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Cover

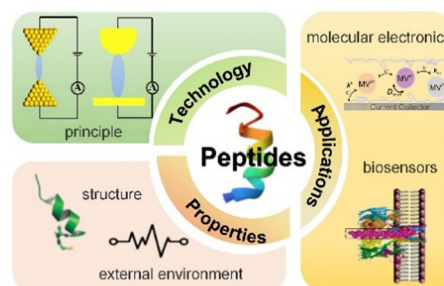
See Sagnik Das,
Hendrike Braun *et al.*,
pp. 8043–8051.
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Phys. Chem. Chem. Phys.,
2025, 27, 8043.

PERSPECTIVE

8026

Advances in single-molecule electrical transport studies of peptides

Cunxin Han, Chao Chen,* Hanqing Shi, Wenzhe Chen,
Wei Sun and Bing Li*

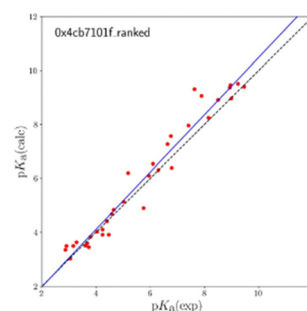


COMMUNICATION

8039

Thermodynamics-informed neural networks and extensive data sets: key factors to accurate blind predictions of apparent pK_a values in the euroSAMPL challenge

Robert Fraczekiewicz



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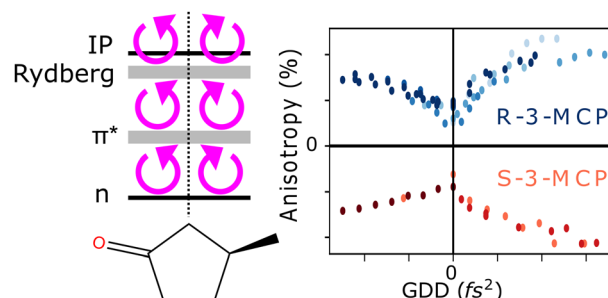


RESEARCH PAPERS

8043

Control of circular dichroism in ion yield of 3-methyl cyclopentanone with femtosecond laser pulses

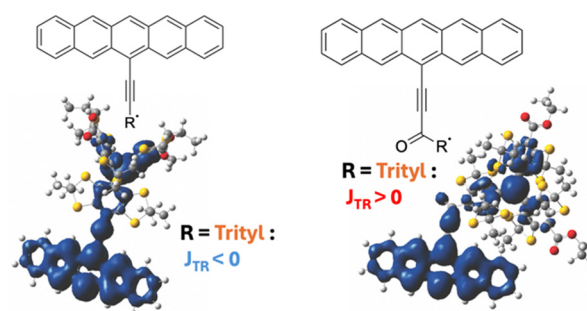
Sagnik Das,* Jayanta Ghosh, Sudheendran Vasudevan, Simon T. Ranecky, Tonio Rosen, Nicolas Ladda, Han-gyeol Lee, Till-Jakob Stehling, Fabian Westmeier, Jochen Mikosch, Arne Senftleben, Thomas Baumert and Hendrike Braun*



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An investigation of contributors to the spin exchange interactions in organic pentacene–radical dyads using quasi-degenerate perturbation theory

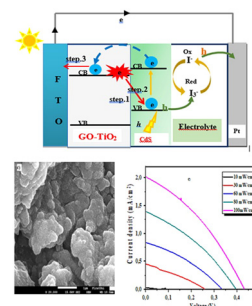
Philip S. Weiss, Amiel S. Paz and Claudia E. Avalos*



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Investigation of the GO effect on CdS quantum dot sensitized PV-cells based on the GO–TiO₂ nanocomposite photoanode: modeling using the Lambert function

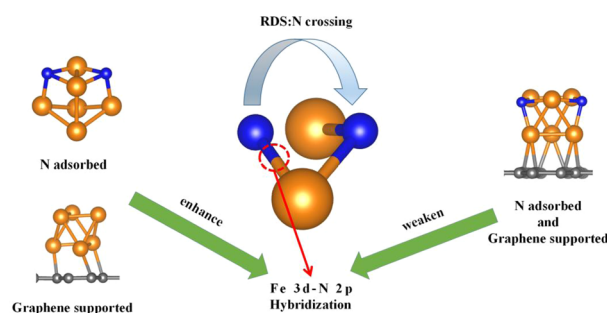
N. Yahyaoui,* S. Mansouri and F. Yakuphanoglu



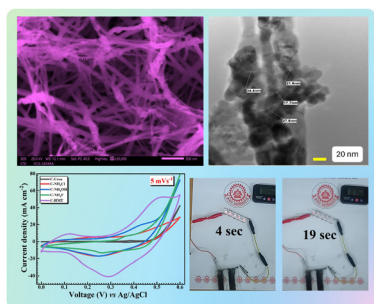
8090

The critical role of Fe 3d–N 2p orbital hybridization in ammonia decomposition on graphene-supported Fe₆N_x clusters: a DFT study

