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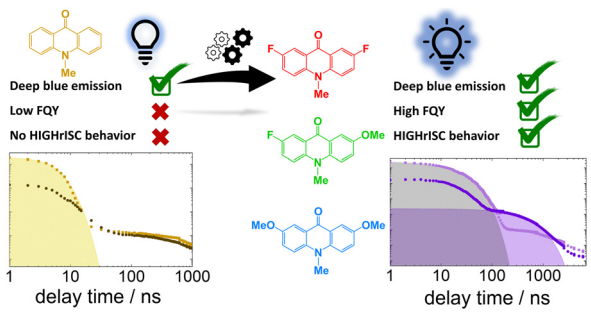
**Cover**
See Peter Gilch *et al.*, pp. 10444–10455. Image reproduced by permission of Pauline Morys from *Phys. Chem. Chem. Phys.*, 2025, **27**, 10444.

## RESEARCH PAPERS

10444

**Substituted acridones: simple deep blue HIGHrISC emitters in an aprotic environment**

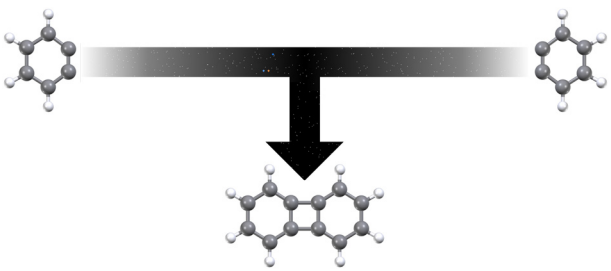
Matthias Jantz, David Klaverkamp, Lennart Bunnemann, Martin Kleinschmidt, Constantin Czekelius and Peter Gilch*




10456

**Polycyclic (anti)aromatic hydrocarbons: interstellar formation and spectroscopic characterization of biphenylene and benzopentalene**

Athena R. Flint, Vincent J. Esposito and Ryan C. Fortenberry*



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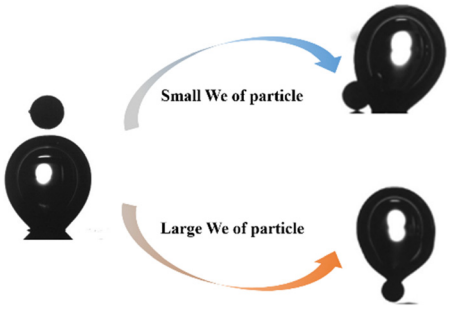
**Experimental study of the effect of particle collision on bubble dynamics behavior**

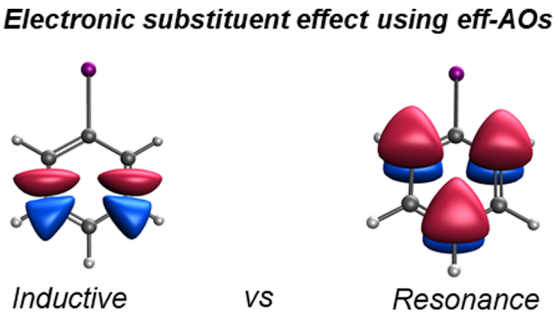
Xiaoxiang Li, Ying Zhang, Weichen Tang, Xin Chen and Fei Dong*




10482

**Capturing electronic substituent effect with effective atomic orbitals**

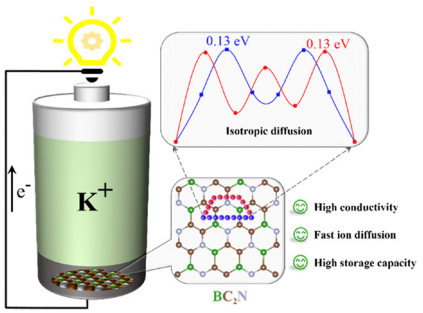
Gerard Comas-Vilà and Pedro Salvador*




10492

**$BC_2N$ monolayer as a high-performance anode material for potassium-ion batteries**

Jingguo Wang, Wenyuan Zhang, Yanling Si* and Guochun Yang*

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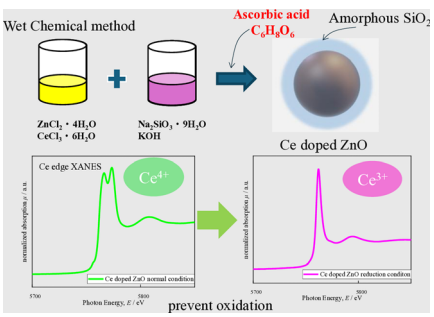
**Preparation of $Ce^{3+}$ doped ZnO nanoparticles *via* a wet chemical method and analysis of their local structure**

Hiroki Amano, Ryota Abe, Shotaro Watanabe, Yuu Kusumoto and Yuko Ichiyanagi



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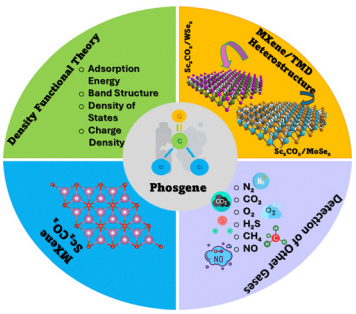
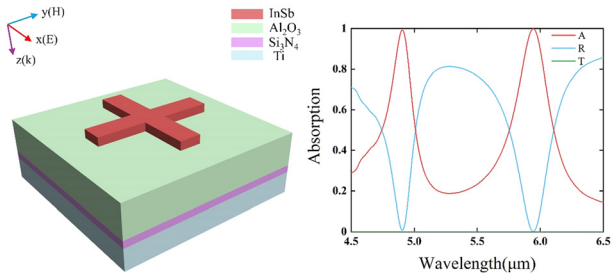



