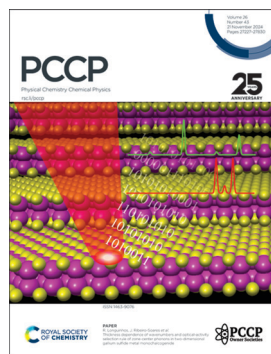


## IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 26(43) 27227–27830 (2024)



### Cover

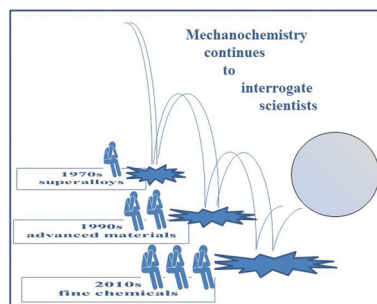
See R. Longuinhos, J. Ribeiro-Soares *et al.*, pp. 27260–27269. Image produced and designed by Raphael Longuinhos Monteiro Lobato, with the approval of the co-authors from *Phys. Chem. Chem. Phys.*, 2024, 26, 27260.

## EDITORIAL

27245

### Fundamental basis of mechanochemical reactivity

Adam A. L. Michalchuk and Francesco Delogu

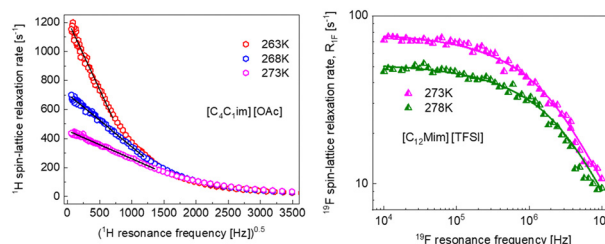


## REVIEW

27248

### Dynamics of ionic liquids by means of nuclear magnetic resonance relaxation – overview of theoretical approaches

Danuta Kruk,\* Elzbieta Masiewicz, Roksana Markiewicz and Rajendra Kumar Singh



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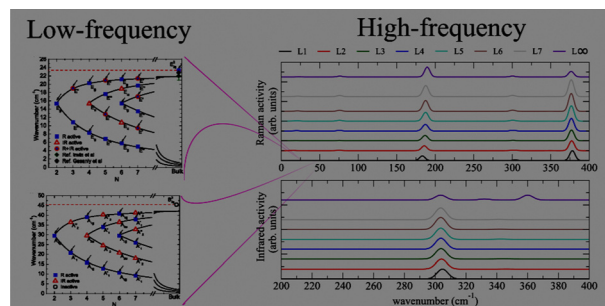
Fundamental questions  
Elemental answers

## RESEARCH PAPERS

27260

### Thickness dependence of wavenumbers and optical-activity selection rule of zone-center phonons in two-dimensional gallium sulfide metal monochalcogenide

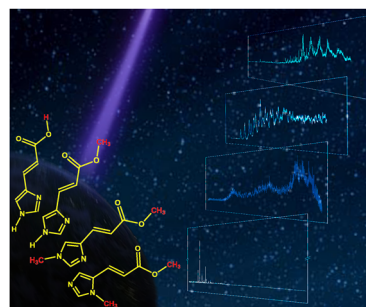
R. Longuinhos,\* Dattatray J. Late, B. C. Viana, R. S. Alencar, M. Terrones, A. G. Souza Filho, A. Jorio and J. Ribeiro-Soares\*



27270

### Urocanic acid as a novel scaffold for next-gen nature-inspired sunscreens: I. electronic laser spectroscopy under isolated conditions

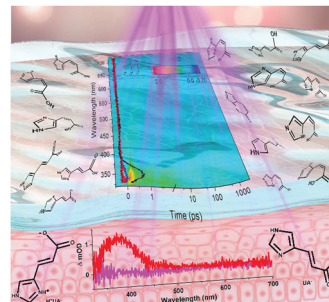
Jiayun Fan, Alexander K. Lemmens, Hans Sanders, Michiel Hilbers, Wim Roeterdink and Wybren Jan Buma\*



27281

### Urocanic acid as a novel scaffold for next-gen nature-inspired sunscreens: II. Time-resolved spectroscopy under solution conditions

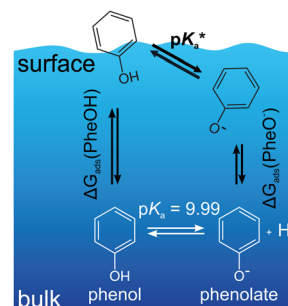
Jiayun Fan, Jack M. Wooley, Hans Sanders, Vasilios G. Stavros\* and Wybren Jan Buma\*