Kaixun Yi, Fengyun Ding, Habibullah, Wanglai Cen* and Tao Gao*



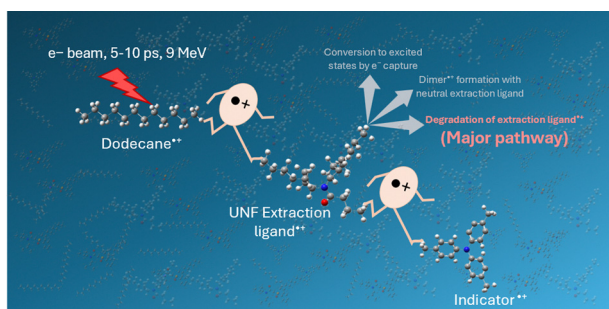
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Additive-assisted oriented growth of cobalt oxide: controlled morphology and enhanced supercapacitor performance

Radhika S. Desai, Vinayak S. Jadhav, Sidharth R. Pardeshi, Pramod S. Patil, Mohammad Rafe Hatshan, Yedluri Anil Kumar and Dhanaji S. Dalavi*

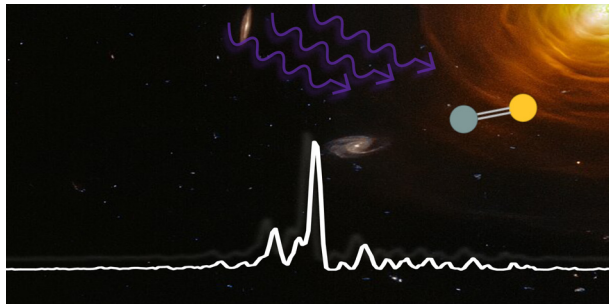
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Ultrafast pre-solvated dodecane hole capture and subsequent damage of used nuclear fuel extraction ligands DEHBA, DEH/BA, HONTA, CMPO, HEH[EHP] and TBP

Rupali G. Deokar and Andrew R. Cook*

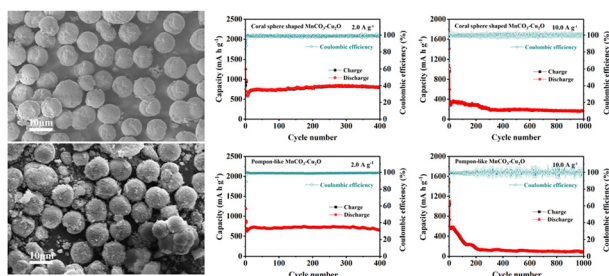
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VUV threshold photoelectron spectroscopy of SiS

Myriam Drissi,* Jean-Christophe Loison,* Béranger Gans, Séverine Boyé-Péronne, Hai-Linh Le, Mengxu Jiang, Laurent Nahon and Gustavo A. Garcia

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A study on the construction of spherical $\text{MnCO}_3\text{-Cu}_2\text{O}$ composites with enhanced electrochemical lithium storage performance

Lei Wang,* Guifen Du, Piyu Gong, Chuansheng Cui, Shuo Tao, Haibo Li and Suyuan Zeng*

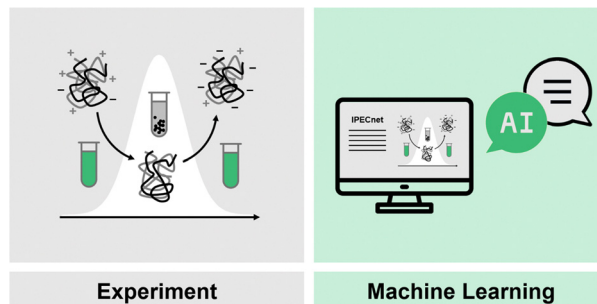


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IPECnet: ML model for predicting the area of water solubility of interpolyelectrolyte complexes

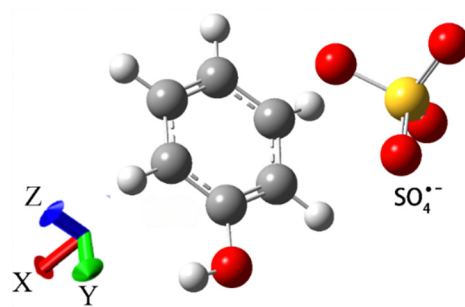
Ilya V. Grigoryan,* Liubov A. Antiufrieva, Anna P. Grigoryan, Vladislava A. Pigareva, Evgenii A. Generalov, Gennady B. Khomutov and Andrey V. Sybachin*



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Enhancement of sulfate radicals degrading phenol in water by an external electric field: a study by DFT calculations

