

## IN THIS ISSUE

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### Cover

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### Inside cover

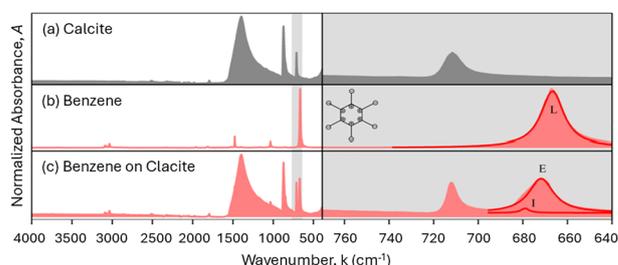
See Stefan Weber *et al.*, pp. 22911–22923. Image reproduced by permission of Sabina Panter from *Phys. Chem. Chem. Phys.*, 2025, 27, 22911.

## REVIEW

22871

### Infrared spectroscopy at the surface of carbonates

Taha Elgayyar,\* Federico Azzolina-Jury and Frédéric Thibault-Starzyk

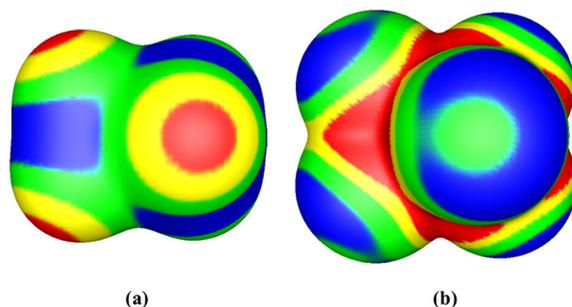


## PERSPECTIVES

22880

### The anomalous nature of fluorine revisited: amazing consequences

Jane S. Murray



# Environmental Science: Atmospheres

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Fundamental questions  
Elemental answers

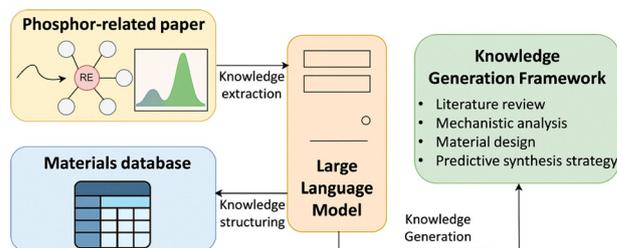


## PERSPECTIVES

22885

### Construction of an artificial-intelligence agent for the discovery of next-generation white-LED phosphors

Zichun Zhou, Han Zhang, Chi Song, Chen Ming\* and Yi-Yang Sun\*

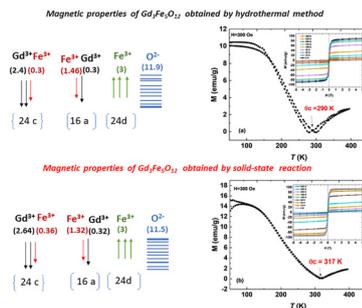


## COMMUNICATIONS

22894

### Cation distribution and its magnetic implications in gadolinium–iron garnets for an enhanced control of compensation temperature

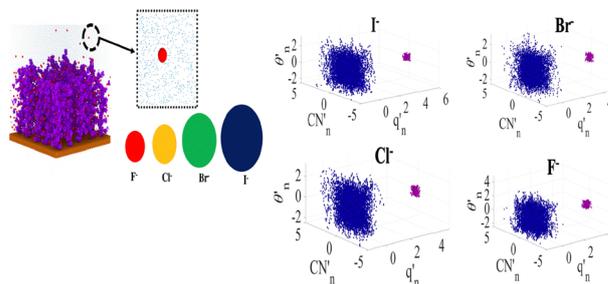
Cristina Bartha, Claudiu Locovei, Andrei Alexandru-Dinu, Cezar Comanescu, Mihai Alexandru Grigoroscuta, Andrei Kuncser, Nicusor Iacob, Magda Galatanu, Aurel Leca, Petre Badica\* and Victor Kuncser\*



22901

### Combined machine learning and atomistic simulations reveal multi-state hydration in cationic brushes in the presence of halide counterions

Raashiq Ishraaq and Siddhartha Das\*

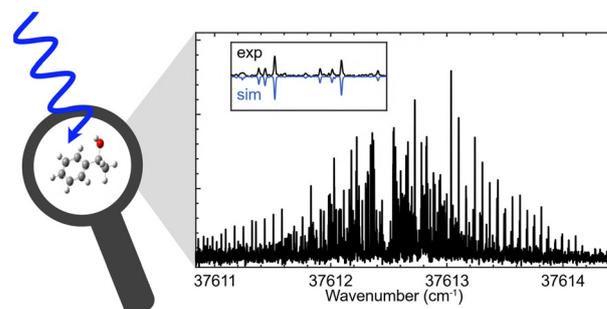


## RESEARCH PAPERS

22906

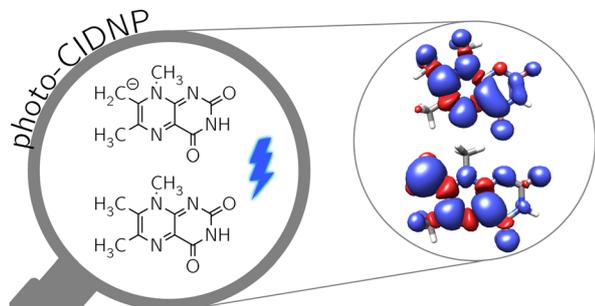
### High-resolution UV spectroscopy of the chiral molecule 1-phenylethanol

