

## IN THIS ISSUE

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### Cover

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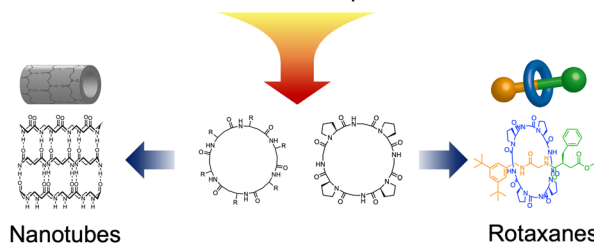
## REVIEW

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

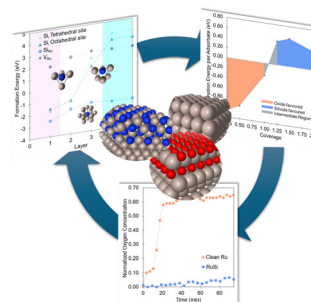


## COMMUNICATION

28793

### Coverage-dependent stability of $\text{Ru}_x\text{Si}_y$ 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



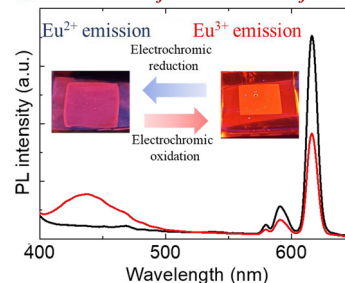
## RESEARCH PAPERS

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\*

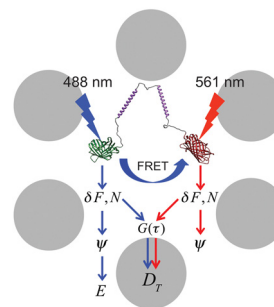
#### Enhanced electrofluorochromism of $\text{Eu}^{2+/3+}$



28808

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

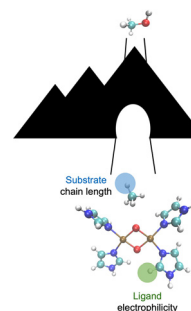
Sarah A. Mersch, Clint McCue, Alexandros Aristidou, Erin D. Sheets, Arnold J. Boersma\* and Ahmed A. Heikal\*



28819

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

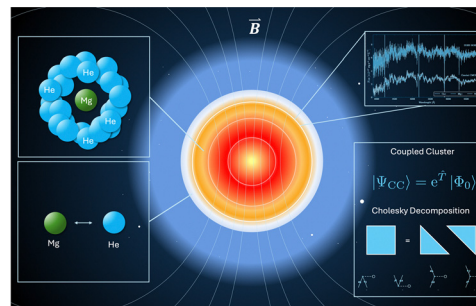
Selin Bac and Shaama Mallikarjun Sharada\*



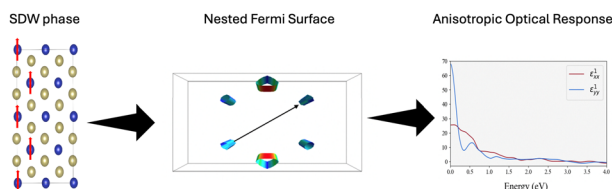
28828

### 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 Stopkowicz\*



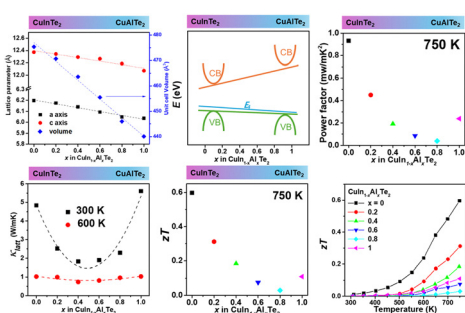
28849



### Magnetic stability, Fermi surface topology, and spin-correlated dielectric response in monolayer 1T-CrTe<sub>2</sub>

Ahmed Elrashidy\* and Jia-An Yan

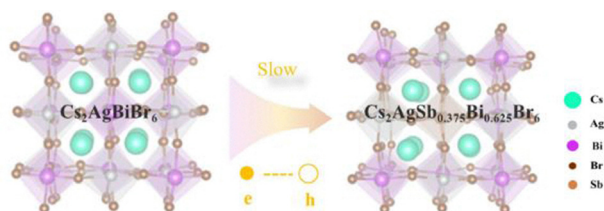
28858



### Significant reduction of lattice thermal conductivity observed in CuInTe<sub>2</sub>-CuAlTe<sub>2</sub> solid-solution alloys