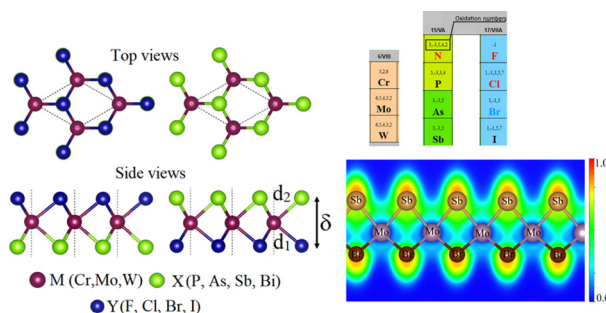
Yong Han,* Huiqing Yang, Qingrui Zhang and Tifeng Jiao*



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Janus group V1B-based pnictogen-halide monolayers: a new class of multifunctional quantum materials from first-principles predictions

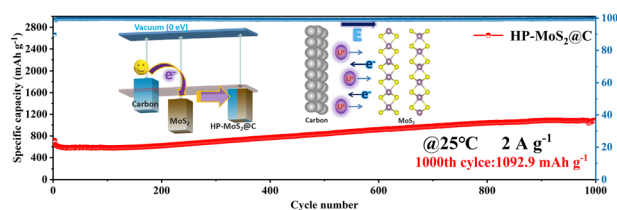
Sergey Gusarov, Chinedu E. Ekuma, Gap Soo Chang, Mina Alizade and Mosayeb Naseri*



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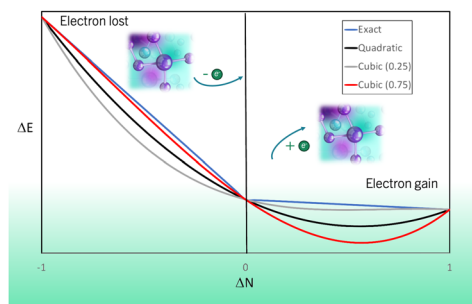
Synthesis of polyhedral MoS₂@C hollow cages using a sacrificial template approach for improved reversible lithium storage

Zhiya Lin, Zhilong Wu, Yuqi Wu, Hai Jia, Xiaojing Hu, Maoxin Yu, Xiaohui Huang* and Shaoming Ying*



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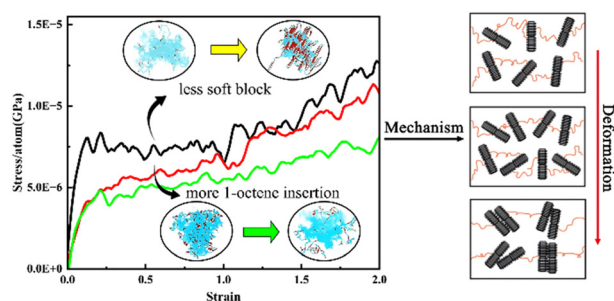
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A redefinition of global conceptual density functional theory reactivity indexes by means of the cubic expansions of the energy

Luis Rincón,* Wendy M. Rodríguez, Jose R. Mora, Cesar Zambrano, Luis E. Seijas, Andres Reyes and F. Javier Torres*

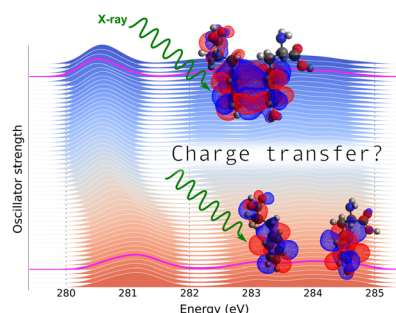
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Molecular dynamics simulation of crystallization and stretching mechanisms in ethylene/1-octene block copolymers: insights into the role of the block structure

Yangyang Zhao, Yiran Cao, Fan Zhang and Xuelian He*

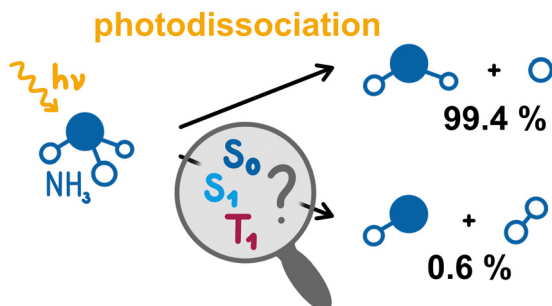
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X-ray absorption spectroscopy reveals charge transfer in π -stacked aromatic amino acids

Carlos Ortiz-Mahecha,* Lucas Schwob, Juliette Leroux, Sadia Bari, Robert H. Meißner* and Annika Bande*

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Revisiting the intricate photodissociation mechanism of ammonia along the minor $\text{NH} + \text{H}_2$ pathway

Brigitta Bachmair, Johannes C. B. Dietschreit and Leticia González*

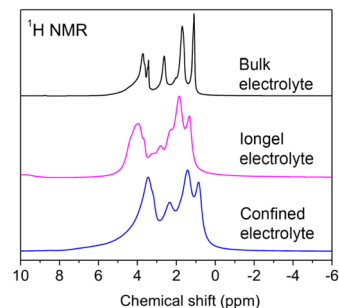


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Ion dynamics in an iongel electrolyte based on fluorine-free ionic liquid probed by multinuclear NMR

