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Cover

See Kazuki Nakamura *et al.*, pp. 28800–28807.
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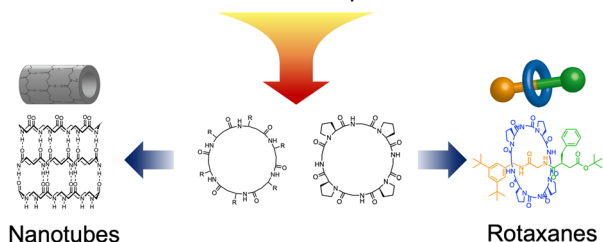
REVIEW

28776

The structural and functional impacts of rationally designed cyclic peptides on self-assembly-mediated functionality

Taichi Kurita and Keiji Numata*

Researcher's rule of thumb Computational simulations

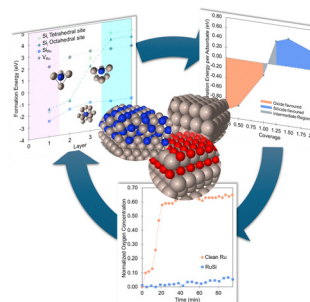


COMMUNICATION

28793

Coverage-dependent stability of Ru_xSi_y on $\text{Ru}(0001)$: a comparative DFT and XPS study

Jonathon Cottom, Stefan van Vliet, Jörg Meyer, Roland Bliem and Emilia Olsson*



Environmental Science: Atmospheres

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Fundamental questions
Elemental answers

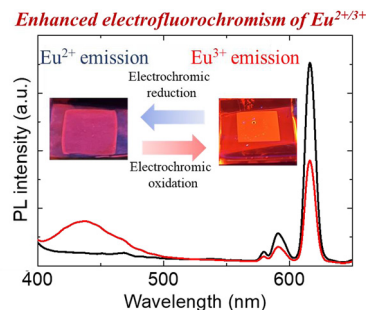


RESEARCH PAPERS

28800

Electrofluorochromism based on the valence change of europium complexes in electrochemical devices with Prussian blue as the counter electrode

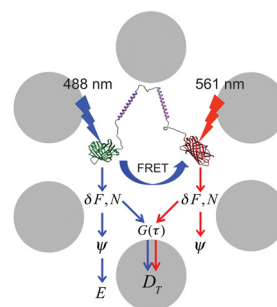
Ryoto Yabuta, Norihisa Kobayashi and Kazuki Nakamura*



28808

Translational diffusion, molecular brightness, and energy transfer analysis of mEGFP-linker-mScarlet-I crowding biosensor using fluorescence correlation spectroscopy

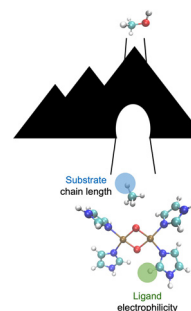
Sarah A. Mersch, Clint McCue, Alexandros Aristidou, Erin D. Sheets, Arnold J. Boersma* and Ahmed A. Heikal*



28819

Quantum effects in CH activation with $[\text{Cu}_2\text{O}_2]^{2+}$ complexes

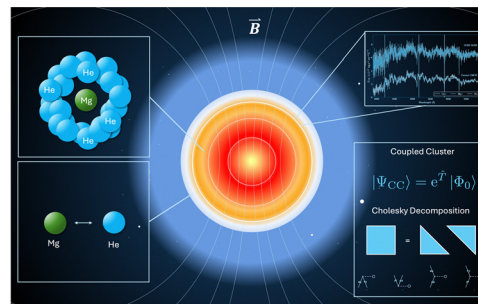
Selin Bac and Shaama Mallikarjun Sharada*



28828

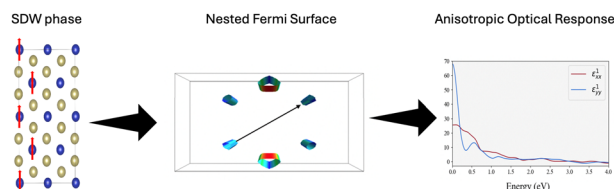
Finite-field Cholesky decomposed coupled-cluster techniques (ff-CD-CC): theory and application to pressure broadening of Mg by a He atmosphere and a strong magnetic field