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

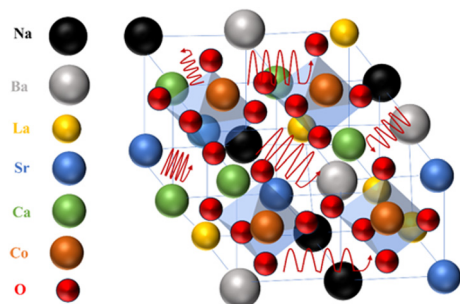
28865



### Effect of Sb-Bi alloying on electron-hole recombination time of Cs<sub>2</sub>AgBiBr<sub>6</sub> 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<sub>0.2</sub>Sr<sub>0.2</sub>Ca<sub>0.2</sub>La<sub>0.2</sub>Na<sub>0.2</sub>)CoO<sub>3</sub> high entropy cobaltate-based perovskite

Tathagata Bhattacharya, Ritwik Banerjee and Tanmoy Maiti\*

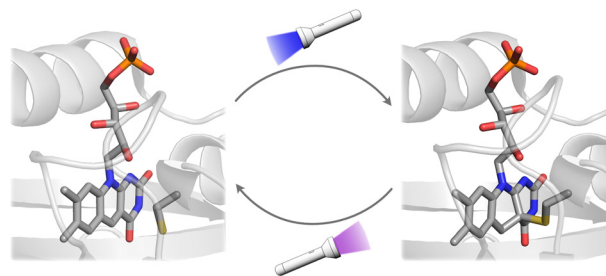


## RESEARCH PAPERS

28884

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

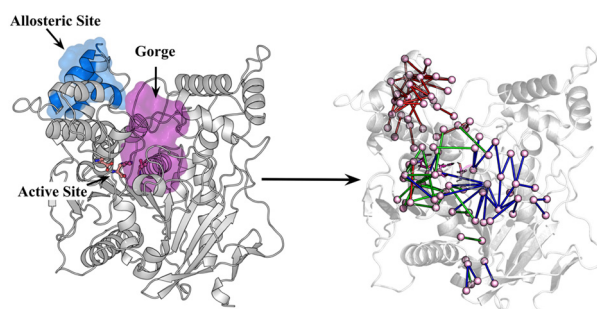
Sabrina Panter, Jakob Wörner, Jing Chen, Boris Illarionov, Adelbert Bacher, Markus Fischer and Stefan Weber\*



28894

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

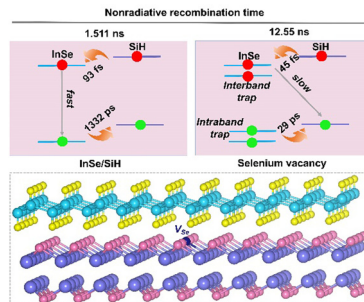
Abhinandan Das, Krishnendu Sinha and Suman Chakrabarty\*



28904

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

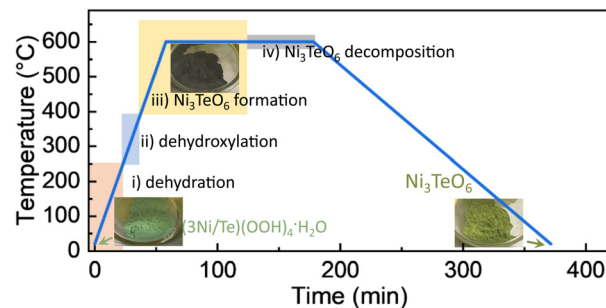
Qi Zhao and Jinlu He\*



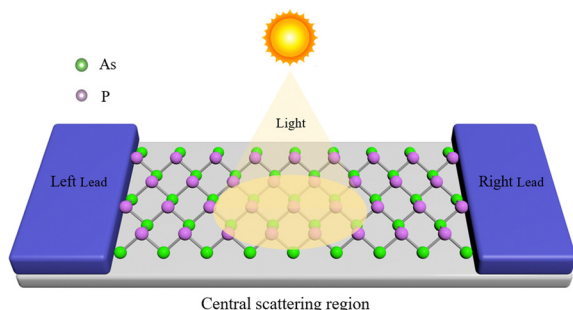
28913

### Insights into $\text{Ni}_3\text{TeO}_6$ calcination *via in situ* synchrotron X-ray diffraction

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



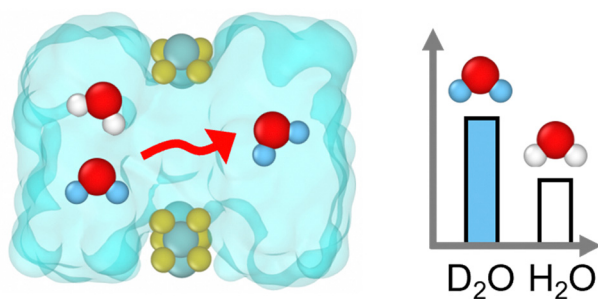
28922



### Tunable electronic and optoelectronic characteristics of two-dimensional $\beta$ -AsP monolayer: a first-principles study