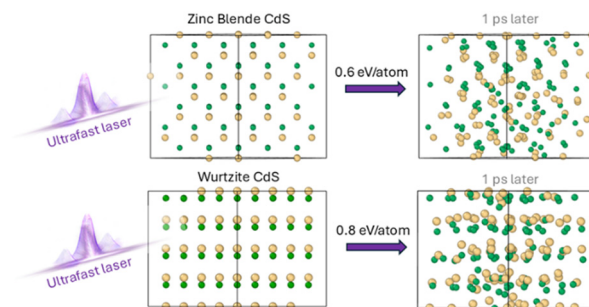
Andrei Filippov,* Maiia Karlsson-Broström, Rustam Gimatdinov, Faiz Ullah Shah and Oleg N. Antzutkin*



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Ultrafast X-ray induced damage and nonthermal melting in cadmium sulfide

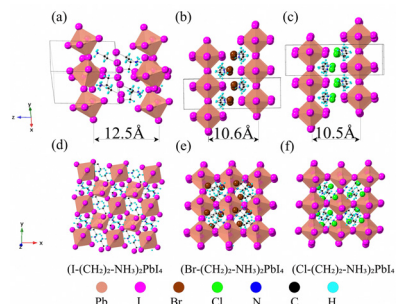
Nikita Medvedev* and Aldo Artímez Peña



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Effect of halogen substitution in spacer cations on two-dimensional Ruddlesden–Popper perovskites

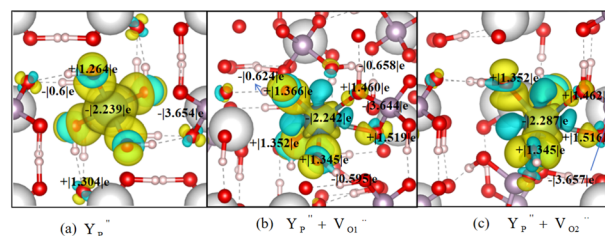
Qiang Huang, Xiaoyan Gan,* Linfei Yang, JianHua Liao, Liling Guo and Hanxing Liu



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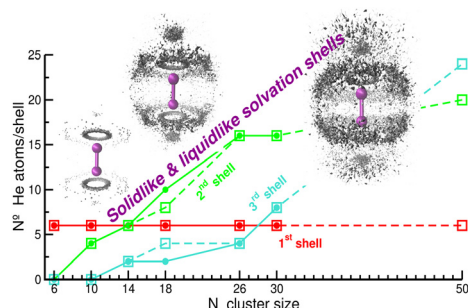
Theoretical prediction of cluster configuration transitions and electro-optical properties of Y_p defects in KH_2PO_4 via density functional theory

Xu Lu, Wei Hong, Tingyu Liu,* Huifang Li and Jianghai Wang



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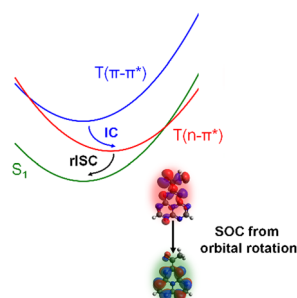
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Microsolvation of cationic alkali dimers in helium: quantum delocalization and solid-like/liquid-like behaviors of He shells

Raquel Yanes-Rodríguez, Pablo Villarreal and Rita Prosimiti*

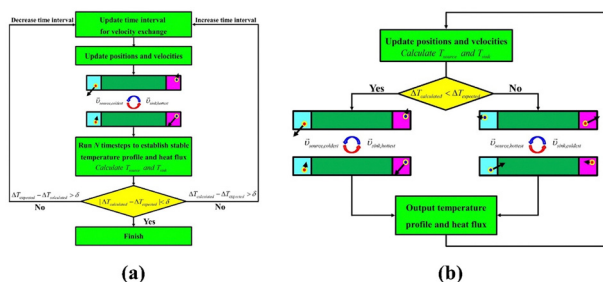
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An efficient reverse intersystem crossing process exploiting non-bonding states in an inverted singlet–triplet gap system

Hwon Kim and Seung Kyu Min*

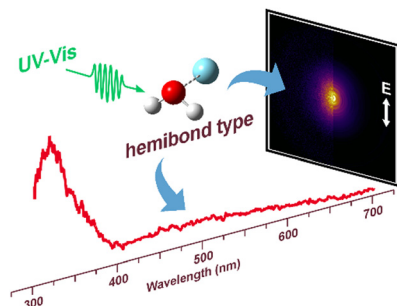
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A modified Müller-Plathe method capable of quickly establishing an expected temperature difference in classical and *ab initio* molecular dynamics simulations for thermal transport calculations

Xiaoliang Zhang,* Kunpeng Yuan, Yufei Gao,* Xiaojing Gong,* Sheng-Ying Yue* and Dawei Tang