27292

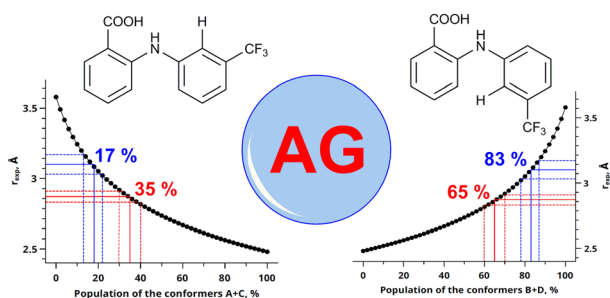
### Surface accumulation and acid–base equilibrium of phenol at the liquid–vapor interface

Clemens Richter,\* Rémi Dupuy, Florian Trinter, Tillmann Buttersack, Louisa Cablitz, Shirin Gholami, Dominik Stemer, Christophe Nicolas, Robert Seidel, Bernd Winter and Hendrik Bluhm\*



## RESEARCH PAPERS

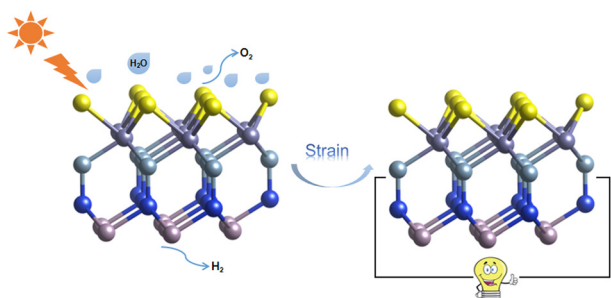
27301



### Structural and sorption characteristics of an aerogel composite material loaded with flufenamic acid: insights from MAS NMR and high-pressure NOESY studies

Valentina V. Sobornova, Valeriya V. Mulloyarova, Konstantin V. Belov, Alexey A. Dyshin, Peter M. Tolstoy, Mikhail G. Kiselev and Ilya A. Khodov\*

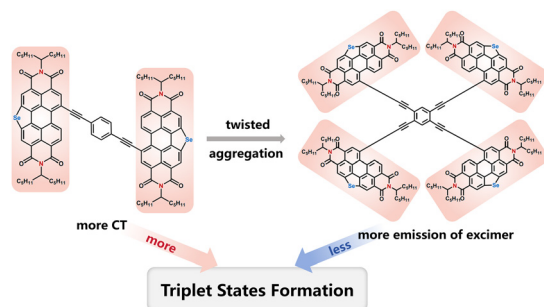
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### Two-dimensional Janus XWZAZ' (X = S, Se, Te; A = Si, Ge; Z, Z' = N, P, As): candidates for photocatalytic water splitting and piezoelectric materials

Zhen Gao, Hongbo Wu, Yao He\* and Kai Xiong\*

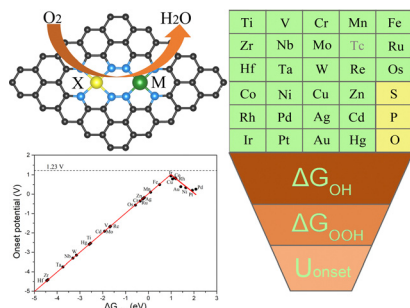
27325



### The efficient triplet states formation of Se-modified PDI dimers and tetramers in solvents

Feijun Huang, Wenli Su, Yubo Yang, Hang Wang, Zhishan Bo, Pengfei Jing and Wenkai Zhang\*

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### Theoretical screening of the metal-nonmetal pair anchored on N-doped graphene for the oxygen reduction reaction

Ji Zhang, Peng Zhang, Aimin Yu, Dong-sheng Li and Chenghua Sun\*

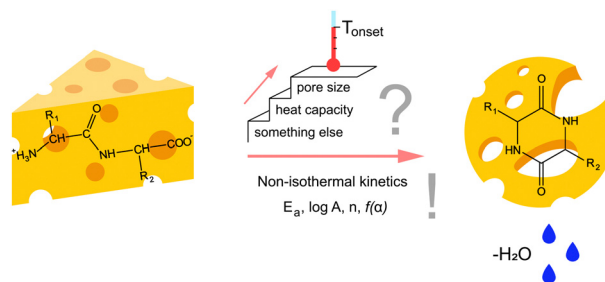


## RESEARCH PAPERS

27338

### Cyclization of alanyl–valine dipeptides in the solid state. The effects of molecular radiator and heat capacity

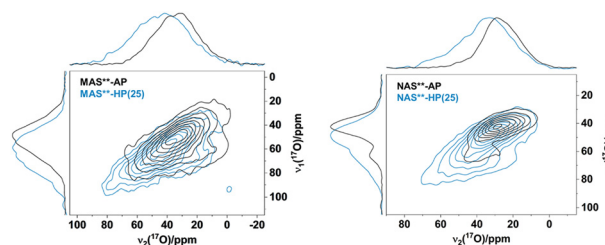
Daria V. Tkachenko, Radik A. Larionov, Sufia A. Ziganshina, Khasan R. Khayarov, Aleksandr E. Klimovitskii, Olga B. Babaeva, Valery V. Gorbachuk and Marat A. Ziganshin\*