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

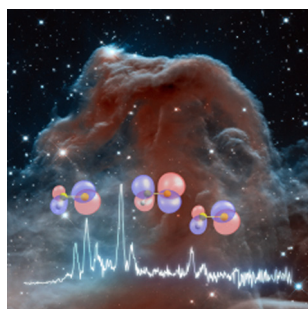
28929



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

Jinu Jeong, Chenxing Liang and Narayana R. Aluru\*

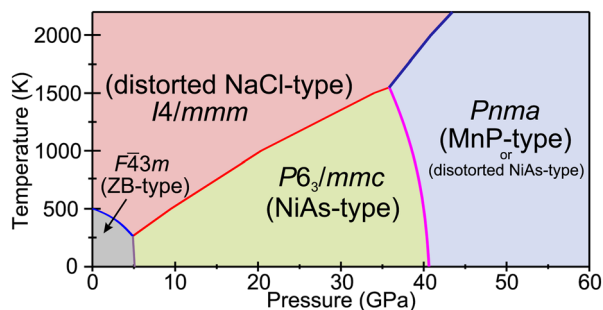
28939



### 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

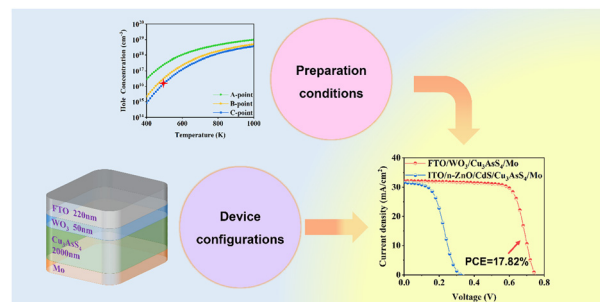
Nursultan E. Sagatov,\* Aitolkyn S. Omarkhan, Assyl-Dastan B. Bazarbek,\* Abdirash T. Akilbekov and Dinara N. Sagatova



28958

### Optimization of preparation conditions and design of device configurations for $\text{Cu}_3\text{AsS}_4$ solar cells: a combined study of first-principles calculations and SCAPS-1D device simulations

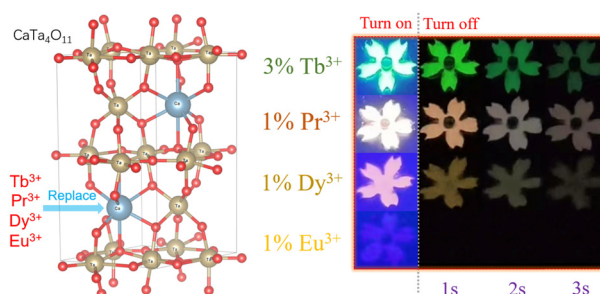
Yi Huang, Changqing Lin, Yang Xue, Binyuan Huang and Dan Huang\*



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

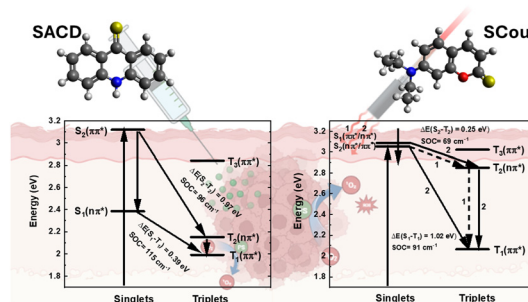
Yuhan Fan, Yongze Cao,\* Meiling Li, Sai Xu, Yichao Wang, Xizhen Zhang, Jinsu Zhang and Baojiu Chen\*