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Observation of the hemibond formation in (H₂O–Ar_n)⁺ radical cation clusters by electronic spectroscopy and ion imaging technique

Mizuhiro Kominato, Takumi Koshiba, Fuminori Misaizu* and Asuka Fujii*

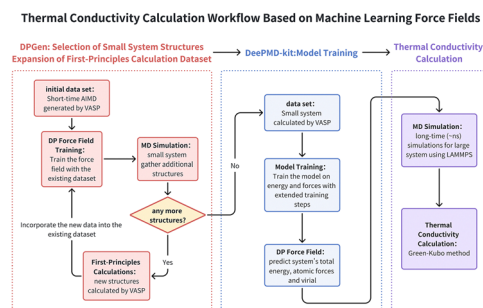


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An active learning force field for the thermal transport properties of organometallic complex crystals

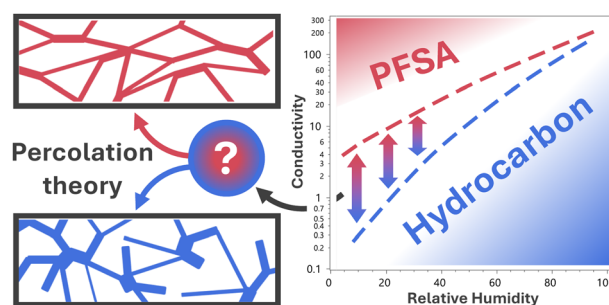
Wenjie Zhang, Weitang Li and Zhigang Shuai*



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Understanding the hydrocarbon – PFSA ionomer conductivity gap in hydrogen fuel cells

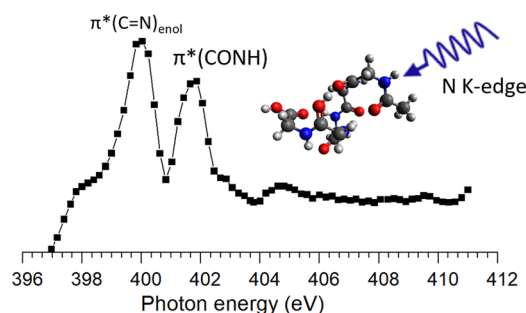
William Bangay,* Michael Yandrasits and Wayne Hayes



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Tautomerism of a backbone protonated peptide revealed by soft X-ray action spectroscopy

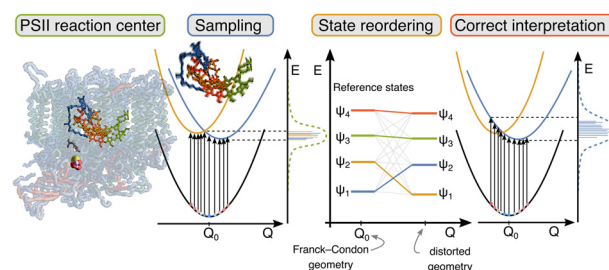
Juliette Leroux, Carlos Ortiz-Mahecha, Kaja Schubert, Florian Trinter, Isaak Unger, Lucas Schwob and Sadia Bari*



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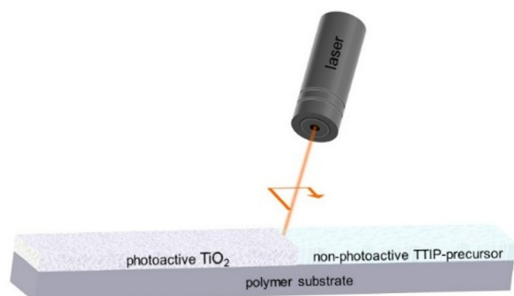
Analyzing spectral distributions of charge transfer character in ensembles: a case study on the reaction center of photosystem II

Adam Šrut, Sinjini Bhattacharjee, Dimitrios A. Pantazis* and Vera Krewald*



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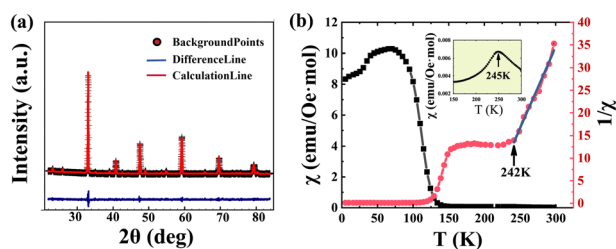
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Stabilization of TiO₂-based photocatalytic coating on polymer substrates with complex geometry using laser annealing

Hong T. Duong, Bastien O. Burek and Jonathan Z. Bloh*

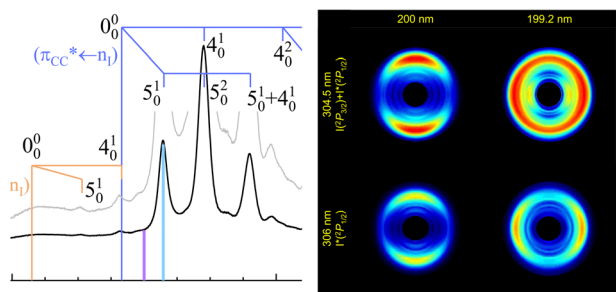
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Dynamic behavior of resistivity irreversibility induced by thermal cycling in perovskite charge ordering manganites