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### Densification of sodium and magnesium aluminosilicate glasses at ambient temperature: structural investigations by solid-state nuclear magnetic resonance and molecular dynamics simulations

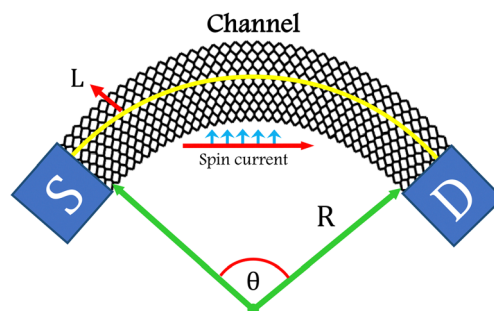
Millena Logrado, Yara Hellen Firmo Gomes, Tomiki Inoue, Shingo Nakane, Yoshinari Kato, Hiroki Yamazaki, Akihiro Yamada and Hellmut Eckert\*



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### Spintronic performance of bent zigzag phosphorene nanoribbons: effects of mechanical deformation and gate voltage

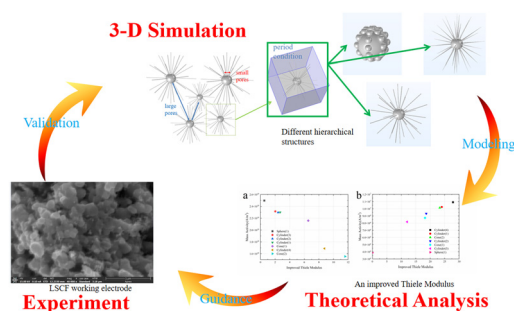
Rouhollah Farghadan



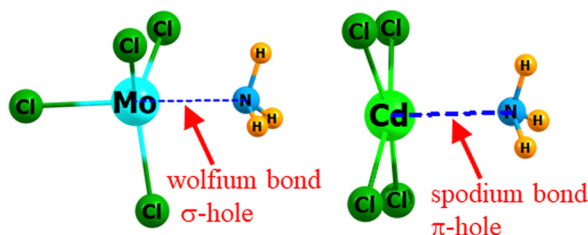
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### Strategy for predicting catalytic activity of catalysts with hierarchical nanostructures

Zidi Zhu, Daoming Huan, Jingchao Yuan, Dan Zhang,\* Aijun Li and Jiujun Zhang



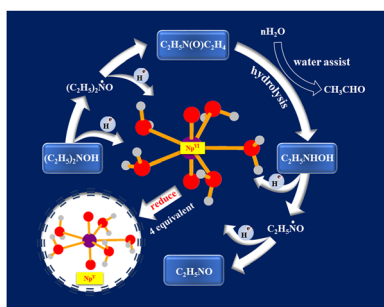
27382

 $\sigma$  and  $\pi$ -hole bonds of transition metals

## Participation of transition metal atoms in noncovalent bonds

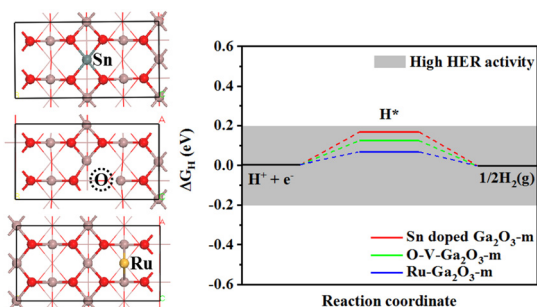
Steve Scheiner

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Uncovering the reduction mechanism of Np(vi) with *N,N*-diethyl hydroxylamine: a scalar-relativistic DFT investigation

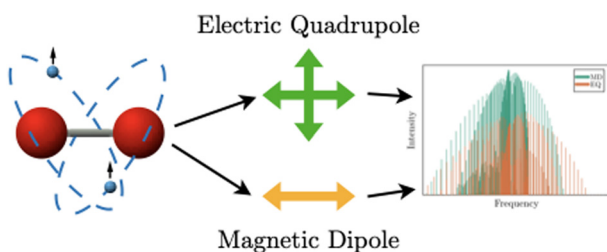
Xin Huang, Xiaobo Li, Qunyan Wu,\* Congzhi Wang, Jianhui Lan, Hongqing Wang and Weiqun Shi\*

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Theoretical design of active Ga<sub>2</sub>O<sub>3</sub> monolayer-based catalysts for electrocatalytic HER

Rongzhi Wang and Jin-Cheng Zheng\*

27419

An *ab initio* spectroscopic model of the molecular oxygen atmospheric and infrared bands