28980

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

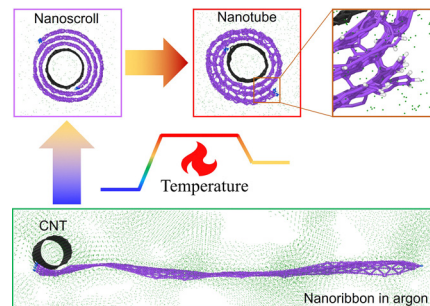
Chris Acquah, Sean Hoehn, Sarah Krul, Steffen Jockusch, Shudan Yang, Sourav Kanti Seth, Eric Lee, Han Xiao and Carlos E. Crespo-Hernández\*



28992

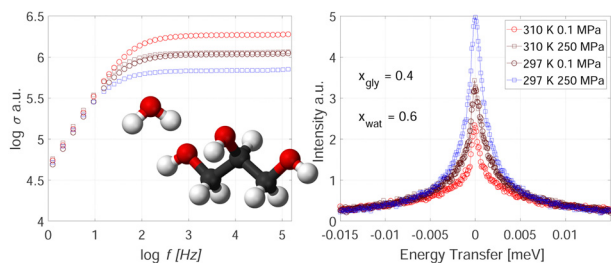
### An annealing approach to form a nanotube from graphdiyne ribbon: a theoretical prediction

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



## RESEARCH PAPERS

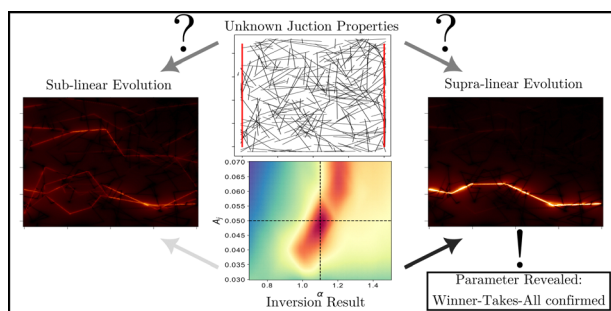
29003



### Density scaling and isodynes in glycerol–water mixtures

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

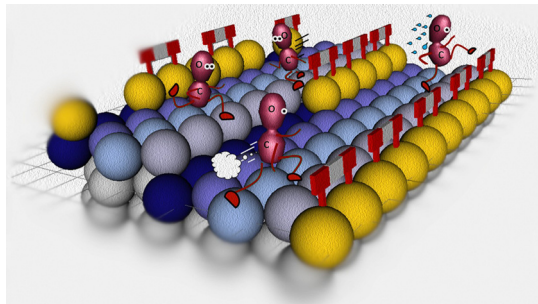
29015



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

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

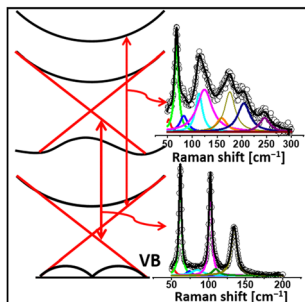
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### The decisive role of Au in CO diffusion on Pt surfaces: a DFT study

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

29036



### 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

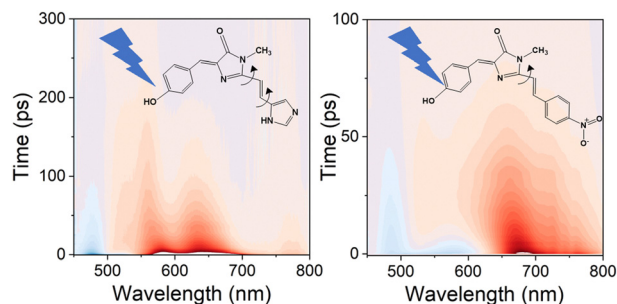


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29048

**Substituent effects on the photophysics of the kaede chromophore**

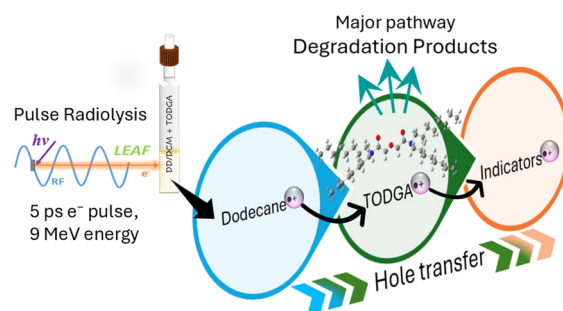
Anam Fatima, Giovanni Bressan, Eleanor K. Ashworth, Philip C. B. Page, James N. Bull\* and Stephen R. Meech\*



