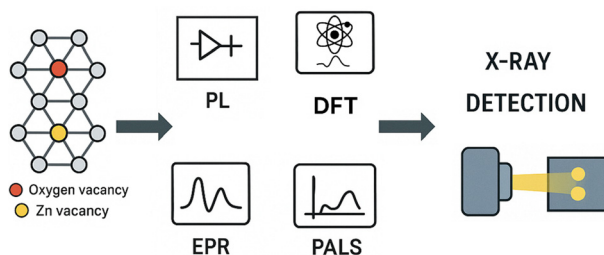
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Computational investigation of coordinating electrolytes with vanadium ions in redox flow batteries

Christopher S. Mills and Anna L. Garden*

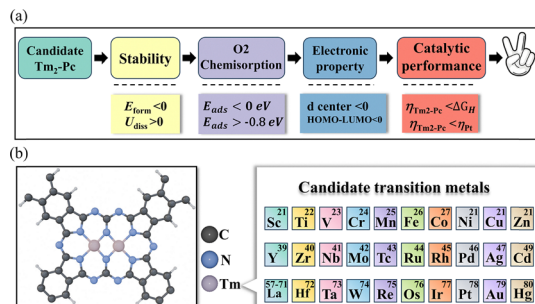
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Identification of defects in pure and Al/Ga-doped ZnO to improve X-ray detector performance: experimental and simulation methods

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Systematic screening of transition metal dual-atom-doped phthalocyanine electrocatalysts for the oxygen reduction reaction

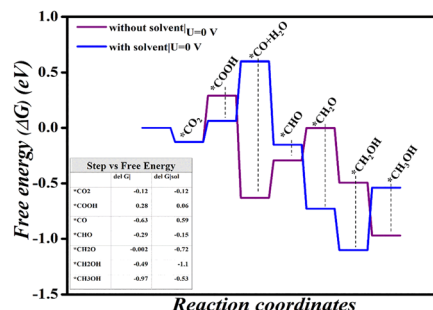
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Electrochemical CO₂ reduction to methanol over Ni@Ti₃CN MXene: a first-principles DFT study

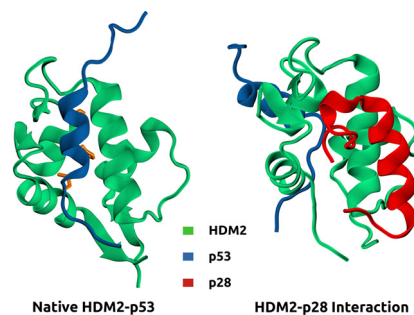
Karthiga Manivannan and Senthilkumar Lakshmiopathi*



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Azurin-based peptide p28 disrupts p53–HDM2 interactions: insights from *in silico* studies

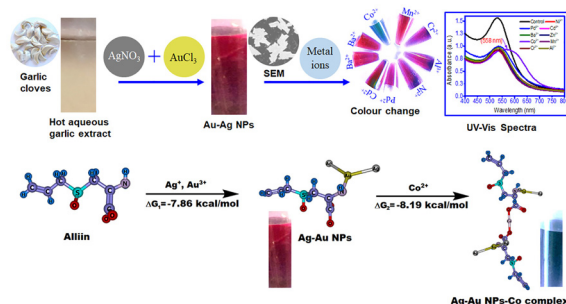
Albin Joy, Anand Srivastava and Rajib Biswas*



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Optimized colorimetric detection of cobalt ions (Co²⁺) using alliin–Ag–Au nanoparticles

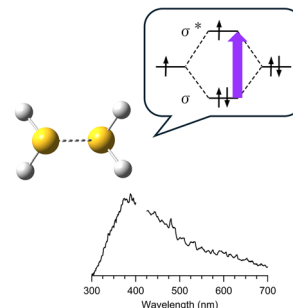
Rintumoni Paw, Kangkan Sarmah, Moushumi Hazarika, Ankur K. Guha and Chandan Tamuly*



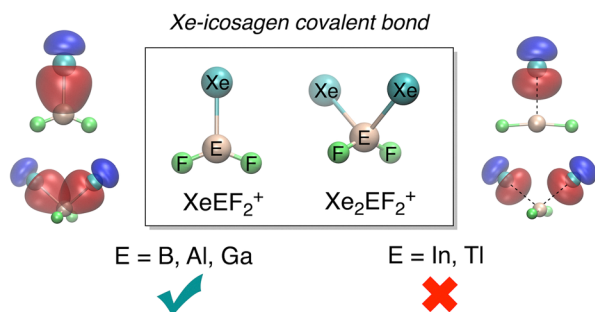
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Electronic spectra of (H₂S)_n⁺ (n = 2–6) and [(H₂S)₂–(H₂O)_m]⁺ (m = 1–2) in the gas phase

Mitsuaki Shioura, Mizuhiro Kominato and Asuka Fujii*



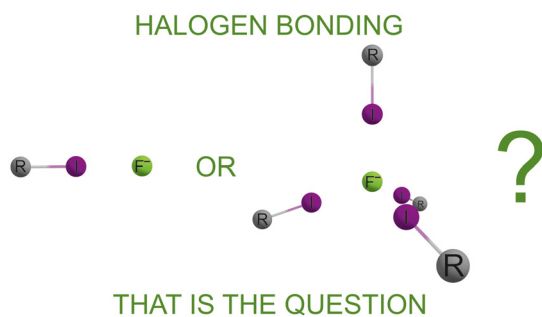
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Covalent bonding and extreme shielding in xenon–icosagen fluoride cations

Erick Cerpa,* Jose A. Guerrero-Cruz, Gabriel Merino, J. Oscar C. Jimenez-Halla and Abril C. Castro*

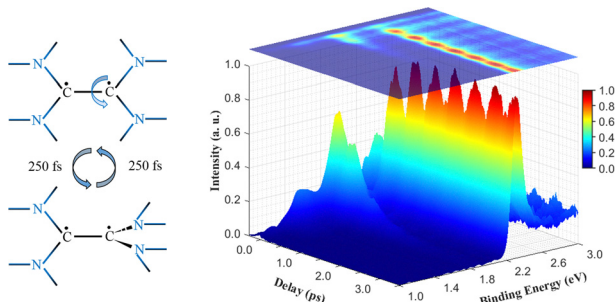
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Multidentate halogen bond acceptors: from fluorides to iodides. Anticooperativity in halogen-bonded clusters

Justyna Dominikowska*

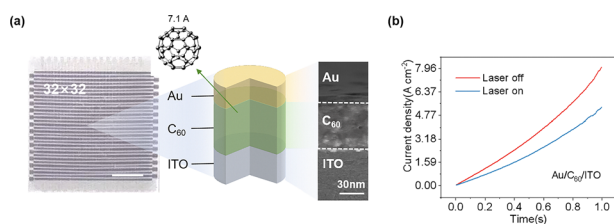
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A time-, angle- and kinetic-energy-resolved photoelectron spectroscopic study of tetrakis(dimethylamino)ethylene