Shilpa Yadav, JuHyeon Lee, Gerard Meijer and Sandra Eibenberger-Arias\*



## RESEARCH PAPERS

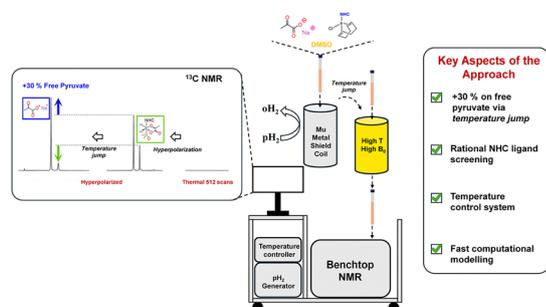
22911



## Investigation of 6,7,8-trimethylumazine and its radicals by NMR and photo-CIDNP spectroscopy

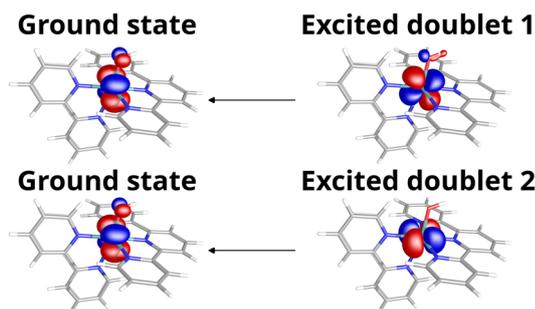
Sabrina Panter, Boris Illarionov, Jing Chen, Adelbert Bacher, Markus Fischer and Stefan Weber\*

22924

(De)coding SABRE of [1-<sup>13</sup>C]pyruvate

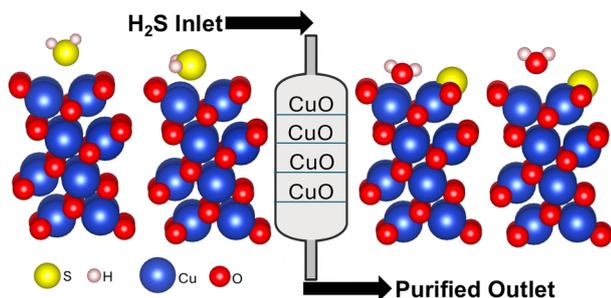
Salvatore Mamone, Federico Floreani, Ahmed Mohammed Faramawy, Claudia Graiff, Lorenzo Franco, Marco Ruzzi, Cristina Tubaro and Gabriele Stevanato\*

22937

Multiconfigurational electronic structure calculations explain the role of ligands in *g*-tensor anisotropy for Ru<sup>III</sup> complexes

Pavel Pokhilko\* and Yulia Pushkar\*

22954

On the mechanism of reactive sorption of H<sub>2</sub>S on CuO (111) and ( $\bar{1}\bar{1}\bar{1}$ ) surfaces: a first-principles study

David Jiang, Nicole Chiang, Tirso López-Ausens and Philippe Sautet\*

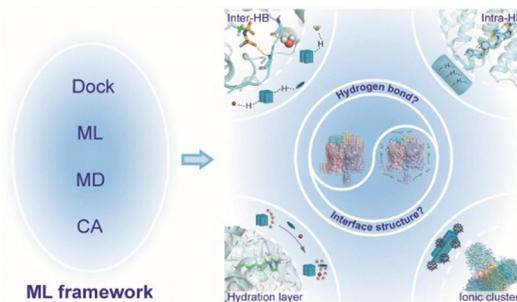


## RESEARCH PAPERS

22964

### Insights into ionic liquid-enhanced membrane protein stability through machine learning and molecular simulations

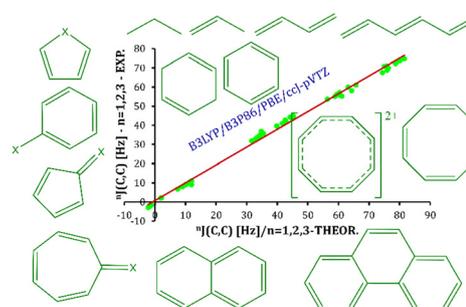
Ju Liu, Guiming Zhang, Cheng Song, Yanlei Wang,\*  
Jing Ren\* and Hongyan He



22974

### SD aromaticity index: a new assessment of aromaticity based on Ramsey spin dipolar contribution to NMR spin–spin coupling constants

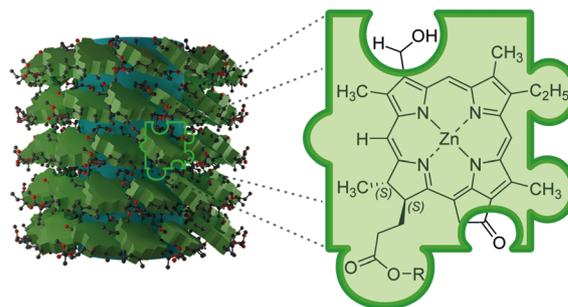
M. Natalia C. Zarycz,\* M. Ayelén Schiel, Héctor A. Baldoni  
and Ricardo D. Enriz



22990

### Substituent effects on the supramolecular arrangement in bio-inspired chlorin nanotubes

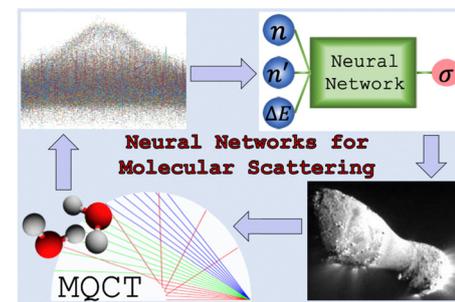
Michael Bühler, Richard Einsele and Merle I. S. Röhr\*



23000

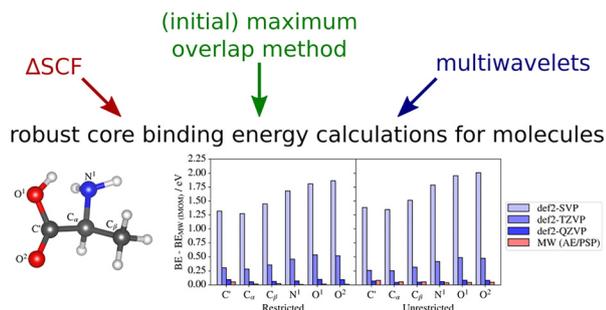
### Neural network ensemble for computing cross sections of rotational transitions in H<sub>2</sub>O + H<sub>2</sub>O collisions