Yunwen Qiu, Zhen Xu, Chunlan Ma, Shuhao Wang, Hao Yang, Yan Zhu, Caixia Wang, Wei Tong and Jiyu Fan*

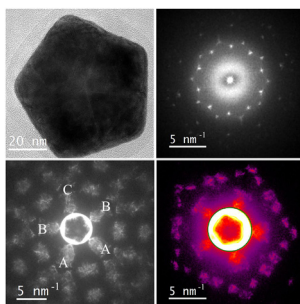
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Non-adiabatic photodissociation dynamics of vinyl iodide from $n\sigma^*$ and $n\pi^*$ transitions

Marta L. Murillo-Sánchez, Sonia Marggi Poullain, Paulo Limão-Vieira, Alexandre Zanchet, Nelson de Oliveira, Jesús González-Vázquez and Luis Bañares*

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Study of decahedral multimetallic nanoparticles using large-angle convergent-beam electron diffraction

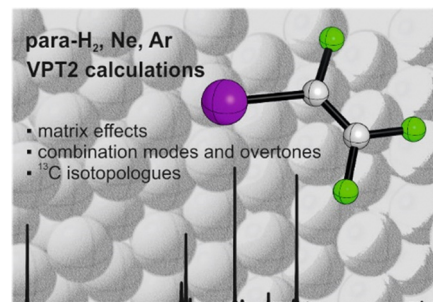
Blake Rogers, Carlos E. Rufino da Silva,*
Juan Pedro Palomares-Báez,*
J. Jesús Velázquez Salazar, José Luis Rodríguez López,
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Miguel José Yacamán

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Matrix-isolation IR spectra of iodotrifluoroethylene (C_2F_3I)

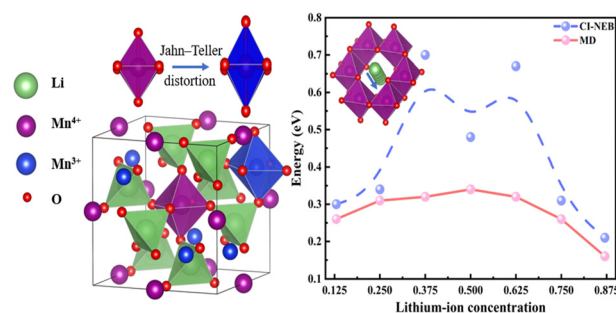
Malte Feßner, Julien Bloino and Christian Merten*



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Decoding lithium-ion dynamics: unveiling the role of concentrations and local environments in spinel $Li_xMn_2O_4$

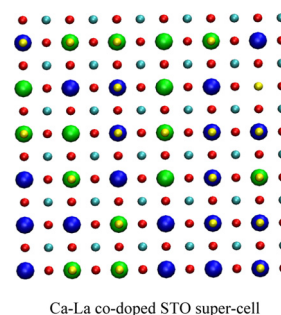
Yingxin Duan, Xiao Liu, Xuhong Wu, Zhi Yang, Ruiping Liu, Lin Xue, Fenglian Li, Jian-Li Shao and Li-Chun Xu*



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A theoretical study of oxygen anion diffusion through La and Ca doped $SrTiO_3$ lattice structures: molecular dynamics and ML approaches

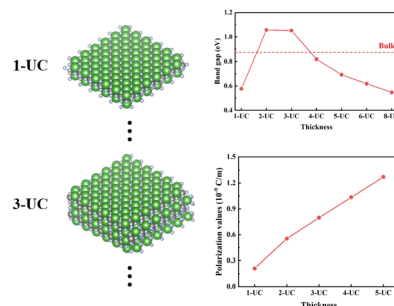
Kapil Sharma, Hrushikesh M. Gade* and Neetu Kumari*



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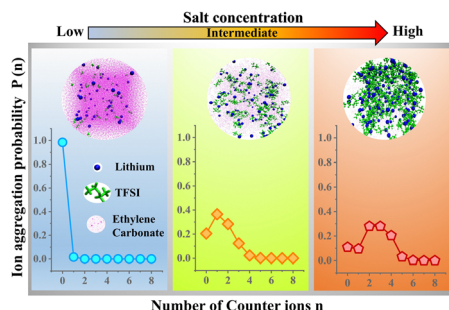
Electronic structures and ferroelectric properties of $LaWN_3$ ultrathin films