Yuhuan Tian, Zhichao Chen, Wenping Wu, Likai Wang, Zhigang He, Dongyuan Yang,* Guorong Wu* and Xueming Yang

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Tunable negative photoconductance states in a C₆₀ device with optically induced trap center reconfiguration

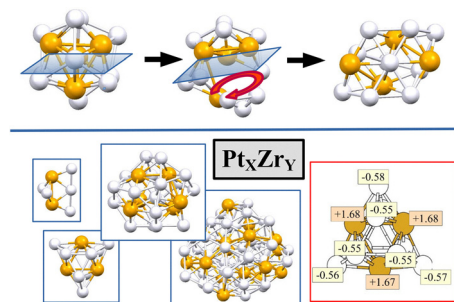
Xiude Yang, Jie Li,* Zhen Zhang, Xiuxia Wang, Zhonglin Chen, Ping Li, Bo Wu, Guangdong Zhou* and Jin Ye*



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Structural and chemical properties of Pt-rich Pt_xZr_y nanoalloys

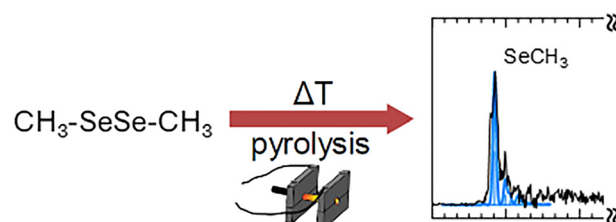
Luis M. Molina* and Julio A. Alonso



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Threshold photoelectron spectroscopy of small organo-selenium radicals

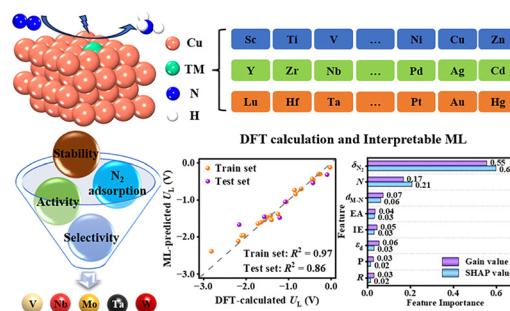
Emil Karaev, Dorothee Schaffner, Marius Gerlach, Sira Grätz, Patrick Hemberger and Ingo Fischer*



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Screening copper-based single-atom alloy catalysts for electrochemical nitrogen reduction

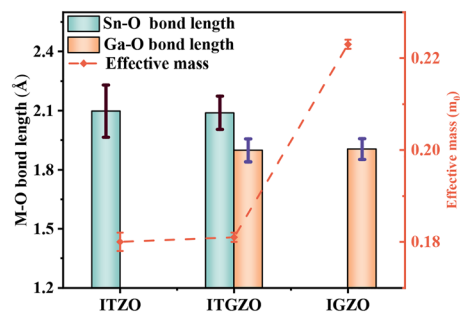
Hengzhi Liu and Yang-Gang Wang*



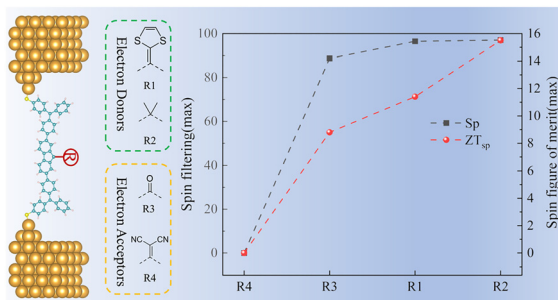
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Theoretical assessment of multi-doping strategies in amorphous indium oxide for synergistically enhancing carrier mobility and bias stability

Jiejun Pan, Zhibin Liu, Xionghui Tan, Kaixuan Chen, Pingqi Gao* and Can Han*



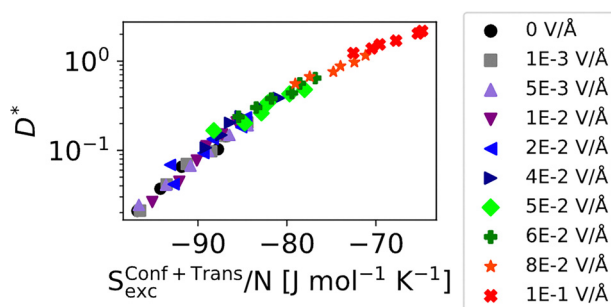
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Substituent-controlled quantum interference tuning of spin and thermoelectric transport in triphenylmethyl diradical junctions

Zhenhai Cui, Yongfeng Xiong, Qiuming Liu, Ziqiang Liu, Tong Chen and Lin Huang*

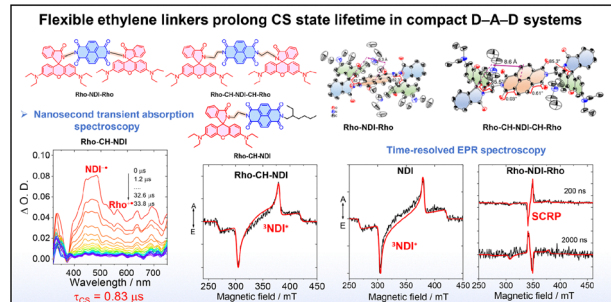
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Excess entropy scaling explains the enhanced dynamics of the ionic liquid 1-ethyl-3-methylimidazolium chloride in external electric fields

Fernando J. Carmona Esteva, Yong Zhang, Katerina Duncheskie, Edward J. Maginn* and Yamil J. Colón*

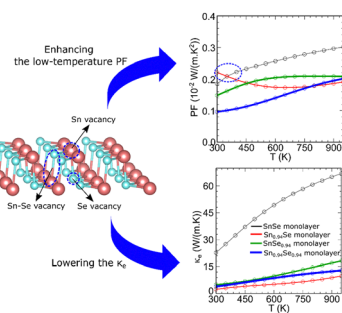
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Long-lived charge separated states in spiro-compact rhodamine-naphthalenediimide D-A-D systems: synthesis and time-resolved optical and electron paramagnetic resonance spectroscopic studies

Balamurugan Tharmalingam, Andrey A. Sukhanov, Yuying Pei, Greta Sambucari, Talita Ramos, Jianzhang Zhao,* Violeta K. Voronkova* and Mariangela Di Donato*

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Tailoring the electronic and thermoelectric properties of the SnSe monolayer via vacancy defects: insights from density functional theory

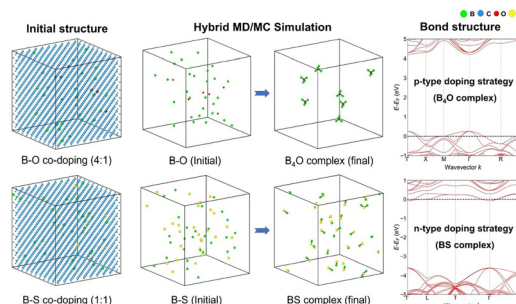
Erik Bhakti Yutomo,* Suci Faniandari and Muhammad Fahmi