Simon Blaschke, Marios-Petros Kitsaras and Stella Stopkiewicz*



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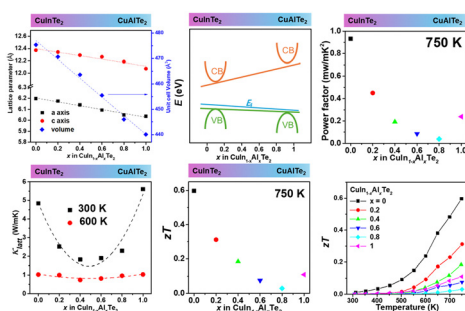
28849



Magnetic stability, Fermi surface topology, and spin-correlated dielectric response in monolayer 1T-CrTe₂

Ahmed Elrashidy* and Jia-An Yan

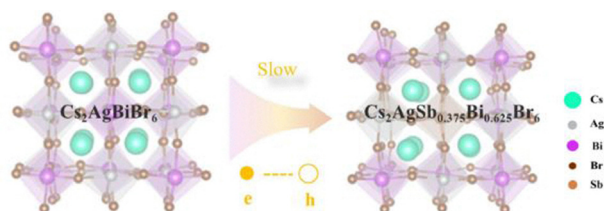
28858



Significant reduction of lattice thermal conductivity observed in CuInTe₂-CuAlTe₂ solid-solution alloys

Seungchan Seon, BeomSoo Kim, Okmin Park, Hyungyu Cho and Sang-il Kim*

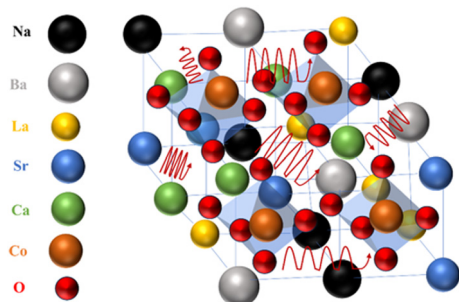
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Effect of Sb-Bi alloying on electron-hole recombination time of Cs₂AgBiBr₆ double perovskite

Yuzhuo Lv, Chang Liu, Yuhang Ma, Guodong Liu, Fei Wang, Yuhong Xia, Chundan Lin, Changjin Shao and Zhenqing Yang*

28874



Thermoelectric behavior of (Ba_{0.2}Sr_{0.2}Ca_{0.2}La_{0.2}Na_{0.2})CoO₃ high entropy cobaltate-based perovskite

Tathagata Bhattacharya, Ritwik Banerjee and Tanmoy Maiti*

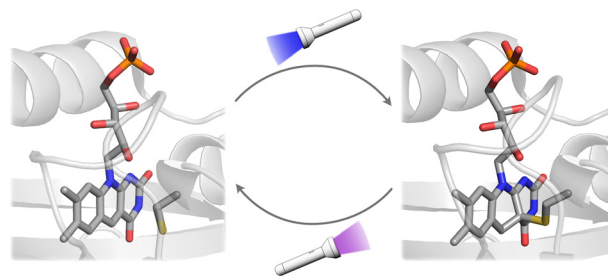


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Insights into the photoswitch based on 5-deazaFMN and LOV2 from *Avena sativa*: a combined absorption and NMR spectroscopy study

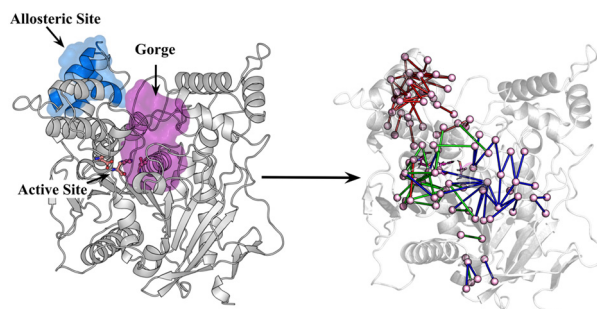
Sabrina Panter, Jakob Wörner, Jing Chen, Boris Illarionov, Adelbert Bacher, Markus Fischer and Stefan Weber*



28894

Elucidating the molecular mechanism of noncompetitive inhibition of acetylcholinesterase by an antidiabetic drug chlorpropamide: identification of new allosteric sites

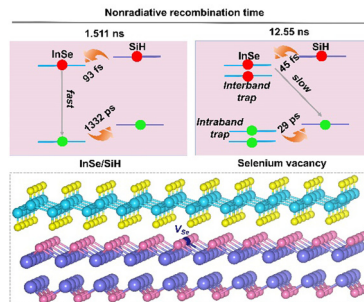
Abhinandan Das, Krishnendu Sinha and Suman Chakrabarty*