Wilfrid Somogyi,\* Sergey N. Yurchenko and Gap-Sue Kim

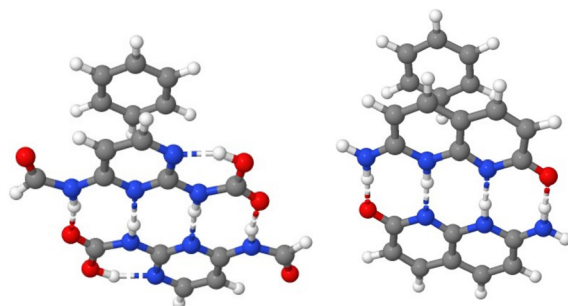


## RESEARCH PAPERS

27431

**The effect of hydrogen bonding on the  $\pi$  depletion and the  $\pi$ - $\pi$  stacking interaction**

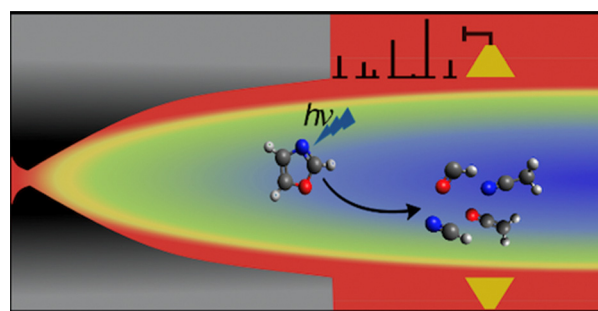
Usman Ahmed, Dage Sundholm\* and Mikael P. Johansson\*



27439

**Product branching in the photodissociation of oxazole detected by broadband rotational spectroscopy**

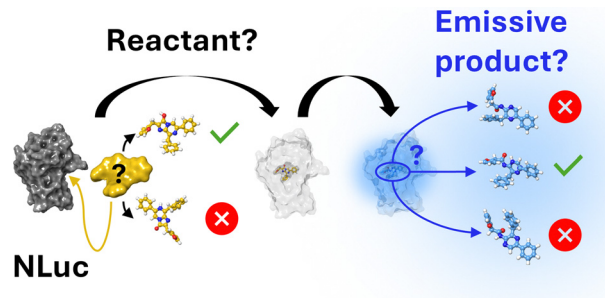
Briony Downes-Ward, Abbas Behzadfar, Shameemah Thawoos and Arthur G. Suits\*



27447

**Behind the glow: unveiling the nature of NanoLuc reactants and products**

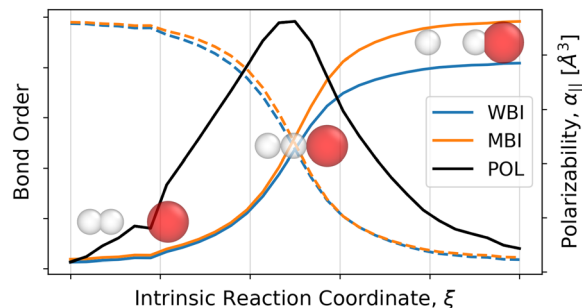
Alessandro Bonardi, Michele Turelli, Giorgio Moro, Claudio Greco, Ugo Cosentino\* and Carlo Adamo\*



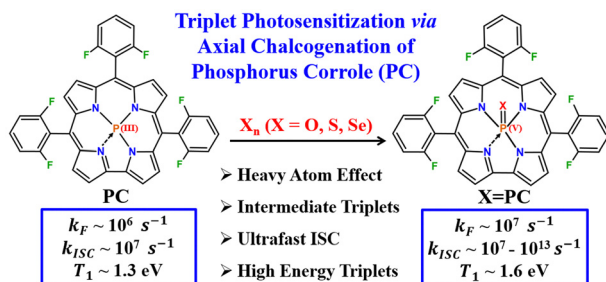
27459

**Near equivalence of polarizability and bond order flux metrics for describing covalent bond rearrangements**

Lukas Kim and Teresa Head-Gordon\*



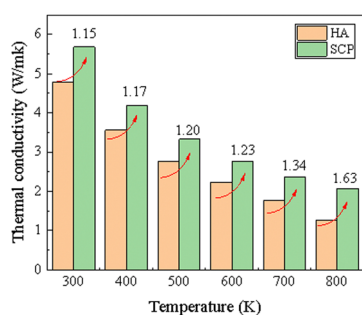
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## Tailoring intersystem crossing in phosphorus corroles through axial chalcogenation: a detailed theoretical study

Annette Mariya Tedy and Arun K. Manna\*

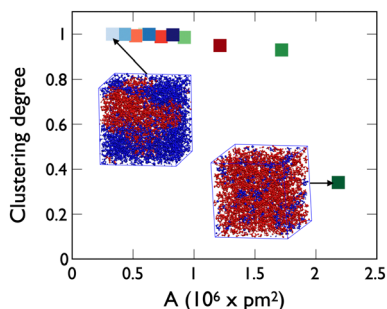
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## Thermal conductivity study of 2D Si<sub>4</sub>C<sub>8</sub> materials by anharmonic phonon renormalization

Peng Gao, Xihao Chen,\* Xingwu Yan, Longxin Zhang, Xiang Meng, Fuqiang Zhai\* and Donglin Guo\*