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Atomistic simulation study of diamond doping based on machine learning potential

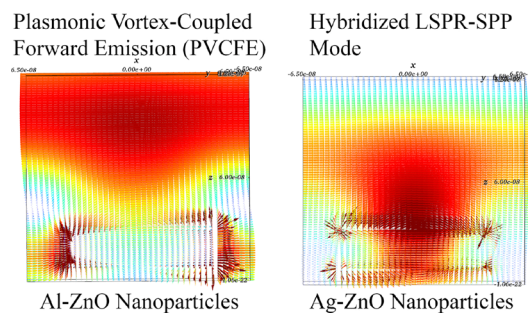
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Plasmonic vortex-coupled forward emission (PVCFE): a novel light coupling mechanism in aluminium nanostructures for high-efficiency, stable, and cost-effective organic photovoltaics

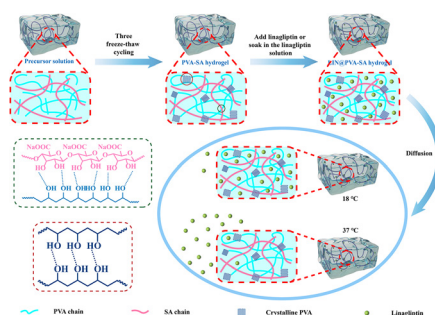
Mahdi Aghlmandi Sadigh Bagheri*



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Mechanically robust PVA/SA semi-IPN hydrogels for highly effective temperature-triggered linagliptin delivery

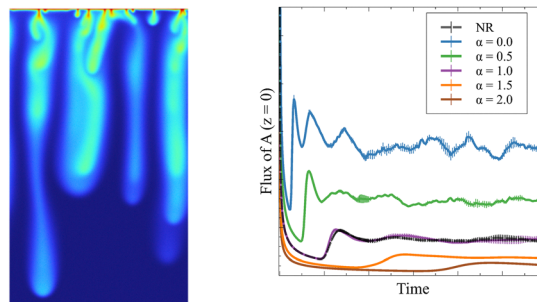
Yue Wang, Guineng Li, Yeying Li, Mutian Yao, Qiaobo Wang, Liang Peng* and Hua Gu*



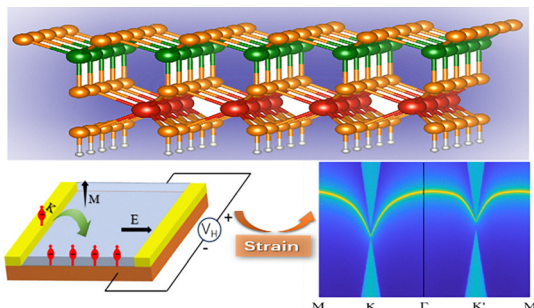
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Effect of variable solubility on reactive convective dissolution

S. Kabbadj, A. De Wit and L. Rongy*



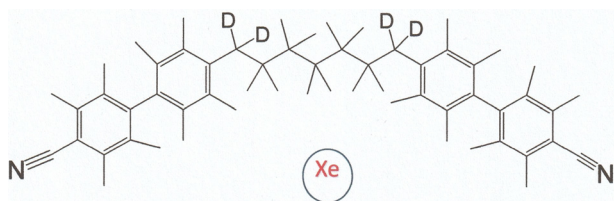
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Janus VAZ₃H (A = Si, Ge; Z = N, P) single layers exhibiting valley polarization, magnetic anisotropy, and topological transition

Yang Yang,* Yanyang Cao, Shao-Jie Zhang, Luogang Xie and Hongyan Lu

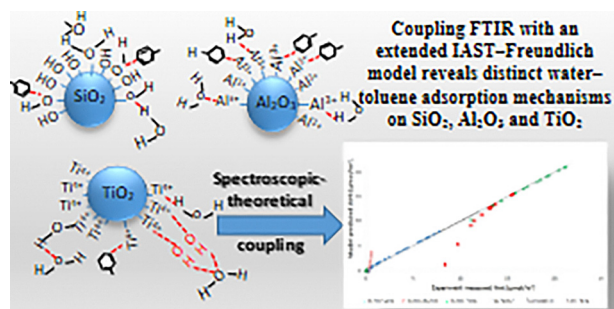
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Properties of CB7CB-D₄ as derived from ¹²⁹Xe and ²H NMR experiments and computations

Jukka Jokisaari* and Juha Vaara

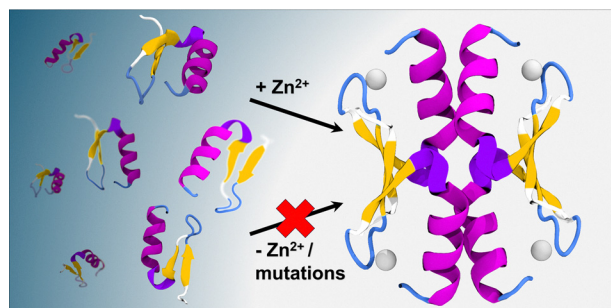
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Deciphering competitive water–toluene adsorption mechanisms on oxide surfaces

Mouna Wissem Guellit,* Abderrahim Choukchou-Braham, Chewki Ziani-Cherif and Sanâa El Korso

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Zinc-mediated multimerization of the N-terminal CCHC zinc finger domain of BCL11B: a key to stability and a potential therapeutic target

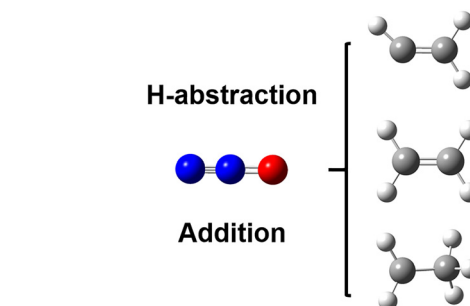
Anne Susemihl, Felix Nagel, Piotr Grabarczyk, Christian Andreas Schmidt and Mihaela Delcea*



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A theoretical study on the mechanism of C_2H_3-5 oxidation by N_2O

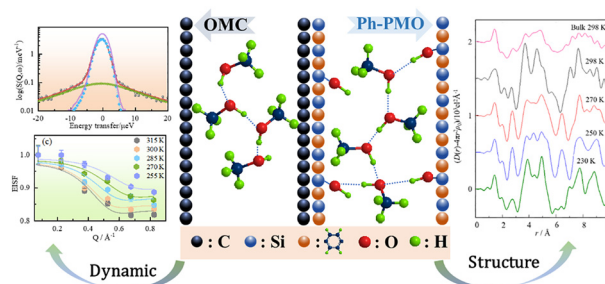
Huanhuan Wang, Long Qin, Bingzhi Liu, Shaohua Zhu, Zhandong Wang and Ran Sui*