Bikramaditya Mandal, Dmitri Babikov, Phillip C. Stancil,  
Robert C. Forrey, Roman V. Krems and  
Naduvalath Balakrishnan\*



## RESEARCH PAPERS

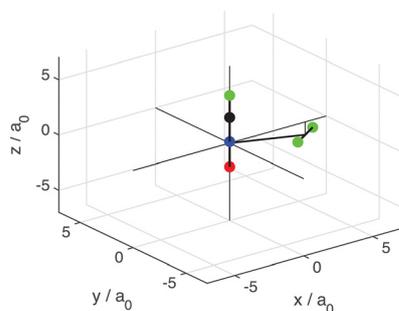
23013



### Combining the maximum overlap method with multiwavelets for core-ionisation energy calculations

Niklas Göllmann, Matthew R. Ludwig, Peter Wind, Laura E. Ratcliff\* and Luca Frediani

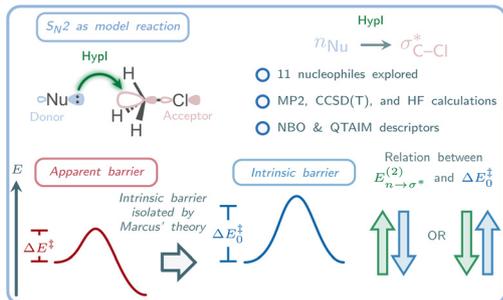
23022



### Rotational excitation of fulminic acid (HCNO) in collisions with molecular hydrogen

Paul J. Dagdigan

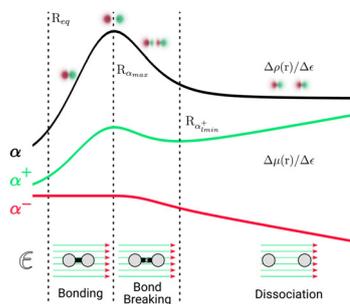
23030



### How the $n_{Nu} \rightarrow \sigma_{C-Cl}^*$ hyperconjugation interaction affects intrinsic reactivity in an $S_N2$ reaction

Leonardo Saravia F., Jorge Gutiérrez-Flores, Eduardo H. Huerta,\* Jorge Garza, Rubicelia Vargas\* and Marcos Hernández-Rodríguez\*

23044



### Unraveling chemical bonding mechanisms through dipole moment variations under external electric fields

Jorge Charry,\* Matteo Barborini and Alexandre Tkatchenko\*

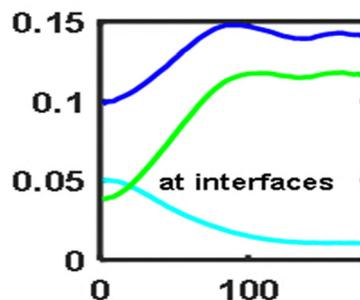


## RESEARCH PAPERS

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## Origin of the nonresonant signal in sum-frequency vibrational spectroscopy at the water interface

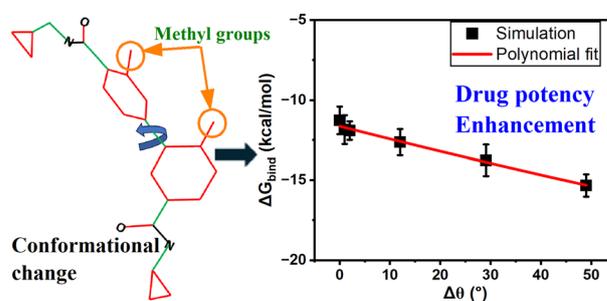
Ren-Hui Zheng\* and Wen-Mei Wei\*



23065

## Mechanism of drug-potency enhancement via methylation

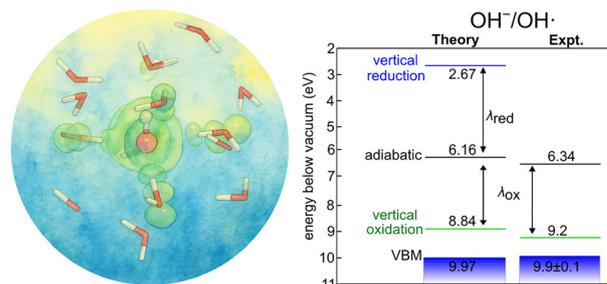
Goga Ram and Nirmalya Bachhar\*



23079

## Electronic energy levels of aqueous hydroxyl species

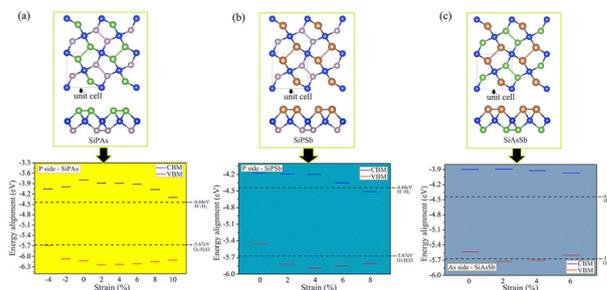
Francesco Ambrosio,\* Wei Chen and Alfredo Pasquarello\*



23091

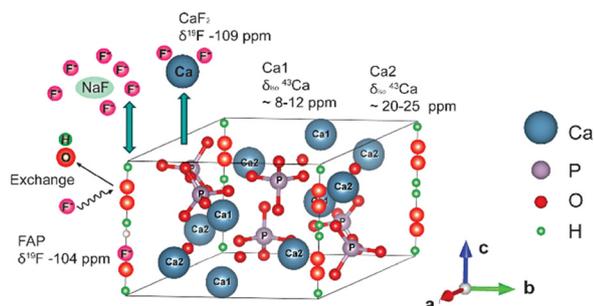
## Pentagonal Janus SiXY monolayers: a new frontier for 2D photocatalysis with high solar-to-hydrogen efficiency