Wan Chen, Kai Gao, Chunju Hou and Yi Yang*



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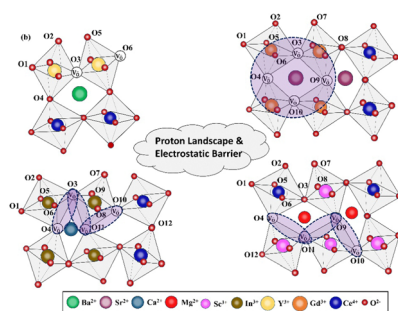
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On the nature of ion aggregation in EC-LiTFSI electrolytes

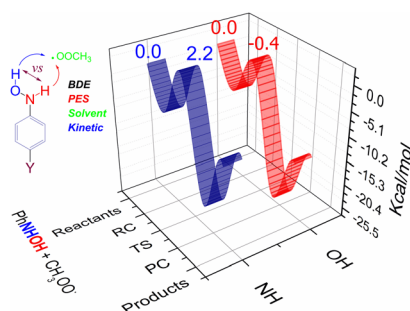
Hema Teherpuria, Prabhat K. Jaiswal and Santosh Mogurampelly*

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Proton–polaron and energy landscape among acceptor doped ACeO_3 ($A = \text{Ba}^{2+}, \text{Sr}^{2+}, \text{Ca}^{2+}, \text{Mg}^{2+}$) proton conductors: a first principles approach

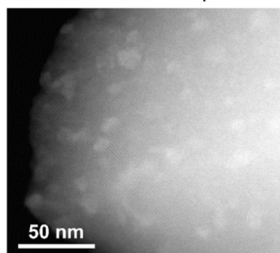
D. Vignesh and Ela Rout*

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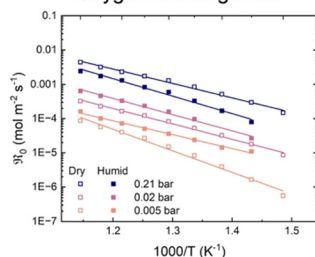
Revisiting the radical trapping activity of N–H and O–H in *N*-phenylhydroxylamine: a DFT study

Pham Thi Thu Thao, Dinh Quy Huong, Nguyen Minh Thong, Mai Van Bay, Son Tung Ngo, Quan Van Vo and Pham Cam Nam*

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Exsolved Co_3O_4 nanoparticles

Oxygen exchange rate

Oxygen exchange kinetics of $\text{BaGd}_{0.3}\text{La}_{0.7}\text{Co}_2\text{O}_{6-\delta}$ with exsolved Co_3O_4 nanoparticles in dry and humid atmospheres

Jónína B. Guðmundsdóttir, Vincent Thoréton, Bo Jiang, Anuj Pokle, Einar Vøllestad, Reidar Haugsrud and Jonathan M. Polfus*

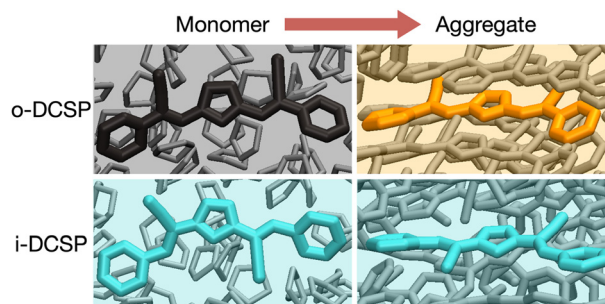


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Theoretical insights into aggregation-induced emission of bis(cyanostyryl)pyrrole derivatives

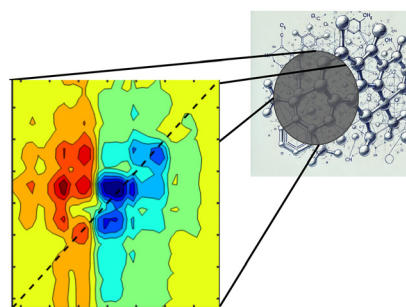
Cherumannil Femina, Toshiya Yamagami,
Norifumi Yamamoto,* Reji Thomas and
Pookkottu K. Sajith*



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H-Bonding structures of 1-ethyl-3-methylimidazolium trifluoroacetate: a vibrational spectroscopic study

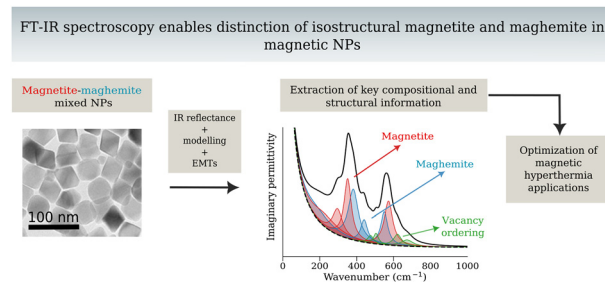
Kallol Mukherjee, Sarah Hall and Amber T. Krummel*



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Quantifying lattice vibrational modes and optical conductivity in mixed magnetite–maghemite nanoparticles