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An X-ray scattering and quasielastic neutron scattering study on the structure and dynamic properties of low-temperature methanol confined in ordered microporous carbon and mesoporous organosilica pores

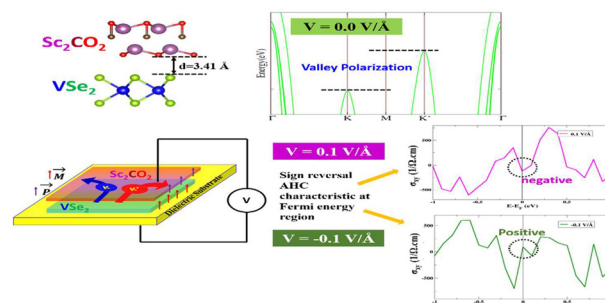
Hongyan Liu, Zhuanfang Jing, Keke Chai, Yongquan Zhou,* Koji Yoshida, Takeshi Yamada and Toshio Yamaguchi*



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Electrically tunable anomalous Hall conductivity in ferrovalley–ferroelectric heterostructure VSe_2/Sc_2CO_2

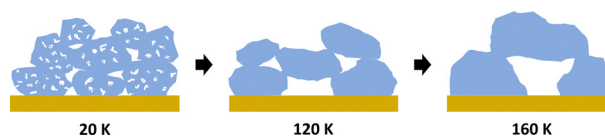
Mayuri Bora,* Himangshu Sekhar Sarmah* and Subhradip Ghosh



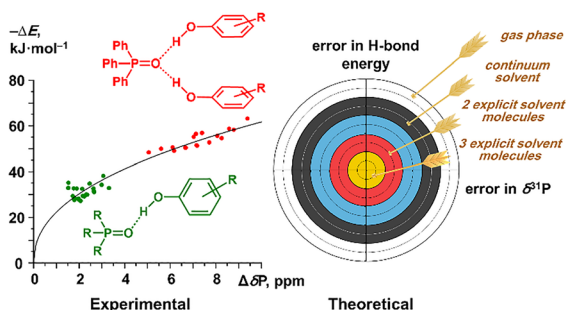
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Molecular and pore-scale structure evolution in amorphous solid water

Zachary Amato,* Sabrina Gärtner, Pierre Ghesquière, Thomas F. Headen, Tristan G. A. Youngs, Daniel T. Bowron, Leide P. Cavalcanti, Sarah E. Rogers, Natalia Pascual, Olivier Auriacombe, Ellen Daly, Rachael E. Hamp, Catherine R. Hill, T. P. Ragesh Kumar and Helen J. Fraser



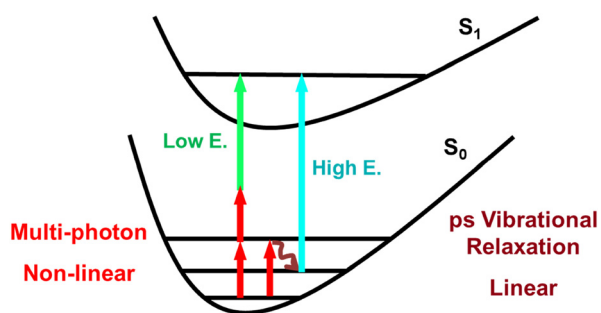
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^{31}P NMR chemical shift of phosphine oxides measures the total strength of multiple anticooperative H-bonds formed between the P=O group and proton donors

Omar Alkhuder, Mikhail A. Kostin and Peter M. Tolstoy*

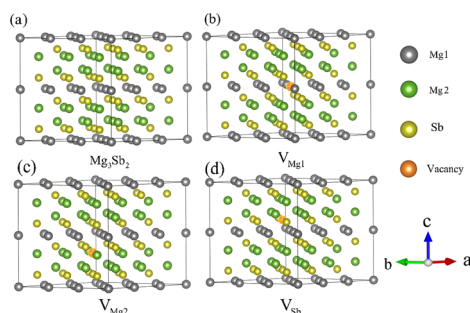
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The interplay of nonlinear multi-photon processes and vibrational population effect on vibration-modulated fluorescence

Qirui Yu, Yuanzhou Shi, Jianxin Guan, Xinmao Li, Zhihao Yu and Junrong Zheng*

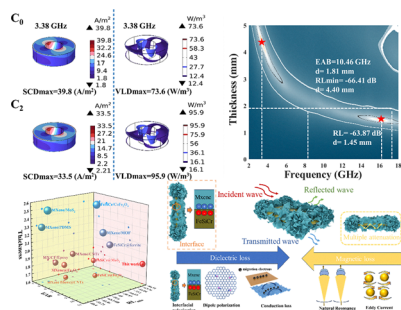
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Vacancy-induced phonon localization and lattice softening for reduced thermal conductivity in Mg_3Sb_2

Sheng Zhang, Jinbao Zhang, Liqi Ren, Yijing Shao, Wanyue Yan, Meng Tian, Kunling Peng,* Ping Lin* and Yunzhen Du*

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Research on two-dimensional FeSiCr/mesoporous MXene composites and their absorption properties

Zhengxing Li, Quan Fang, Zhongyue Song, Juan Liu,* Honghui Jiang* and Tongxiang Liang*

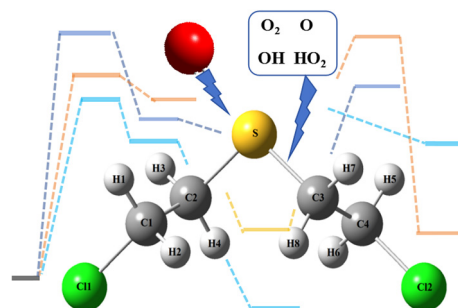


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High-accuracy theoretical studies on the gas-phase reaction mechanisms of sulfur mustard with reactive oxygen species (OH/O₂/HO₂/O)

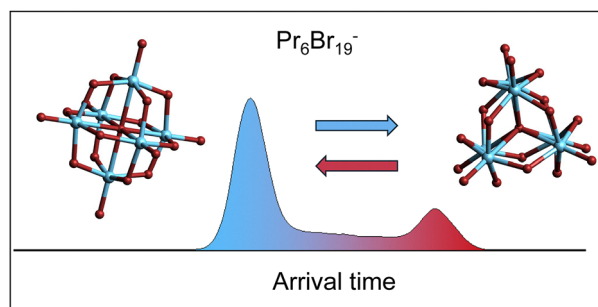
Xuefeng Liu, Shangpeng Hao, Xin Gao, Lin Yang, Huanhuan Wang* and Haitao Wang*



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A cyclic ion mobility and DFT study of the structures, isomer space and isomer interconversion of lanthanide bromide clusters, Ln_xBr_{3x+1}⁻, x = 1–6