Gang Guo,\* Congsheng Xu\* and Ping Li



## RESEARCH PAPERS

23105



### Calcium environments, proton defects, and facet-dependent fluoride interactions in hydroxyapatite nanostructures probed by multinuclear solid-state NMR

Yuan Li, Brianna Duarte and Gregory P. Holland\*

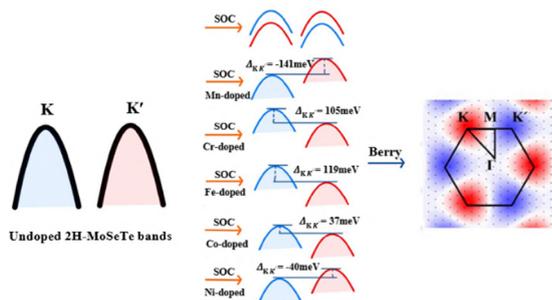
23116



### Magnesium perfluorinated pinacolborate in diglyme: understanding microscopic structures in rechargeable magnesium batteries

Nadezhda A. Andreeva and Vitaly V. Chaban\*

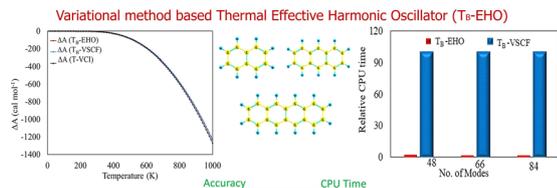
23127



### A first-principles study on the effects of 3d transition metal dopants on the valleytronic properties of Janus-type 2H-MoSeTe monolayers

Kai Cheng,\* Peng Wu, Haoran Cui, Shijie Guo, Jianpei Xing,\* Sandong Guo and Yan Su

23139



### A reduced-parameter variational strategy for accelerated evaluation of thermal density matrices via quantum effective harmonic oscillators approach

Mokshi Sharma and Tapta Kanchan Roy\*

Variational parameters:  $Q_i^0, \omega_i^2$ 

$$Q_i^0 = \frac{1}{2f_{ii}} \left[ \sum_{jj} f_{ij} Q_j^0 Q_j^0 + \sum_{jj} f_{ij} Q_j^0 Q_j^0 + 3 \left( f_{ii} \frac{\langle \coth \theta_i \rangle}{2\omega_i} + \sum_{jj} f_{ij} \frac{\langle \coth \theta_j \rangle}{2\omega_j} \right) Q_i^0 \right] + \left\{ \sum_{jj} f_{ij} \frac{\langle \coth \theta_j \rangle}{2\omega_j} + \sum_{jj} f_{ij} \frac{\langle \coth \theta_j \rangle}{2\omega_j} \right\} Q_i^0$$

$$\omega_i^2 = 2f_{ii} + 2 \sum_{jj} f_{ij} Q_j^0 Q_j^0 + 6f_{ii} \frac{\langle \coth \theta_i \rangle}{\omega_i} + \sum_{jj} f_{ij} \frac{\langle \coth \theta_j \rangle}{\omega_j}$$

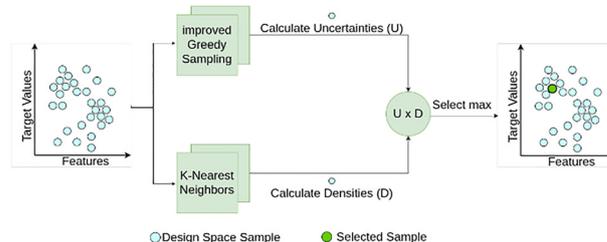


## RESEARCH PAPERS

23152

### Density-aware active learning for materials discovery: a case study on functionalized nanoporous materials

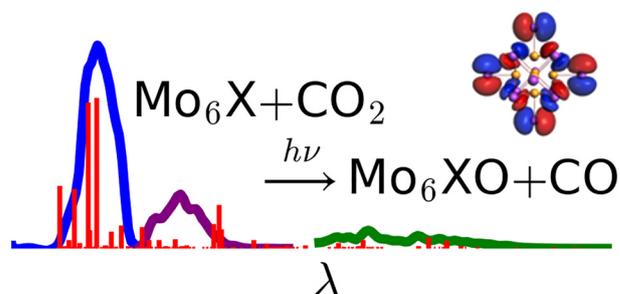
V. Gkatsis, P. Maratos, C. Rekatsinas,\*  
G. Giannakopoulos and P. Krokidas\*



23166

### Gas-phase reactivity of hexanuclear molybdenum $[\text{Mo}_6\text{I}_{14}]^{2-}$ and its photo-fragments towards $\text{O}_2$ and $\text{CO}_2$ : combined mass spectrometry ( $\text{MS}^n$ ) and quantum chemical simulations

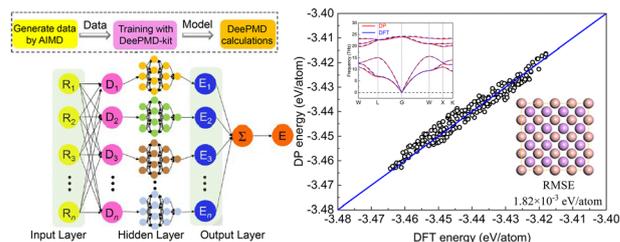
Aikaterini Tsirkou, Nina Tyminska, Richard A. J. O'Hair,  
Fabien Grasset, Yann Molard, Karine Costuas,\*  
Stéphane Cordier\* and Luke MacAleese\*