28904

Synergizing between interband and intraband defect states in prolonging the charge carrier lifetime of InSe/SiH heterojunctions

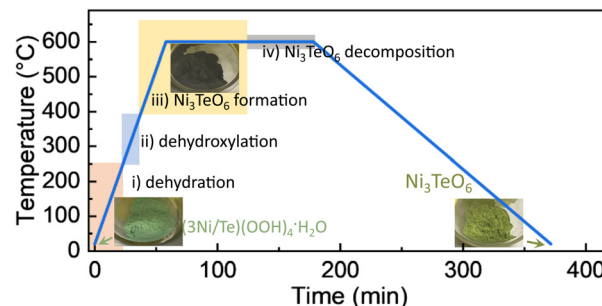
Qi Zhao and Jinlu He*



28913

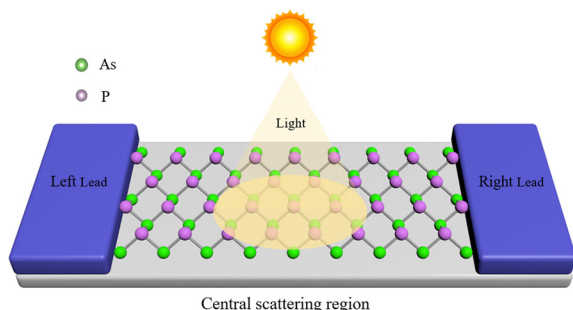
Insights into Ni_3TeO_6 calcination *via in situ* synchrotron X-ray diffraction

Shubo Wang,* Javier Fernández-Catalá, Qifeng Shu, Marko Huttula, Wei Cao and Harishchandra Singh*



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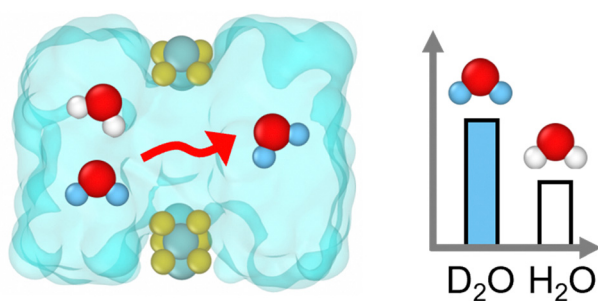
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Tunable electronic and optoelectronic characteristics of two-dimensional β -AsP monolayer: a first-principles study

Zhonghui Xu,* Kaiyu Wei, Zhenyu Wang, Junlin Jiang, Guogang Liu and San-Huang Ke

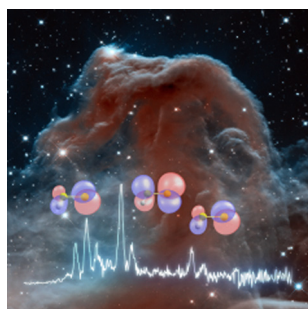
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Data-driven molecular dynamics simulation of water isotope separation using a catalytically active ultrathin membrane

Jinu Jeong, Chenxing Liang and Narayana R. Aluru*

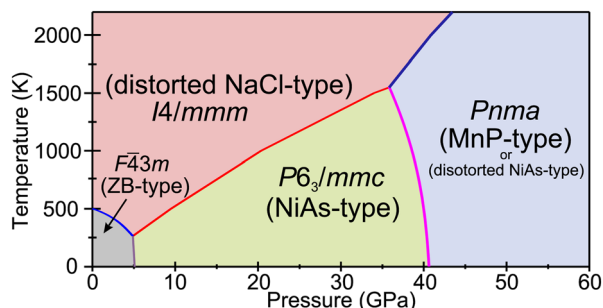
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Threshold photoelectron spectroscopy of organosulfur radicals

Emil Karaev, Marius Gerlach, Dorothee Schaffner, Sarah E. Dutton, Maggie D. Phillips, Patrick Hemberger,* AnGayle K. Vasiliou* and Ingo Fischer*

28947



Structure searching and phase relationships in MnN up to 50 GPa: a DFT study

Nursultan E. Sagatov,* Aitolkyn S. Omarkhan, Assyl-Dastan B. Bazarbek,* Abdirash T. Akilbekov and Dinara N. Sagatova