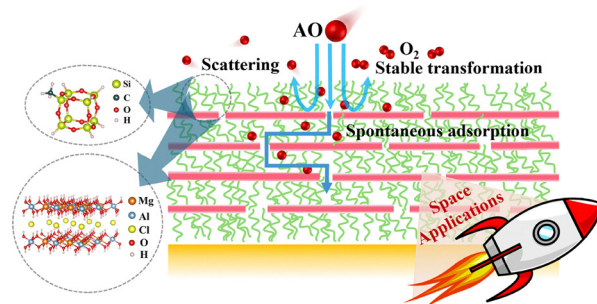
Yuto Nakajima, Patrick Weis,* Florian Weigend,* Marcel Lukanowski, Fuminori Misaizu and Manfred M. Kappes*



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First-principles insights into atomic oxygen protection coatings composed of scale-like layered double hydroxide nanosheets

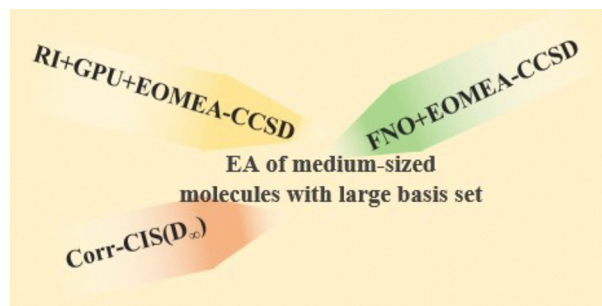
Denghang Tang, Rui Sun, Jiayu Zheng, Mengyun Xu, Haogeng Li, Hongyu Gu,* Yuzhi Zhang,* Yi-Yang Sun and Lixin Song



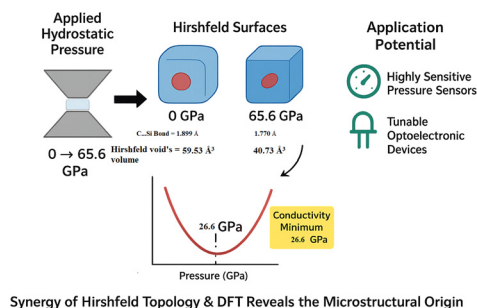
620

Electron affinities with GPU-accelerated density-fitting EOM-CCSD, approximate EOM-CCSD methods and EOM-CCSD with frozen natural orbitals

Yanmei Hu, Zhifan Wang and Fan Wang*



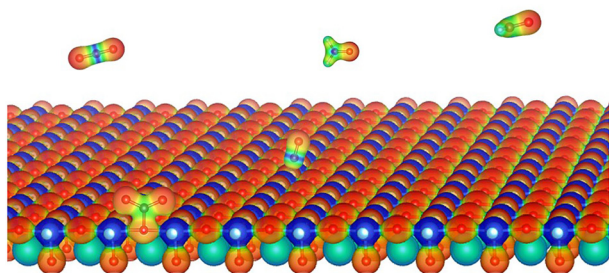
632



Pressure-induced tunability and conductivity minimum in 3C-SiC for optoelectronic applications

Z. Y. Khattari* and M. Albaddawi

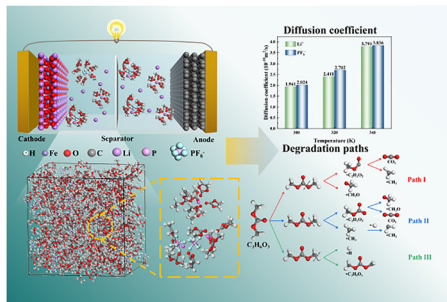
644



The adsorption characteristics and mechanism of C1 molecules on two-dimensional SrTiO₃ films

Yuanbin Xue, Cuihuan Geng, Xiaojing Bai and Huali Hao*

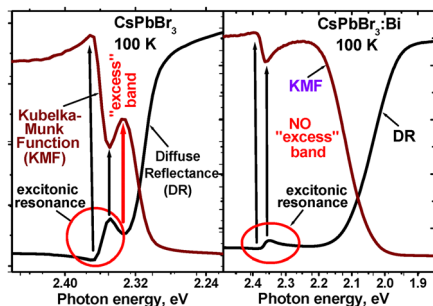
651



Thermal runaway mechanism of LiFePO₄ battery electrolytes: a molecular dynamics and density functional theory simulation study

Jun Xie,* Ping Huang, Guowei Xia, Yixiao Zhang, Yutong Zhang, Kun Tian and Qing Xie

662



Manifestation of excitonic resonance in diffuse reflectance spectra of halide perovskites

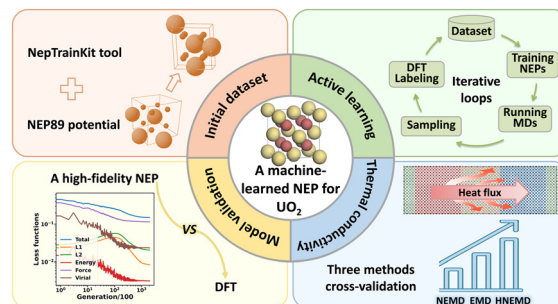
Vyacheslav N. Kuznetsov,* Yuri V. Chizhov, Nadezhda I. Glazkova, Galina V. Kataeva, Ruslan V. Mikhaylov, Vladimir K. Ryabchuk, Alexei V. Emeline and Nick Serpone*



671

Active learning-enhanced neuroevolution potential for predictive modeling of UO_2 thermophysical properties

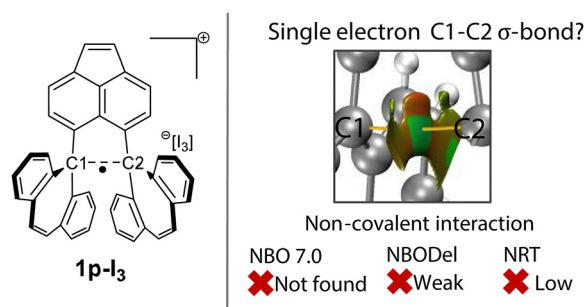
Junying Zhong, Lei Zhang and Tao Bo*



683

Dissecting the single-electron C–C bond: NBO and AIM perspectives

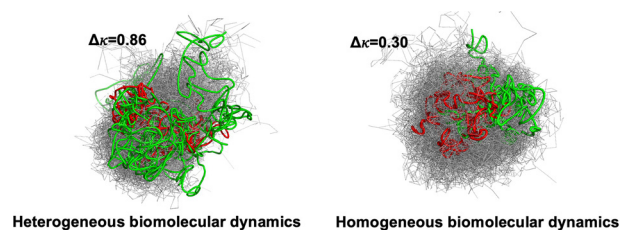
Leonardo I. Lugo-Fuentes, Darien I. Martínez-Valencia, J. Oscar C. Jiménez-Halla and Joaquín Barroso-Flores*



692

Differential sequence charge clustering and mixing ratio affect stability and dynamics of heterotypic peptide condensates