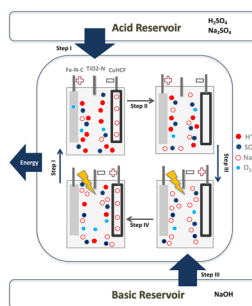
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## Structural insights into carboxylic-acid based DES across H-bond donor ratios: impact of CL&Pol refinement

Jon Zubeltzu\* and Elixabete Rezabal

27498



## Electrochemical system of nitrogen-doped TiO<sub>2</sub>, Fe-N-C, and copper hexacyanoferrate electrodes for photo-assisted energy conversion in acidic wastewater treatment

Bianca Tainá Ferreira, Matheus Martins and Fritz Huguenin\*

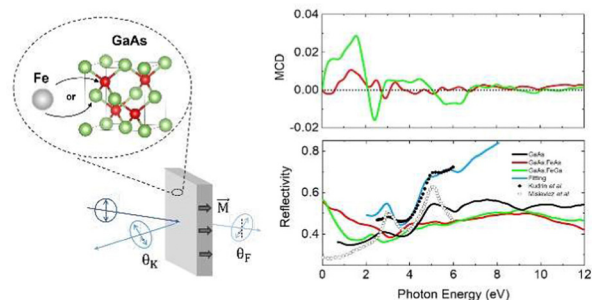


## RESEARCH PAPERS

27510

**Magneto-optical properties of heavily Fe-doped GaAs: a density functional approach**

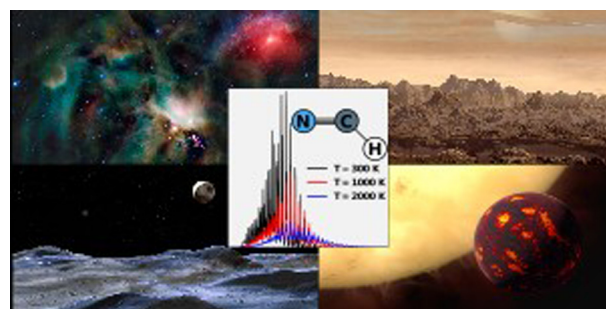
J. Zarpellon,\* D. H. Mosca and J. Varalda



27519

**A time-independent, variational method for studying the photodissociation of triatomic molecules**

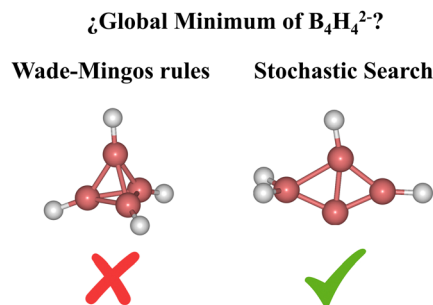
Marco Pezzella, Georgi Mitev, Sergei N. Yurchenko, Jonathan Tennyson\* and Alexander O. Mitrushchenkov



27530

**Exploring the potential energy surface of  $B_4H_4^{2-}$ : an exception of the Wade–Mingos rules**

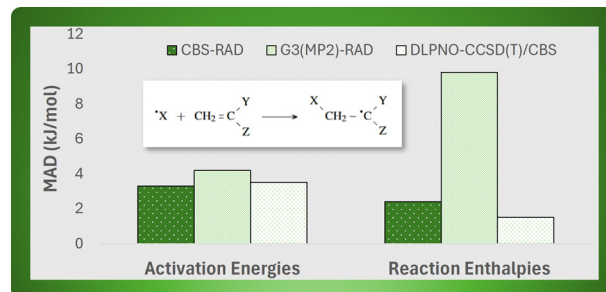
Rodrigo Báez-Grez, Alejandro Vásquez-Espinal\* and Ricardo Pino-Rios\*



27536

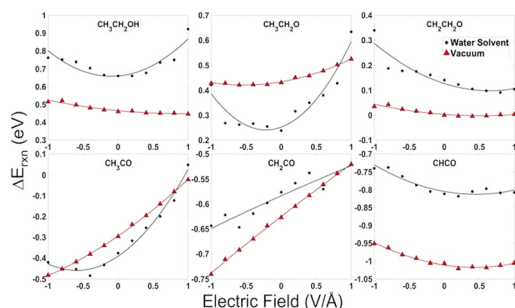
**Comparing coupled cluster and composite quantum chemical methods for computing activation energies and reaction enthalpies of radical propagation reactions**