29060

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

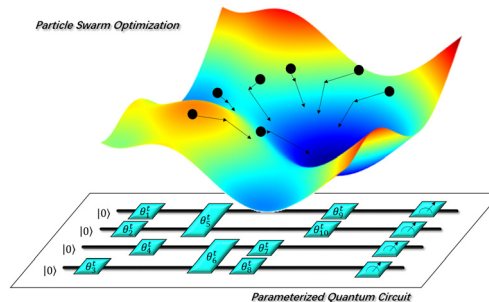
Rupali G. Deokar and Andrew R. Cook\*



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**Particle swarm optimization for a variational quantum eigensolver**

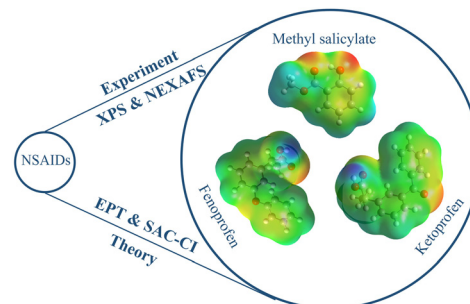
Hao Mei, Jianyu Zhao, Qing-Song Li, Zhao-Yun Chen, Jing-Jing Zhang, Qingchun Wang,\* Yu-Chun Wu\* and Guo-Ping Guo\*



29082

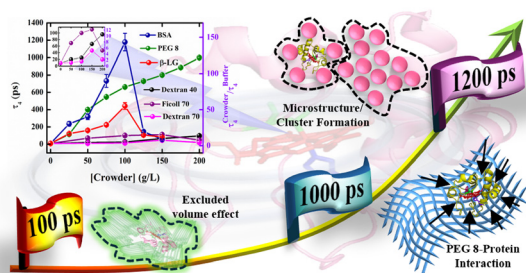
**Insights into the electronic structure of non-steroidal anti-inflammatory drugs: soft X-ray study of fenoprofen, ketoprofen and methyl salicylate in the gas phase**

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



## RESEARCH PAPERS

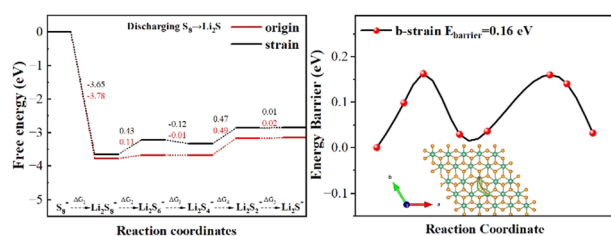
29095



### Capturing ultrafast energy flow of a heme protein in crowded milieu

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

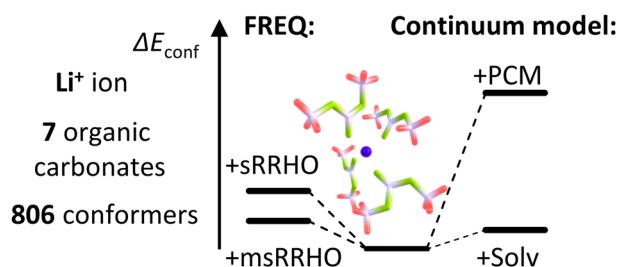
29110



### Uniaxial tensile strain impact on 1T-NbS<sub>2</sub> monolayers as cathode material for lithium-sulfur batteries

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

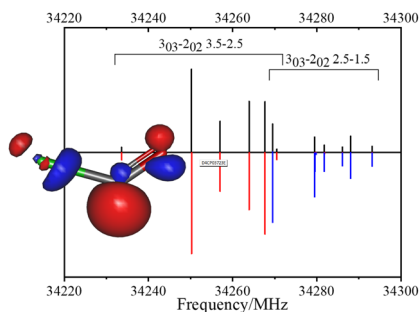
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### A comprehensive guide for accurate conformational energies of microsolvated Li<sup>+</sup> clusters with organic carbonates

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

29133



### Fourier-transform microwave spectroscopy of the ClCO radical

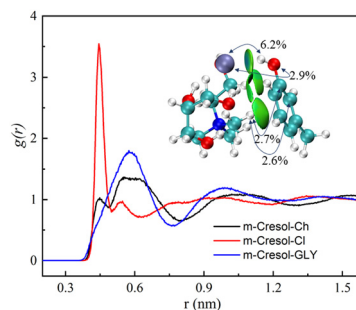
Chin-Hua Chang, Chen-Hand Tsai and Yasuki Endo\*



29140

### 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\*