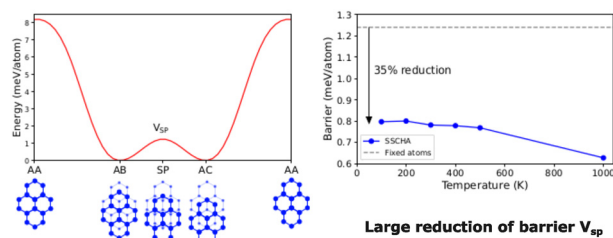
Milan Kumar Hazra



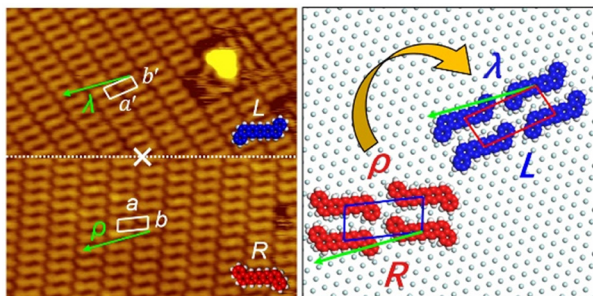
707

Free energy barrier and thermal-quantum behavior of sliding bilayer graphene

Jean Paul Nery,* Lorenzo Monacelli and Francesco Mauri*



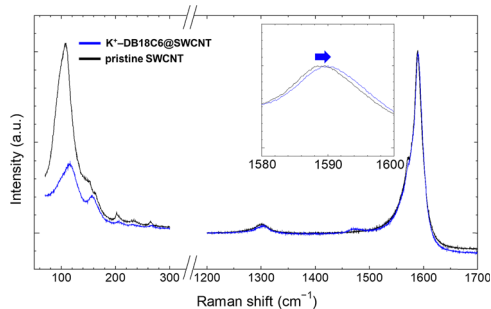
715



Collective chirality flipping of dibenzopentacene molecules induced by an electric field

Li-Ting Yuan, Chen-Yu Hu, Ji-Yong Yang, Gang Yao, Ming-Long Tao, Kai Sun and Jun-Zhong Wang*

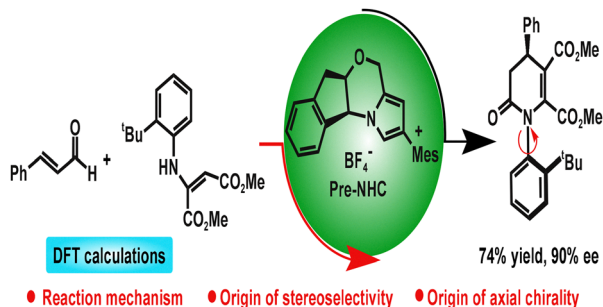
721



Enhancement of oxygen reduction activity of iron phthalocyanine electrocatalyst supported on carbon nanotubes through molecular encapsulation

Tatsuya Akiyama,* Yosuke Ishii* and Shinji Kawasaki*

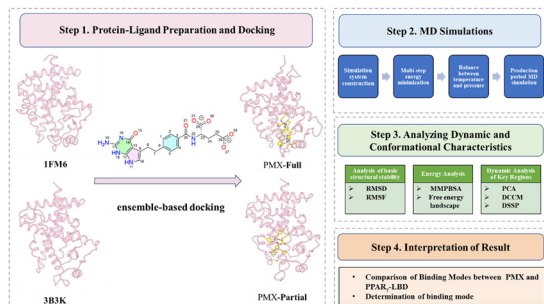
730



Mechanisms and regio- and stereoselectivities in NHC-catalyzed [3+3] annulations for the synthesis of axially and centrally chiral dihydropyridinones

Yanlong Kang, Mingchao Zhang, Yan Li* and Zhiqiang Zhang

742



Molecular insight into pemetrexed as a partial agonist of PPAR_γ through molecular dynamics simulations

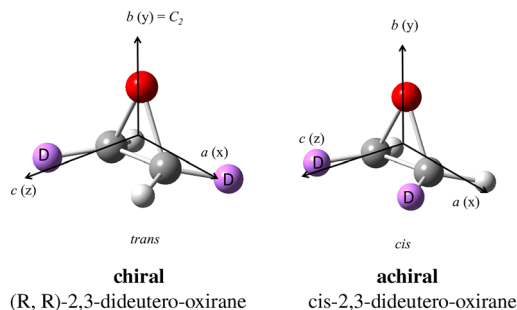
Yifan She, Jiasheng Zhao, Shunlin Ren, Lei Zhang, Shengli Zhang and Zhiwei Yang*



751

Isotopic chirality and high-resolution gigahertz and terahertz spectroscopy of *trans*-2,3-dideutero-oxirane (*tc*-CHDCHDO)

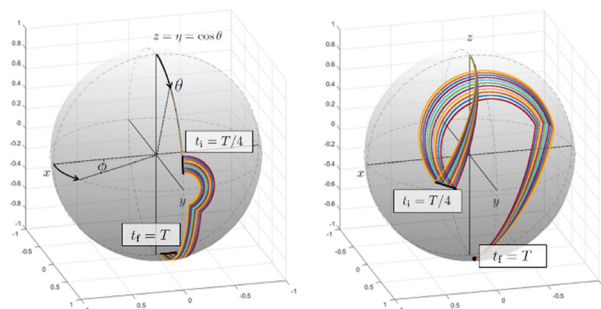
Ziqiu Chen,* Sieghard Albert, Karen Keppler, Gunther Wichmann, Martin Quack,* Volker Schurig and Oliver Trapp



764

The robustness of composite pulses elucidated by classical mechanics: stability around the globe

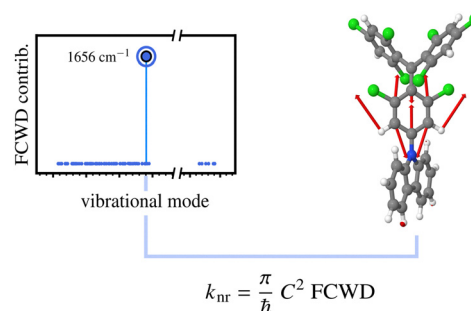
Jonathan Berkheim* and David J. Tannor



776

Dissecting non-radiative decay in donor-functionalized radicals with a mode-resolved model

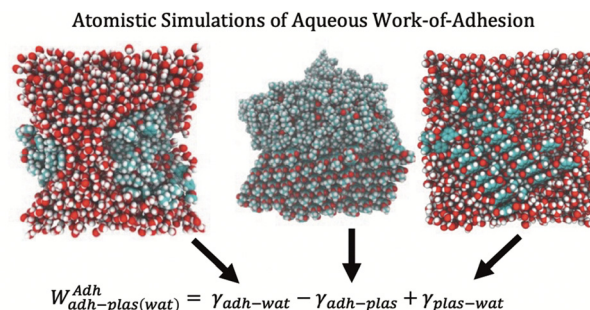
Robert Toews* and Andreas Köhn



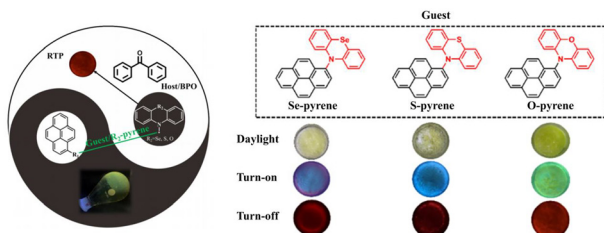
790

Predicting polyacrylate–microplastic interactions with atomistic simulation

Timothy M. E. Jugovic, Henry E. Thurber, Michael T. Robo, Woojung Ji, Madeline E. Clough, Anne J. McNeil and Paul M. Zimmerman*