Timothy B. Huber\* and Ralph A. Wheeler\*



## RESEARCH PAPERS

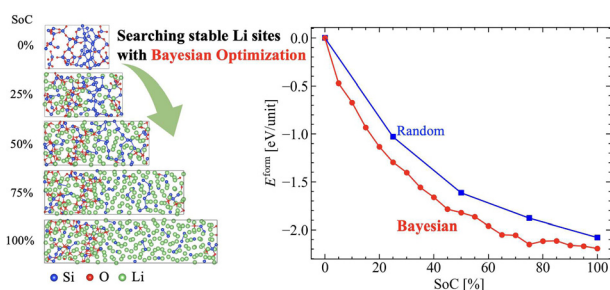
27544



### Modeling interfacial electric fields and the ethanol oxidation reaction at electrode surfaces

Yuhan Mei, Fanglin Che and N. Aaron Deskins\*

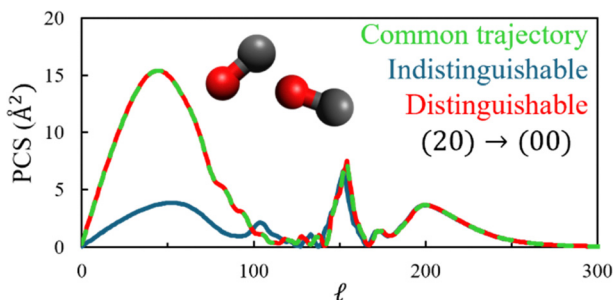
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### First-principles study on the lithiation process of amorphous SiO anode for Li-ion batteries with Bayesian optimization

Ryoya Shintaku, Tomoyuki Tamura,\* Shogo Nogami, Masayuki Karasuyama and Takakazu Hirose

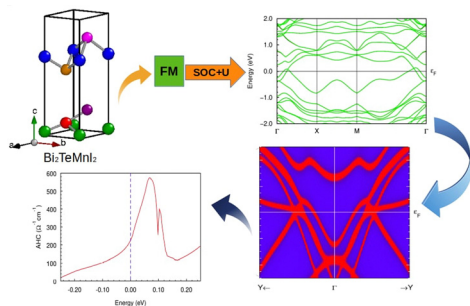
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### Mixed quantum/classical theory for rotationally inelastic scattering of identical collision partners revised

D. Bostan, B. Mandal and D. Babikov\*

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### Emergence of Weyl points and large anomalous Hall conductivity in layered Bi<sub>2</sub>TeMnI<sub>2</sub>

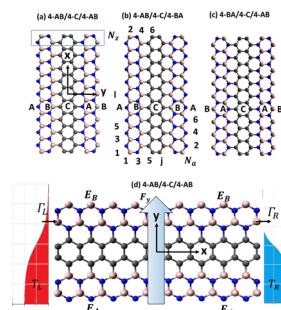
Dipak Bhattarai, Deergh Bahadur Shahi, Dipendra Prasad Kalauni and Madhav Prasad Ghimire\*



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### Impact of valley degeneracy on the thermoelectric properties of zig-zag graphene nanoribbons with staggered sublattice potentials and transverse electric fields

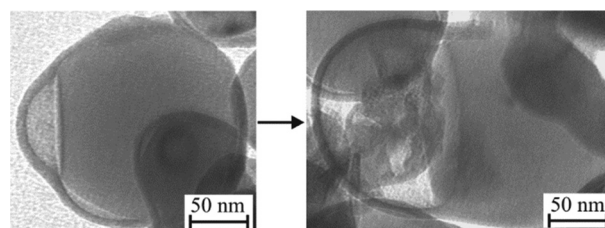
David M. T. Kuo



27602

### Oxidation of fine aluminum particles: thermally induced transformations in particle shells and kinetics of oxide nucleation

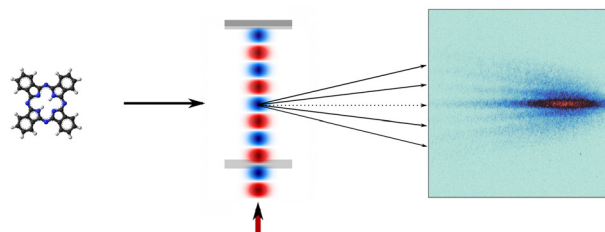
Andrey V. Korshunov



27617

### Diffracting molecular matter-waves at deep-ultraviolet standing-light waves

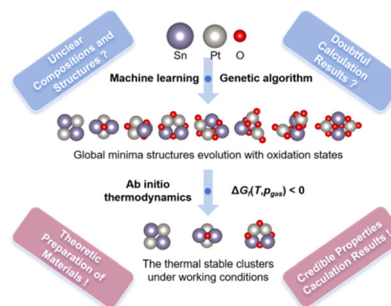
Ksenija Simonović,\* Richard Ferstl, Alfredo Di Silvestro, Marcel Mayor, Lukas Martinetz, Klaus Hornberger, Benjamin A. Stickler, Christian Brand and Markus Arndt



27624

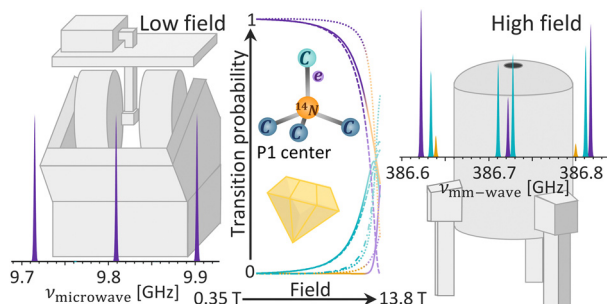
### Machine-learning-accelerated structure prediction of PtSnO nanoclusters under working conditions