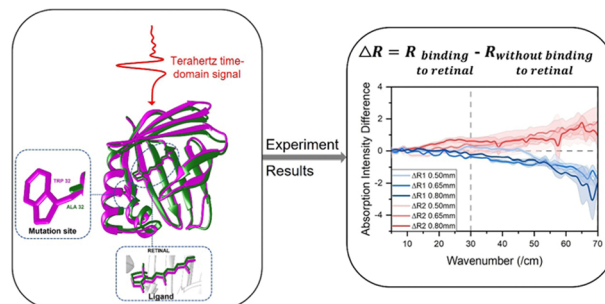
Mireia Sainz-Menchón, Iñigo González de Arrieta,*
Telmo Echániz, Karam Nader, Maite Insausti,
Aurélien Canizarès, Olivier Rozenbaum and
Gabriel A. López



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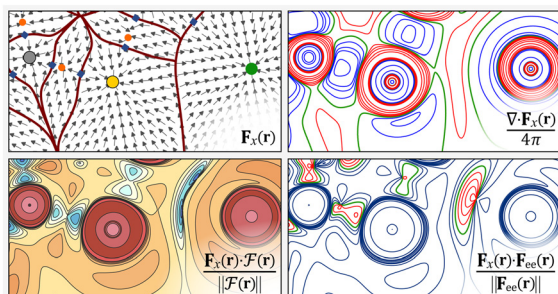
Modulation of terahertz absorption by a single mutation of rhodopsin mimics

Yunyu Wang, Yongnan Hu, Jiajia Meng, Xubiao Peng*
and Qing Zhao*



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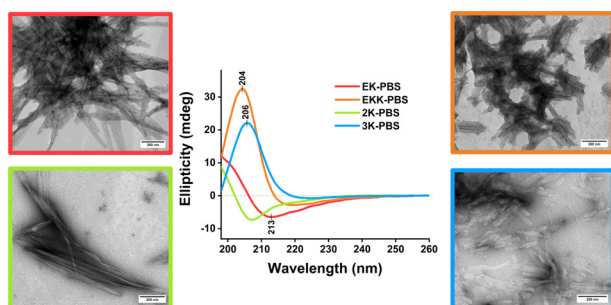
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Evaluating and interpreting the exchange correlation contributions to the total static and interelectron interaction force densities, with a force-field perspective on the exchange charge density

Sergey V. Kartashov and Robert R. Fayzullin*

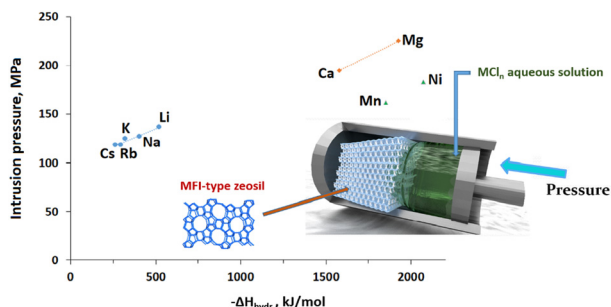
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Charge and length dependent build-up of environment sensitive lamellin β -peptides

Sohini Chakraborty, Kamal el Battioui, Tasvilla Sonallya, Imola Cs. Szigyártó, Kata Horváti, Zoltán Varga, Tünde Juhász and Tamás Beke-Somfai*

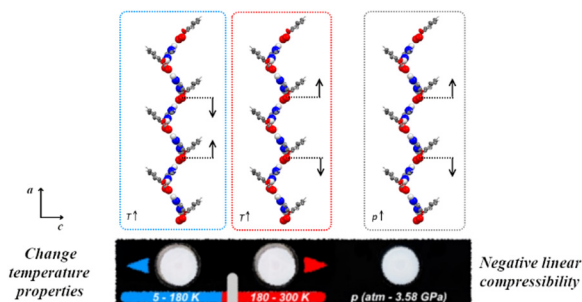
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Influence of cation nature on high pressure intrusion of aqueous salt solutions in pure silica MFI-type zeolite

Amir Astafan, Habiba Nouali, Gérald Chaplais, T. Jean Daou and Andrey Ryzhikov*

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Negative thermal expansion and linear compressibility in 1*H*-imidazol-3-ium 2-hydroxybenzoate with a helical network of hydrogen bonds

Sylvia Zięba*, Alina T. Dubis, Michalina Rusek, Andrzej Katrusiak, Andrzej Gzella and Andrzej Łapiński



CORRECTIONS

8570

Correction: High-level *ab initio* characterization of the OH + CH₃NH₂ reaction

Balázs Gruber and Gábor Czakó*

8571

Correction: Gas-phase, conformer-specific infrared spectra of 3-chlorophenol and 3-fluorophenol

Olga A. Duda, Alexander K. Lemmens, Gerrit C. Groenenboom, Daniel A. Horke and Joost M. Bakker*

8572

Correction: The p-block challenge: assessing quantum chemistry methods for inorganic heterocycle dimerizations

Thomas Gasevic, Markus Bursch,* Qianli Ma, Stefan Grimme, Hans-Joachim Werner* and Andreas Hansen*