23179

### Deep learning interatomic potential for boron phosphide: accurate prediction of mechanical and thermal properties

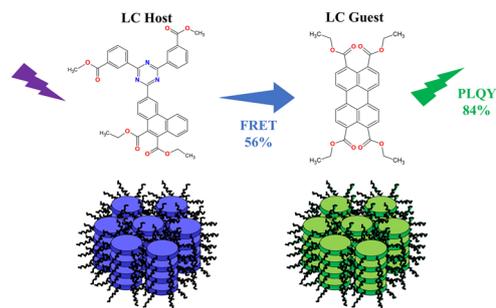
Kai Ren, Chao Lv, Yang Wang, Chao Zhang\* and  
Dong-Qi Wang\*



23187

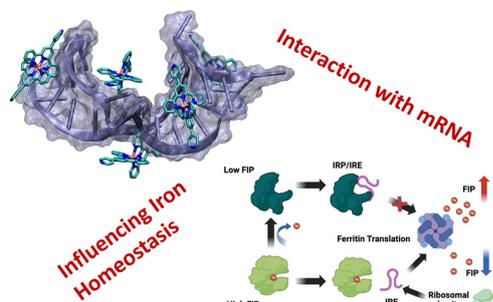
### Columnar liquid crystal as alignable host for perylene-based emitters

Feik Amil de Campos, Carlos H. Stadlober,  
Lorenzo C. Serra, Arthur Felipe Zito Santos,  
Thiago Cazati, Juliana Eccher, André Alexandre Vieira,  
Harald Bock, Andrew P. Monkman and Ivan H. Bechtold\*



## RESEARCH PAPERS

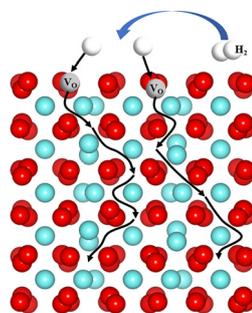
23193



### Influencing iron homeostasis by a transition metal complex interacting with a messenger-RNA stem loop in the iron regulating element

Cécilia Hognon, Aurane Froux, Stéphanie Grandemange\* and Antonio Monari\*

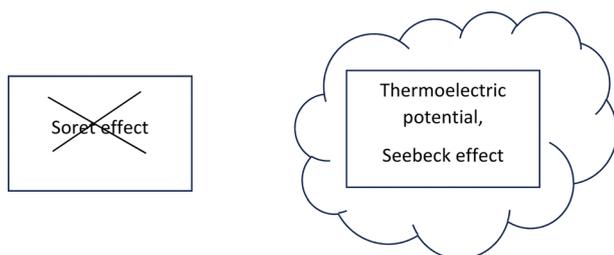
23202



### First-principles study on surface and internal hydrogen diffusion of $Y_2O_3$

Weihao Ye, Chuan-Hui Zhang\* and Liwu Jiang\*

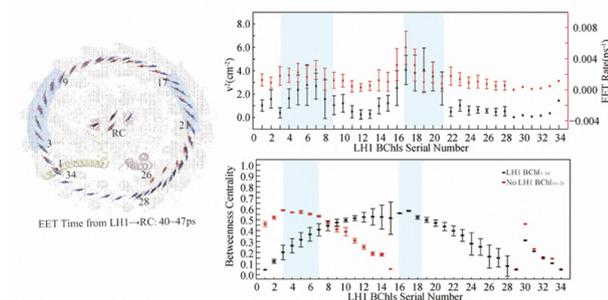
23215



### Soret-decoupled thermoelectric potential in binary highly ionized liquids

Semen N. Semenov\* and Martin E. Schimpf

23223



### Investigation of the excitation energy transfer pathways of photosynthetic RC-LH1 supercomplexes

Meng-Ying Tong, Qian Jiang, Ao Shen, Bern M. Christianson, Li-Hua Bie,\* Lu-Ning Liu\* and Jun Gao\*

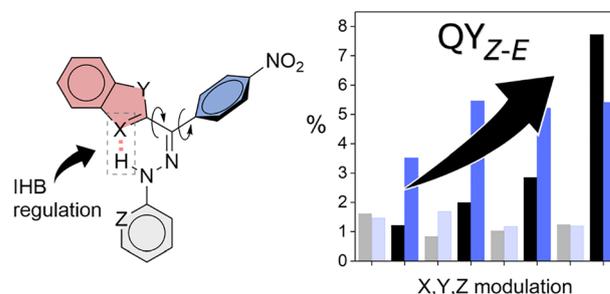


## RESEARCH PAPERS

23234

### Modulation of triarylhydrazone photoswitching efficiency through heteroaryl variations

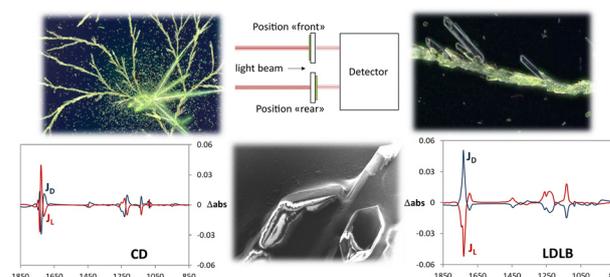
Lea Hegedúsová, Šimon Budzák, Miroslav Medved', Lukáš F. Pašteka, Juraj Filo, Bernard Mravec, Anna M. Grabarz\* and Marek Cigáň\*



23245

### Tuning linear dichroism/birefringence (LDLB) contributions in VCD spectra of tartaric acid-TPPS<sub>4</sub> porphyrin films

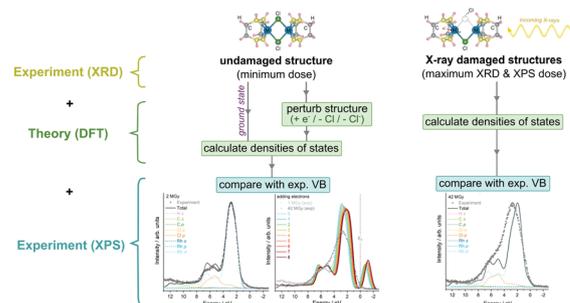
Giuseppe Mazzeo, Marco Fusè, Sergio Abbate, Roberto Zagami, Maria Angela Castriciano, Andrea Romeo, Luigi Monsù Scolaro\* and Giovanna Longhi\*