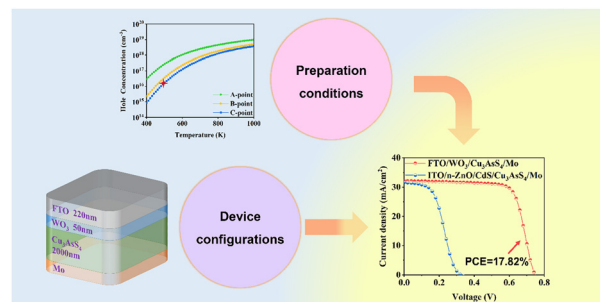


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Optimization of preparation conditions and design of device configurations for Cu_3AsS_4 solar cells: a combined study of first-principles calculations and SCAPS-1D device simulations

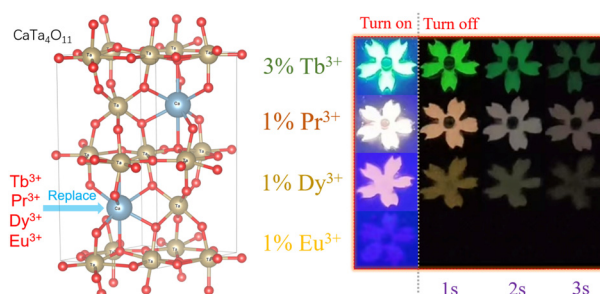
Yi Huang, Changqing Lin, Yang Xue, Binyuan Huang and Dan Huang*



28971

Molten salt synthesized Tb^{3+} , Pr^{3+} or Dy^{3+} single doped $\text{CaTa}_4\text{O}_{11}$ with persistent luminescence

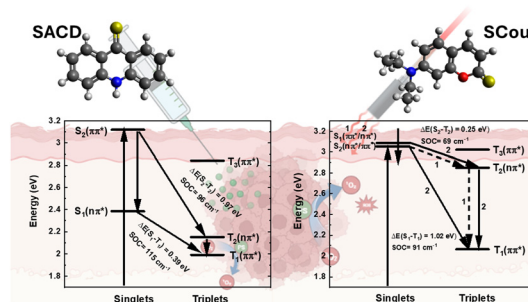
Yuhan Fan, Yongze Cao,* Meiling Li, Sai Xu, Yichao Wang, Xizhen Zhang, Jinsu Zhang and Baojiu Chen*



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Electronic relaxation pathways in thio-acridone and thio-coumarin: two heavy-atom-free photosensitizers absorbing visible light

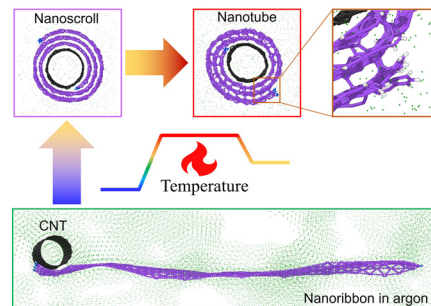
Chris Acquah, Sean Hoehn, Sarah Krul, Steffen Jockusch, Shudan Yang, Sourav Kanti Seth, Eric Lee, Han Xiao and Carlos E. Crespo-Hernández*



28992

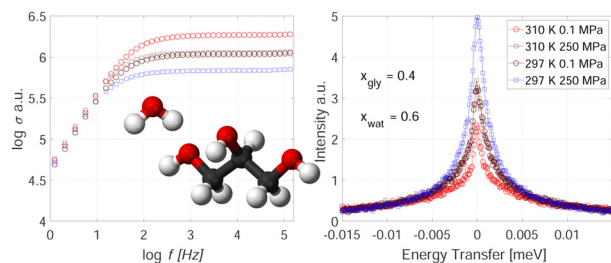
An annealing approach to form a nanotube from graphdiyne ribbon: a theoretical prediction

Bo Song, Kun Cai,* Jiao Shi and Qing-Hua Qin*



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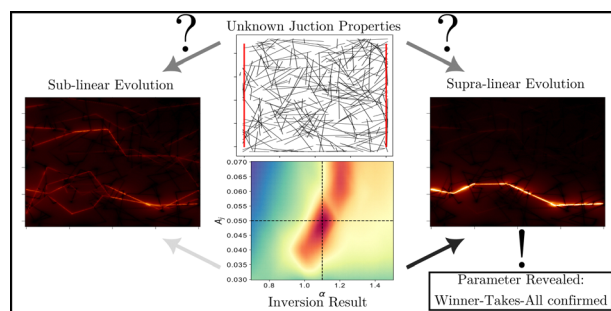
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Density scaling and isodynes in glycerol–water mixtures