Fanke Zeng and Wanglai Cen\*



## RESEARCH PAPERS

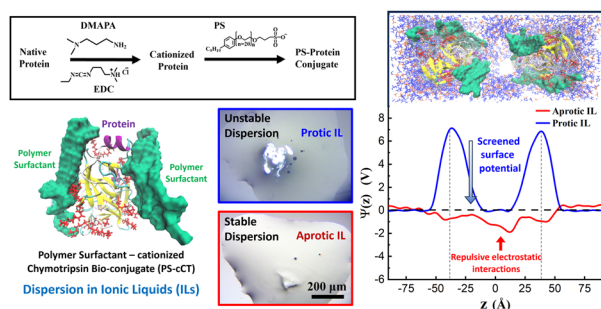
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### On the peculiar EPR spectra of P1 centers at high (12–20 T) magnetic fields

Orit Nir-Arad, Eyal Laster, Mais Daksi, Nurit Manukovsky and Ilia Kaminker\*

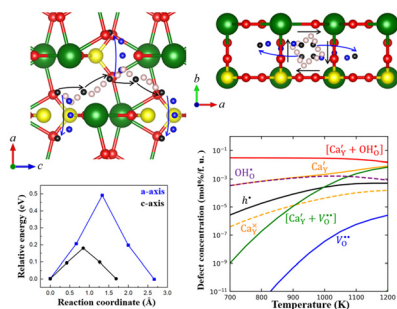
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### Cation effects and charge inversion contribute to the electrostatic stabilisation of protein bioconjugates in neat ionic liquids

Lokesh Soni, Raj Kumar, Kamendra P. Sharma\* and Ajay Singh Panwar\*

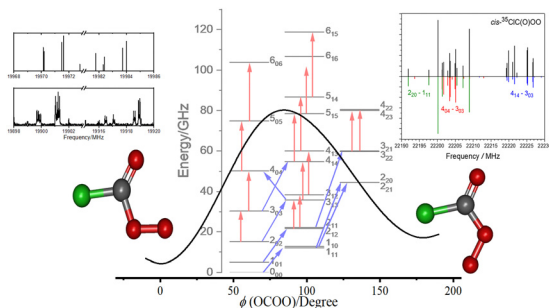
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### First-principles calculations of proton defect properties in Ca-doped YPO<sub>4</sub>

Gyeongseo Lee,\* Takafumi Ogawa, Kazuki Shitara and Akihide Kuwabara\*

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### Insights of the peroxychloroformyl radical ClC(O)OO via microwave spectrum

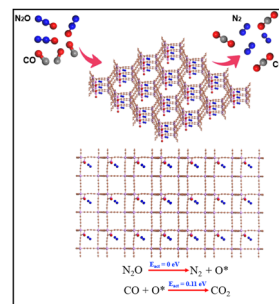
Ching-Hua Chang, Wen Chao, Cheng-Han Tsai, Mitchio Okumura, Frank A. F. Winiberg and Yasuki Endo\*



27677

### Unveiling the potential of aluminum-decorated 3D phosphorus graphdiyne as a catalyst for N<sub>2</sub>O reduction

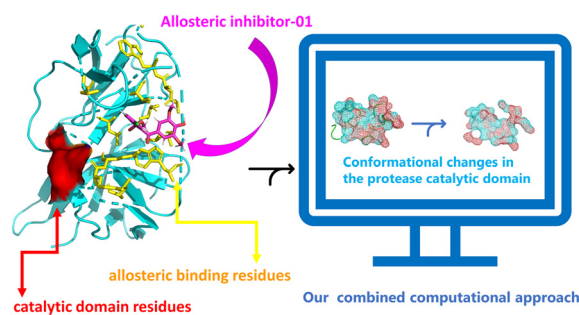
Shehzad Ahmed, Adnan Ali Khan,\* Danish Khan, Awais Ghani,\* Rashid Ahmad, Tian Xiaoqing\* and Imran Muhammad\*



27684

### In silico validation of allosteric inhibitors targeting Zika virus NS2B–NS3 protease

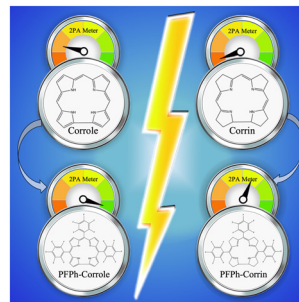
Yeng-Tseng Wang,\* Yuan-Chin Hsieh and Tin-Yu Wu



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### Effect of meso-pentafluorophenyl group on two-photon absorption in heterocorrroles and heterocorrins