23257

### Simulation of radiation damage on [M(COD)Cl]<sub>2</sub> using density functional theory

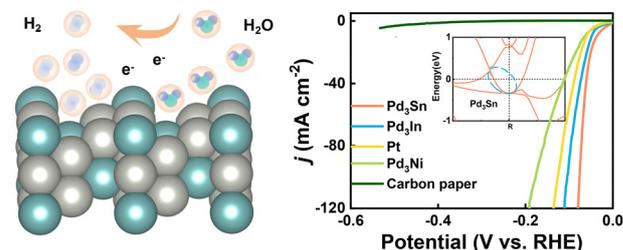
Nathalie K. Fernando,\* Nayera Ahmed, Katherine Milton, Claire A. Murray, Anna Regoutz and Laura E. Ratcliff



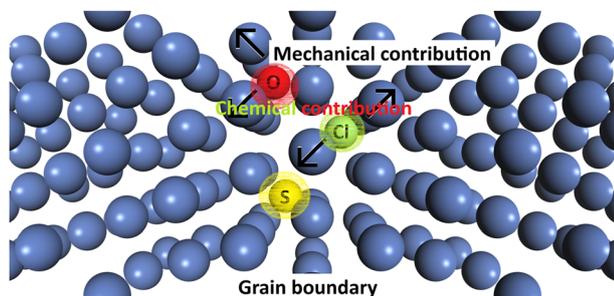
23270

### Topological quantum materials for enhanced hydrogen evolution: role of bulk band structures in Pd-based alloys

Meixia Su, Yuhao Zhang, Youshun Wang, Shuocheng Qiu, Yu Zhao, Xin Chen, Yan Ding, Kun Tao, Erqing Xie and Zhenxing Zhang\*



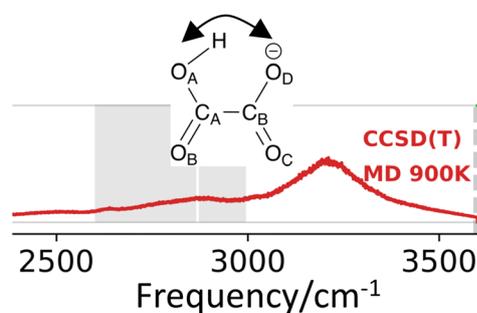
23277



### First-principles study of the effect of the corrosive environmental components on the grain boundary strength in nickel

Azamat Mukhametov, Insaf Samikov, Elena A. Korznikova and Andrey A. Kistanov\*

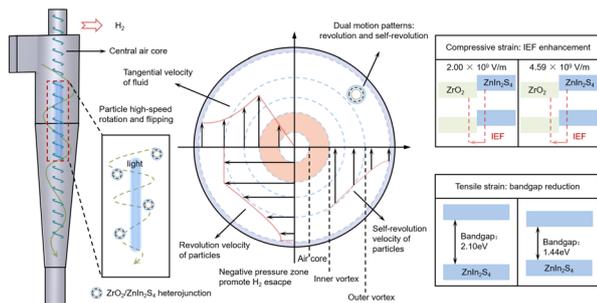
23288



### Dynamics of protonated oxalate from machine-learned simulations and experiment: infrared signatures, proton transfer dynamics and tunneling splittings

Valerii Andreichev, Silvan Käser, Erica L. Bocanegra, Madeeha Salik, Mark A. Johnson and Markus Meuwly\*

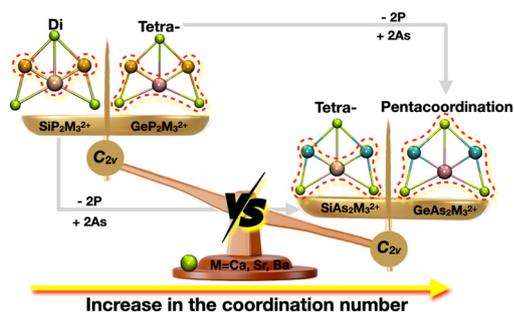
23301



### Strain-driven electronic structure modulation in $\text{ZrO}_2/\text{ZnIn}_2\text{S}_4$ S-scheme heterojunctions: a theoretical study of multiscale modelling

Zhengdai Zhang, Danhui Yang,\* Yizhou Yang,\* Fanghe Zhou, Lixia Zhao, Yawei Wang and Xuejing Yang

23313



### Planar pentacoordinate germanium stabilized by the 18-valence-electron rule: structural and bonding comparison with silicon analogues

Luz Diego, Diego V. Moreno, David Arias-Olivares and Rafael Islas\*

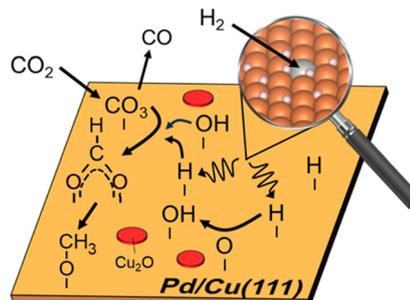


## RESEARCH PAPERS

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### Spillover hydrogen-driven CO<sub>2</sub> hydrogenation on a Pd/Cu(111) single atom alloy model catalyst at room temperature studied by ambient pressure X-ray photoelectron spectroscopy