David B. Noirat, Bernhard Frick, Bo Jakobsen, Markus Appel and Kristine Niss*

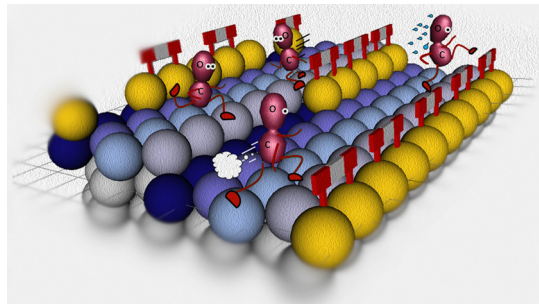
29015



Identifying winner-takes-all emergence in random nanowire networks: an inverse problem

F. R. Duarte,* S. Mukim, M. S. Ferreira and C. G. Rocha

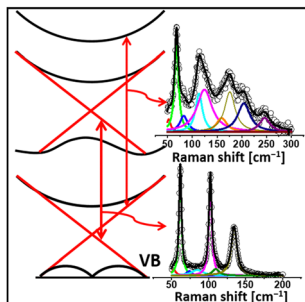
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The decisive role of Au in CO diffusion on Pt surfaces: a DFT study

Ana Lucía Reviglio,* Paula S. Cappellari,* German J. Soldano,* Marcelo M. Mariscal and Gabriel A. Planes

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Polarization-resolved resonant Raman excitation of surface and bulk electronic bands and phonons in MBE-grown topological insulator thin films

N. Kumar,* D. V. Ishchenko, I. A. Milekhin, P. A. Yunin, E. D. Kyrova, A. V. Korsakov and O. E. Tereshchenko

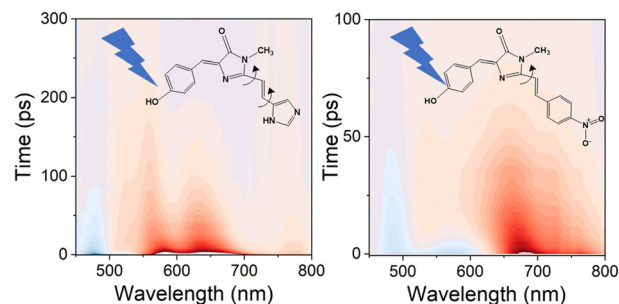


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Substituent effects on the photophysics of the kaede chromophore

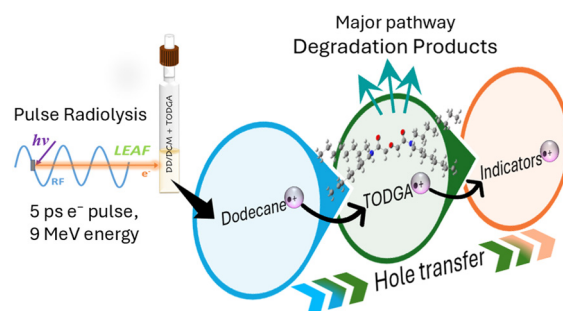
Anam Fatima, Giovanni Bressan, Eleanor K. Ashworth, Philip C. B. Page, James N. Bull* and Stephen R. Meech*



29060

Early-stage oxidation and subsequent damage of the used nuclear fuel extractant TODGA; electron pulse radiolysis and theoretical insights

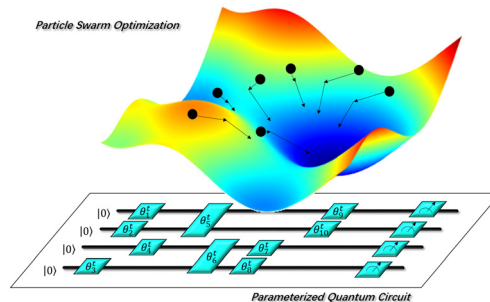
Rupali G. Deokar and Andrew R. Cook*



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Particle swarm optimization for a variational quantum eigensolver