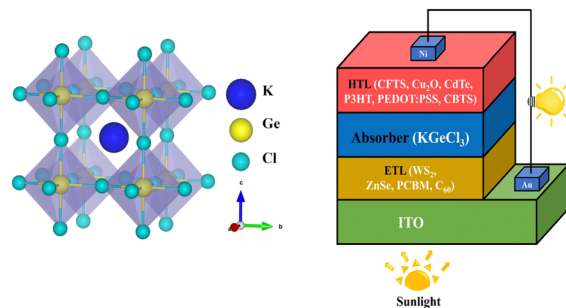
Tejendra Banana, Swati Singh Rajput, Neelam Chandravanshi and Md. Mehboob Alam\*



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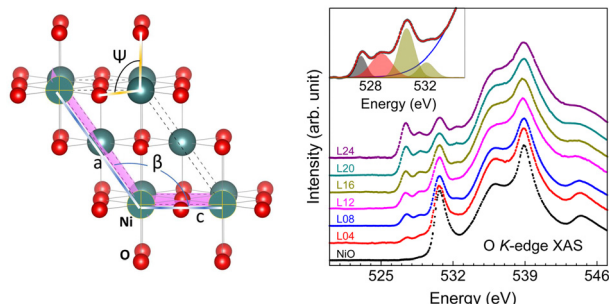
### An in-depth investigation of lead-free KGeCl<sub>3</sub> perovskite solar cells employing optoelectronic, thermomechanical, and photovoltaic properties: DFT and SCAPS-1D frameworks

Md. Tarekuzzaman, Mohammad Hasin Ishraq, Md. Shahazan Parves, M. A. Rayhan, Sohail Ahmad, Md. Rasheduzzaman, K A Al Mamun, M. Moazzam Hossen and Md. Zahid Hasan\*



## RESEARCH PAPERS

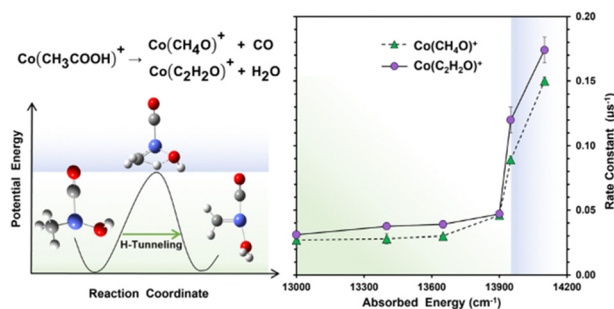
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### Hole-states in Li doped NiO: doping dependence of Zhang-Rice spectral weight

Suman Mandal\* and Krishnakumar S. R. Menon

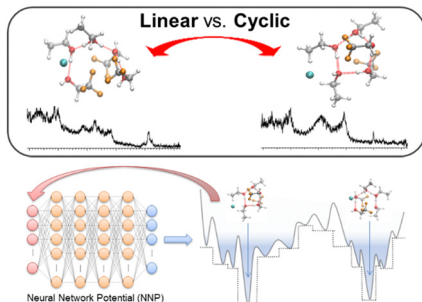
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### Hydrogen tunneling with an atypically small KIE measured in the mediated decomposition of the $\text{Co}(\text{CH}_3\text{COOH})^+$ complex

Simon U. Okafor, Gabriele Pinto, Michael Brdecka, William Smith, Tucker W. R. Lewis, Michael Gutierrez and Darrin J. Bellert\*

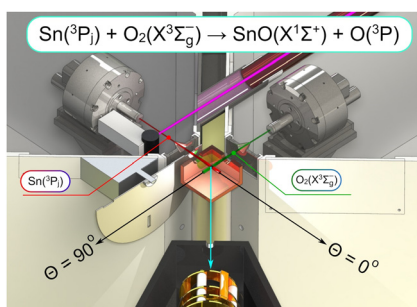
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### Hydrogen bond network structures of protonated 2,2,2-trifluoroethanol/ethanol mixed clusters probed by infrared spectroscopy combined with a deep-learning structure sampling approach: the origin of the linear type network preference in protonated fluoroalcohol clusters

Po-Jen Hsu, Atsuya Mizuide, Jer-Lai Kuo\* and Asuka Fujii\*

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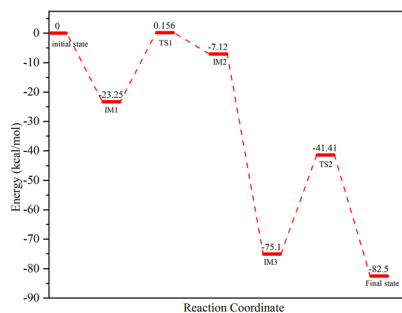
### Experimental and theoretical study of the Sn–O bond formation between atomic tin and molecular oxygen

Iakov A. Medvedkov, Anatoliy A. Nikolayev, Shane J. Goettl, Zhenghai Yang, Alexander M. Mebel\* and Ralf I. Kaiser\*





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## Performance of functionalized graphene oxide with organic radical scavengers in proton exchange membranes

Yu Hu, Jiaxing Wang, Shuai Wang\* and Yuan Feng