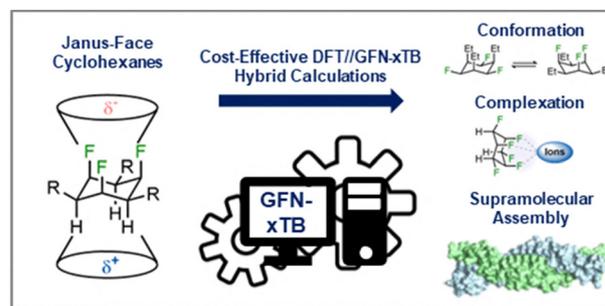
Wataru Osada, Fumihiko Ozaki, Shunsuke Tanaka, Kozo Mukai, Masafumi Horio, Iwao Matsuda, Takanori Koitaya, Susumu Yamamoto and Jun Yoshinobu\*



23336

### Performance of semiempirical DFT methods for the supramolecular assembly of Janus-face cyclohexanes

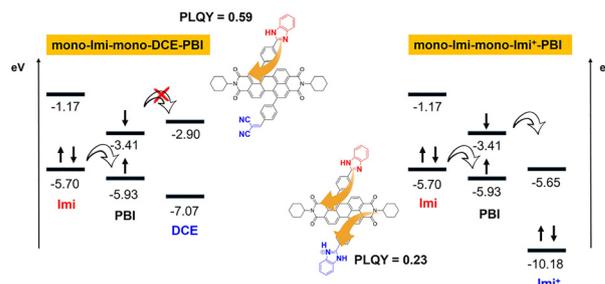
Bruno A. Piscelli, Tiger Swithenbank-Michel, Rodrigo A. Cormanich, David O'Hagan and Michael Bühl\*



23348

### Discrete component model to explain the photophysics of bay-functionalized perylene bisimide derivatives

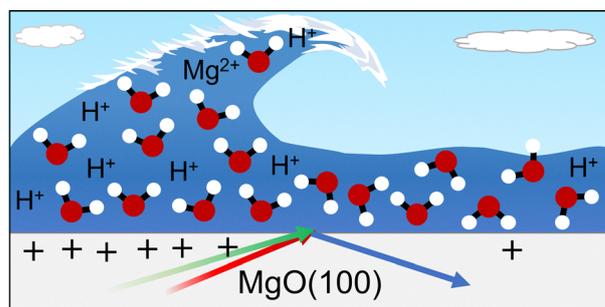
Chenbo Meng and Siegfried Eigler\*



23356

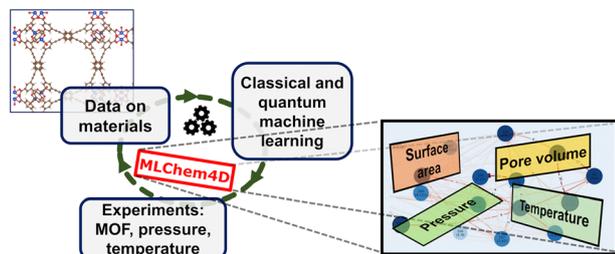
### MgO–water interface: structure and surface dissolution depend on flow and pH

Moritz Zelenka and Ellen H. G. Backus\*



## RESEARCH PAPERS

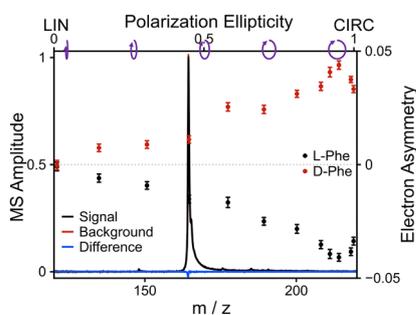
23365



### Seeking metal–organic frameworks for hydrogen storage using classical and quantum active learning

Maicon Pierre Lourenço,\* Rishabh Shukla,\*  
Mosayeb Naseri, Daya Gaur, Utkarsh Singh,  
Sergey Gusarov and Dennis R. Salahub

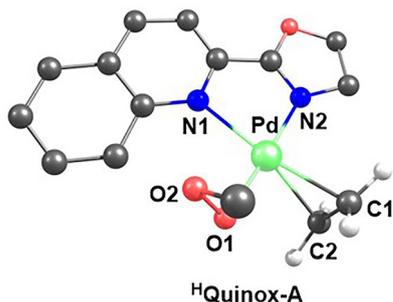
23380



### Single photon photoelectron elliptical dichroism of amino acid anions

Jon Henrik Both and Karl-Michael Weitzel\*

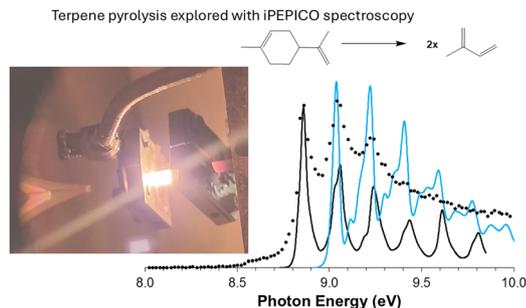
23386



### DFT mechanistic investigation of Wacker-type oxidation of olefins catalyzed by a Pd(II) quinoline-2-oxazoline complex: the effect of electronic asymmetry of the ligand

Tabasum Jan, Tasleema Jan, Muzzaffar Ahmad Bhat and  
Noor U Din Reshi\*

23400



### Monoterpene flash pyrolysis reveals weakly coupled mechanistic domains and fleeting biradical intermediates

Edgar White Buenger, Andras Bodi, Maxi A. Burgos-Paci  
and Paul M. Mayer\*

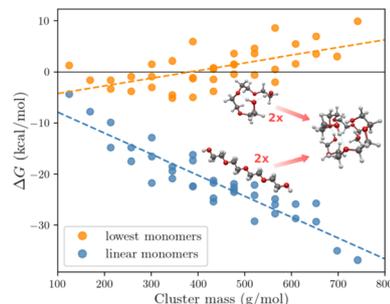


## RESEARCH PAPERS

23410

### Enhanced configurational sampling methods reveal the importance of molecular stiffness for clustering of oxygenated organic molecules