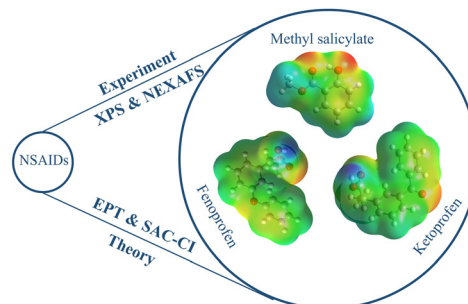
Hao Mei, Jianyu Zhao, Qing-Song Li, Zhao-Yun Chen, Jing-Jing Zhang, Qingchun Wang,* Yu-Chun Wu* and Guo-Ping Guo*



29082

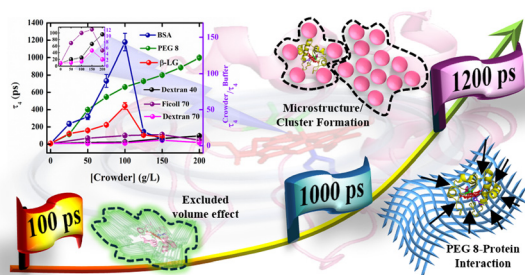
Insights into the electronic structure of non-steroidal anti-inflammatory drugs: soft X-ray study of fenoprofen, ketoprofen and methyl salicylate in the gas phase

Hanan Sa'adeh,* Assimo Maris,* Kevin C. Prince, Oksana Plekan, Cesare Grazioli, Marcello Coreno and Robert Richter



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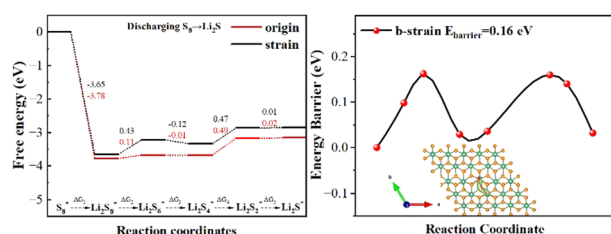
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Capturing ultrafast energy flow of a heme protein in crowded milieu

Shubhangi Majumdar, Ambika Prasad Kar, Jaydeep Basu and Pramit K. Chowdhury*

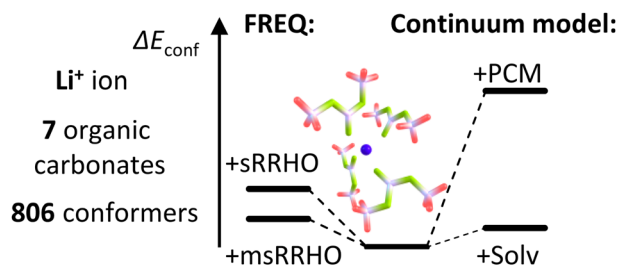
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Uniaxial tensile strain impact on 1T-NbS₂ monolayers as cathode material for lithium-sulfur batteries

Shanling Ren,* Xiaocong Tan, Xin Huang, Zhihong Yang and Yunhui Wang*

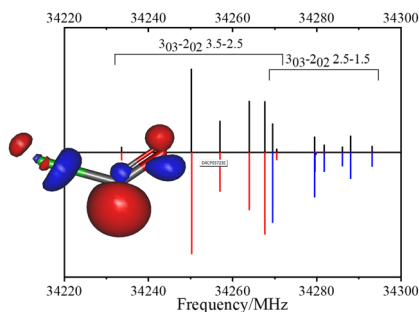
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A comprehensive guide for accurate conformational energies of microsolvated Li⁺ clusters with organic carbonates

Arseniy A. Otlyotov, Andrey D. Moshchenkov, Timofey P. Rozov, Anna A. Tuma, Alexander S. Ryzhako and Yury Minenkov*

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Fourier-transform microwave spectroscopy of the ClCO radical

Chin-Hua Chang, Chen-Hand Tsai and Yasuki Endo*

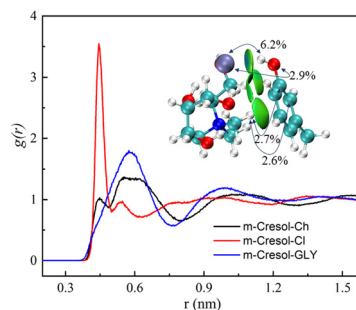


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Extraction mechanism of phenolic compounds by a choline chloride/glycerol solvent: DFT and molecular dynamics studies

Lan Yi,* Jinwen Wang, Jixing Liu, Hao Luo, Xiaoqin Wu and Wen-Ying Li*



29150

Intermolecular hydrogen bonding delineates the stability of non-canonical adenine base pairs: a first-principles study

Nicholas Adu-Effah and Nabanita Saikia*