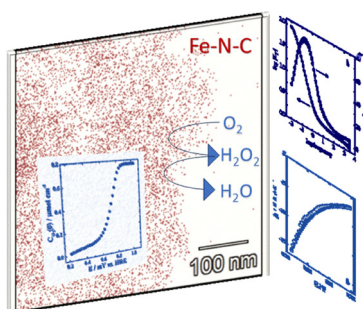
798



Buchwald–Hartwig aminated pyrene-heterocycles with host–guest-enhanced NIR phosphorescence: DFT-guided design toward breast cancer imaging probes

Kaixuan Hu, Shufeng Chen, Xinmin Wang, Lingkai Tang, Yan Cheng, Yuting Song, Hubing Shi, Jing Jing, Jianping Hu* and Ting Luo*

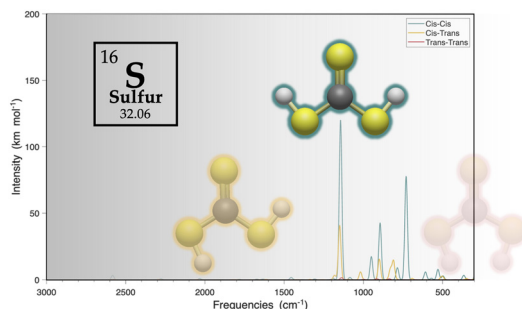
811



Fe–N–C electrocatalysts derived from a 1,10-phenanthroline–iron complex: kinetic insights into the acidic oxygen reduction reaction

Matheus Martins, Bianca Tainá Ferreira, Carlos Sant'ana Vasconcelos, Nelson A. Galote, Fabio Henrique Barros Lima and Fritz Huguenin*

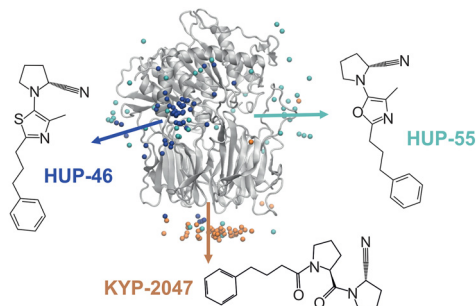
821



Quantum chemical rovibrational spectroscopic data for possible observation of thiocarbonic acid (H_2CS_3) in interstellar environments

Megan McKissick and Ryan C. Fortenberry*

829



Decoding dissociation pathways of ligands in prolyl oligopeptidase

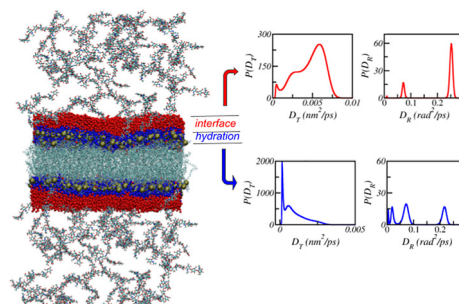
Katarzyna Walczewska-Szewc* and Jakub Rydzewski



841

Heterogeneous water dynamics in hyaluronan–DPPC interfaces

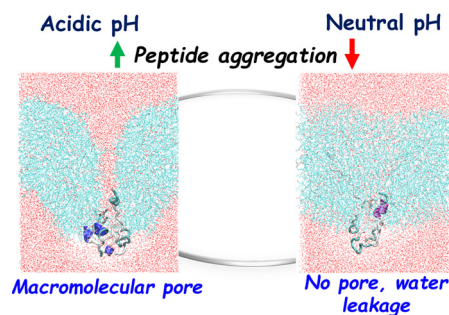
Anirban Paul* and Jaydeb Chakrabarti*



850

pH-dependent peptide aggregation and translocation across octanol and hexane interfaces: insights from umbrella sampling simulations

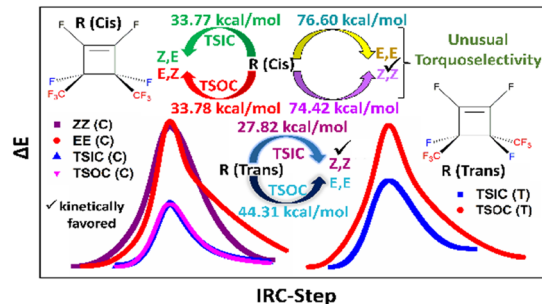
Anjana V. Mathath, Samrat Sarkar and Debashree Chakraborty*



862

Unraveling unusual torquoselectivity in ring-opening electrocyclic reactions: a DFT perspective

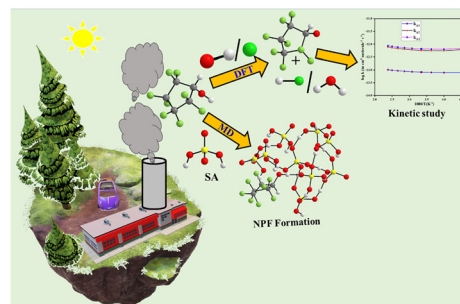
Arpita Poddar, Jesús Sánchez-Márquez, Alejandro Morales-Bayuelo* and Pratim Kumar Chattaraj*



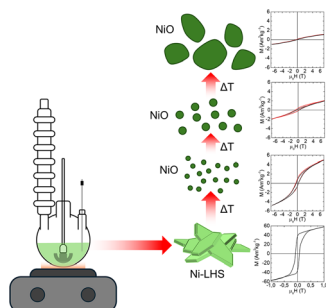
871

A theoretical investigation on the mechanistic and kinetic study of 2,2,3,3,4,4,5,5-octafluorocyclopentanol with OH radicals and Cl atoms and its implications in new particle formation

Suresh Tiwari and Ranga Subramanian*



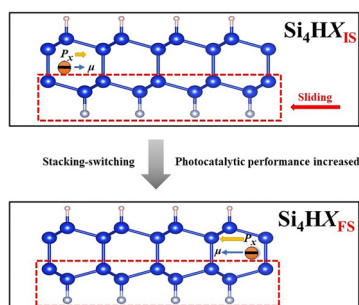
885



Size-dependent magnetic properties of NiO nanoparticles synthesized *via* Ni-hydroxyacetate decomposition