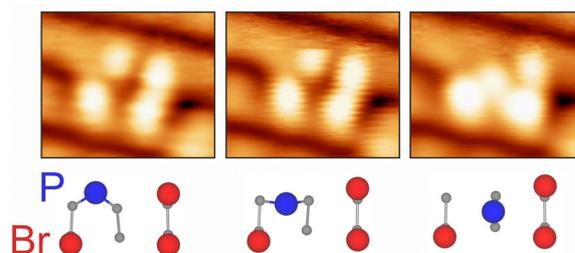
Jaakko Kähärä, Lauri Franzon, Stephen Ingram, Nanna Myllys, Theo Kurtén and Hanna Vehkamäki\*



23421

### Surface diffusion of phosphorus on Si(100) after $\text{PBr}_3$ adsorption

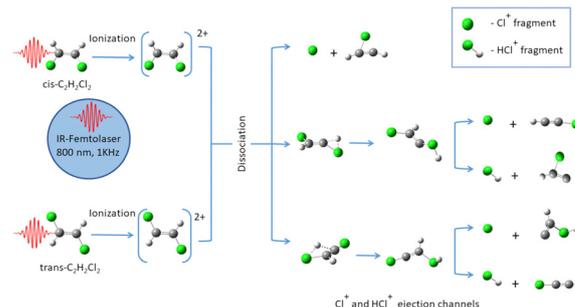
Tatiana V. Pavlova\* and Vladimir M. Shevlyuga



23428

### Strong-field induced ionization and dissociation of *cis*- and *trans*-1,2-dichloroethylene: $\text{Cl}^+$ and $\text{HCl}^+$ fragments

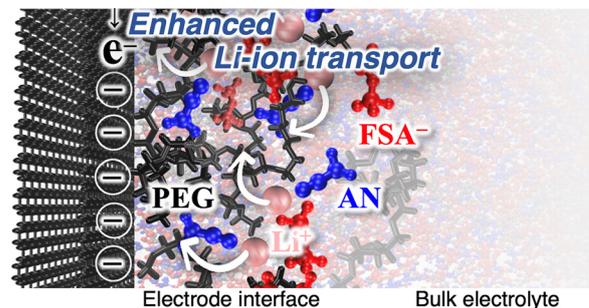
Ephraim Anto, Rituparna Das, Vinitha Nimma, Madhusudhan P, Pranav Bhardwaj, Pooja Chandravanshi, Rajesh Kumar Kushawaha and Koushik Saha\*



23438

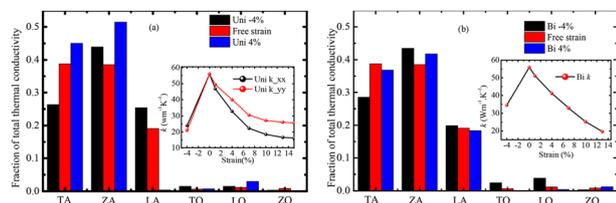
### Ion transport and structural properties of highly concentrated organogel electrolytes based on Tetra-arm PEG networks

Yuna Deguchi, Yuta Yasui, Tomoya Tashiro, Masaru Matsugami, Saki Sawayama and Kenta Fujii\*



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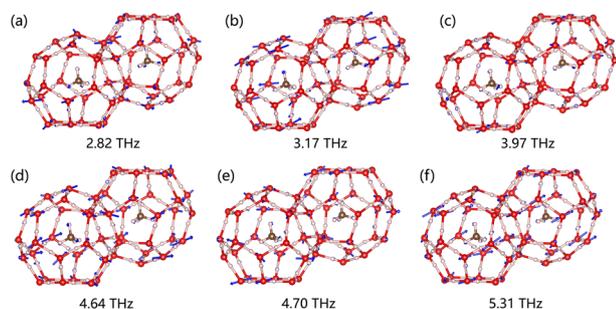
23446



### Comparison of thermal conductivity modulation by uniaxial and biaxial strain in monolayer MoSe<sub>2</sub>: a first-principles calculation

Chunwei Zhang,\* YinLi Sun, Chi Xu, Haixiang Huan, Qian Lu, Liang Li, Linzhen Zhou and Ning Xu\*

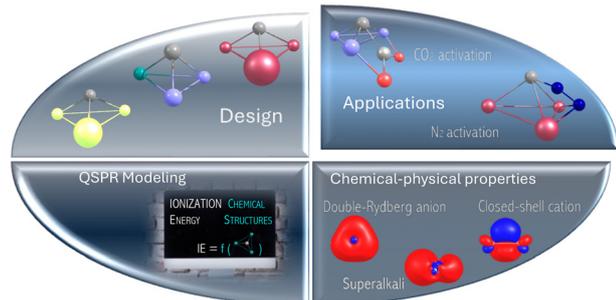
23459



### First-principles investigation of the terahertz absorption spectrum and thermodynamic properties of methane hydrate

Yuchao Li, Chenglong Wang, Xiang Hou, Fangze Deng, Zhihua Han, Yansheng Shao, Keke Cheng, Ke Ma, Yumeng Ma, Huifang Ma,\* Huiyun Zhang and Yuping Zhang\*

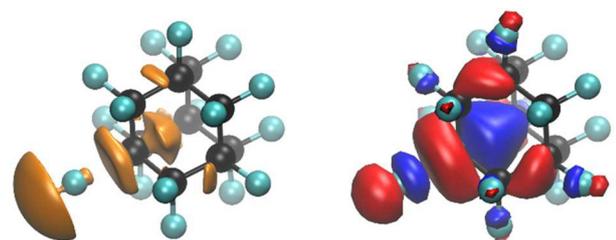
23468



### Tunable reducibility of alkaline earth metal clusters for carbon dioxide and nitrogen molecule activation: a QM-QSPR study

Natalia Wiszowska, Natalia Rogoza and Celina Sikorska\*

23487



### A combined density functional and coupled-cluster theory study on correlation-bound anions of perfluorinated compounds

Charlotte Titeca,\* Garrette Pauley Paran, Frank De Proft and Thomas-Christian Jagau