Miran Baričić,* Pierfrancesco Maltoni, Giulia Franceschin, Thomas Gaudisson, Sophie Nowak, Frederic Mazaleyrat, Davide Peddis and Souad Ammar*

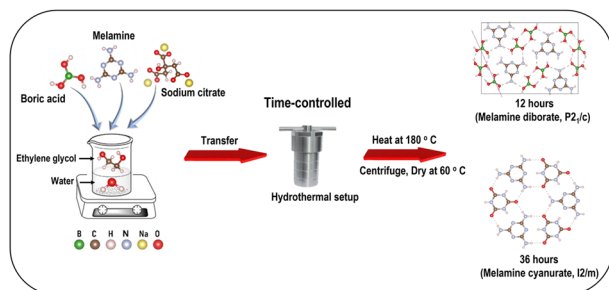
892



Stacking-switching of silicon-based two-dimensional diamane structures to enhance photocatalytic water splitting performance

Min Tao, Chu-Chu Liu, Pan Ma, Xiao Shang, Hai-Bin Du, Xian-Yu Hu, Lu-Chao Du* and Fu-Chun Liu*

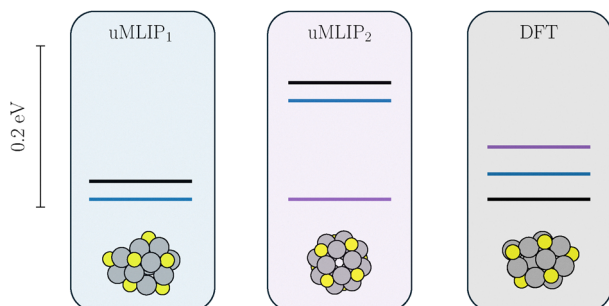
903



Time-dependent solvothermal synthesis of melamine cyanurate and melamine diborate: experimental and theoretical insights

Atika, Zihan Zhang, Klaus Leifer, Jöns Hilborn, Dan Li, Jiefang Zhu, Rajeev Ahuja and Wei Luo*

912



Active Δ -learning with universal potentials for global structure optimization

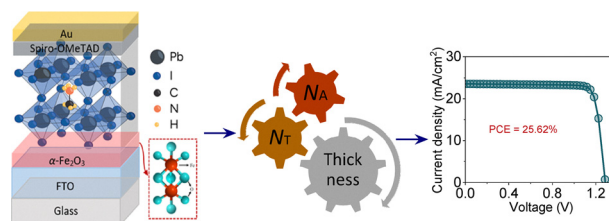
Joe Pitfield, Mads-Peter Verner Christiansen and Bjørk Hammer



927

High-performance hematite-integrated perovskite solar cells

Mustafa Kareem,* Ethar Yahya Salih, Malatesh Akkur, Satish Kumar Samal, Sridharan Sundharam and Sanjeev Kumar

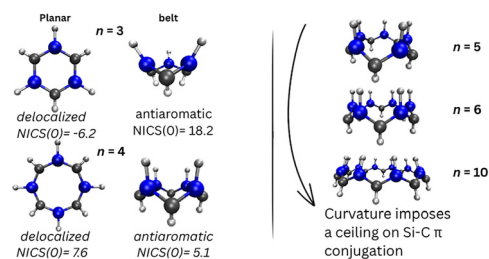


938

Theoretical study of Si/C alternately substituted annulenes with a belt structure

Takako Kudo,* Katherine N. Ferreras, Tajji Nakamura, Akira Imanishi, Ryuta Ikutomo and Mark S. Gordon*

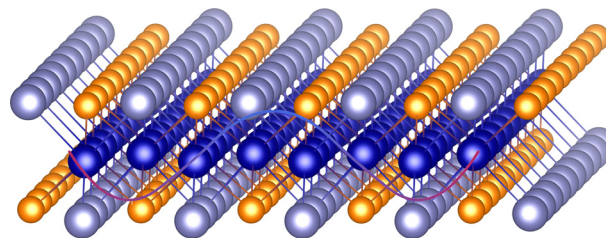
Curvature Driven π Localization in Belt-Shaped Alternating Si/C Annulenes, $H_{2n}Si_nC_n$



953

Strain-selected magnetic ordering in $1T'\alpha$ -CrXY (X, Y = S, Se, Te) monolayers

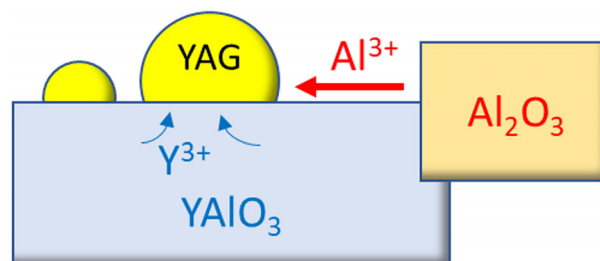
Deju Zhang and Yanning Zhang*



960

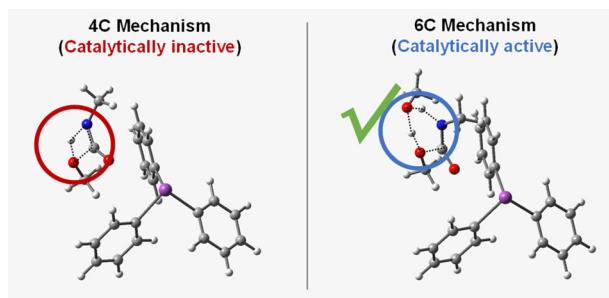
A TMA and DSC study of the kinetics of the solid-state reaction in an Al_2O_3 - Y_2O_3 system

Nathan Kerkad, Loïck Bonnet, Loïc Favergeon, Alexandre Maître and Rémy Boulesteix*



RESEARCH PAPERS

969



The catalytic role of triphenyl bismuth in curing reactions: a theoretical study

Bowen Zhang, Lu Gem Gao, Peng Guo, Ruiqing Lei, Pengchao Zhang, Xuefei Li* and Xuefei Xu*

CORRECTIONS

977

Correction: Electrolyte clusters as hydrogen sponges: diffusion Monte Carlo simulations

A. R. Zane and E. Curotto*

978

Correction: High-temperature and solid-state NMR investigation of the structural evolution and special phase transition in LiF–NaF–BeF₂ mixed salts

Jianchao Sun, Hailong Huang, Ling Han, Xiaobin Fu,* Hongtao Liu* and Yuan Qian*

979

Correction: Excited state dipole moments from Δ SCF: a benchmark

Lukas Paetow and Johannes Neugebauer*



CORRECTIONS

980

Correction: Theoretical study of large-scale graphene on the Cu(111) surface using machine learning potential

Jingli Han, Rubén Cabello, Jordi Bonet Ruiz, Alexandra Elena Plesu Popescu, Sergi Dosta Parras,* Camila Barreneche and Yongpeng Yang*

981

Correction: Triggered release kinetics of living cells from composite microcapsules

Shwan Abdullah Hamad, Simeon D. Stoyanov and Vesselin N. Paunov*