**Unlocking the sensing and scavenging potential of $Sc_2CO_2$ and $Sc_2CO_2$/TMD heterostructures for phosgene detection**

Julaiba T. Mazumder, Mohammed M. Hasan, Fahim Parvez, Tushar Shivam, Dobbidi Pamu, Alamgir Kabir, Mainul Hossain and Ravindra K. Jha*

10523




**A dual-band mid-infrared polarization-insensitive perfect absorber**

Sijing Huang, Mousu Wan, Mingli Sun, Lin Lu, Xiaogang Wang and Bijun Xu*

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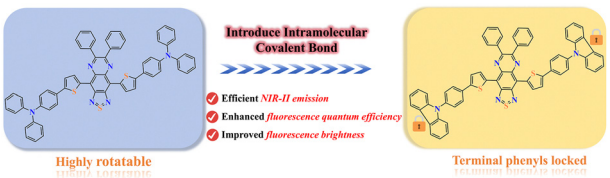


**Improving the fluorescence brightness of NIR-II fluorophores *via* intramolecular covalent bond locking: a theoretical perspective**

Lingling Dong, Yuying Du, Meina Zhang, Jiancai Leng, Wei Hu* and Yujin Zhang*

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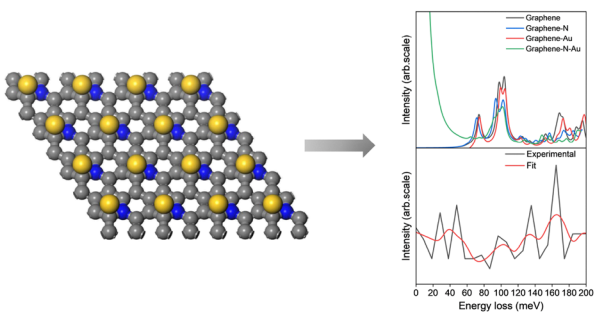


**A theoretical study on synergistic tuning of graphene phonons *via* heteroatom modifications**

Shuang Li, Lifeng Zhang, Langli Luo* and Xing Chen*

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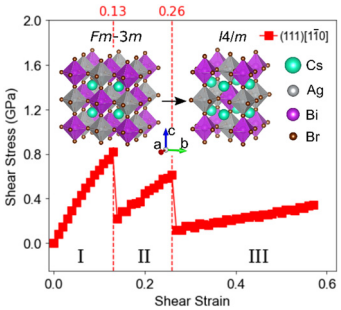
**Ideal strength and deformation mechanism in inorganic halide double perovskite $Cs_2AgBiBr_6$**

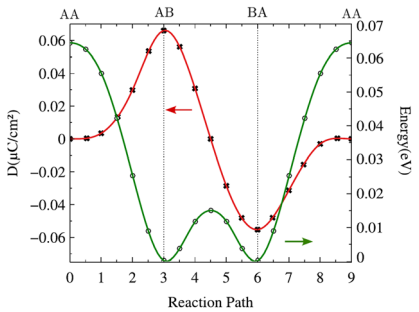
Xiaohan Liu, Yabin Ren, Shihao Wang, Yingzhuo Lun, Bo Yang,* Bonan Zhu, Jiawang Hong* and Gang Tang*




10556

**Switchable half-metallicity in anti-ferromagnetic bilayer $NbS_2$**

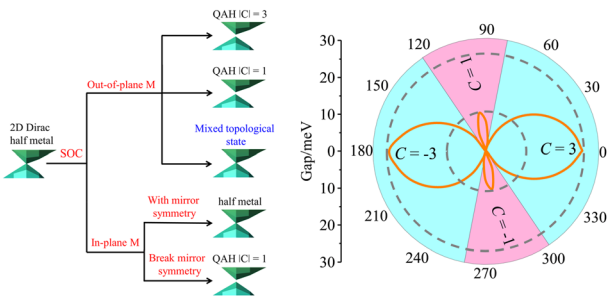
Zhifan Zheng, Shili Yang, Shaohui Yu,* Tengfei Cao, Xiaohong Zheng,* Weiyang Wang and Yushen Liu




10562

**Novel mixed topological state in monolayer $MnSbO_3$**

Yanzhao Wu, Li Deng, Junwei Tong, Xiang Yin, Gaowu Qin and Xianmin Zhang*

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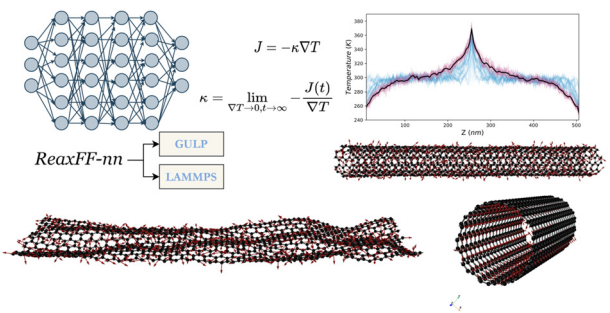
**ReaxFF-nn: a reactive machine-learning potential in GULP/LAMMPS and its applications in the thermal conductivity calculations of carbon nanostructures**

Zhong-Hao Ye, Jia-Hua Liu, Chuan-Guo Chai, Yu-Shi Wen, Shou-Xin Cui, Gui-Qing Zhang, Ke-Jiang Li, Feng Guo* and Xiao-Chun Wang*



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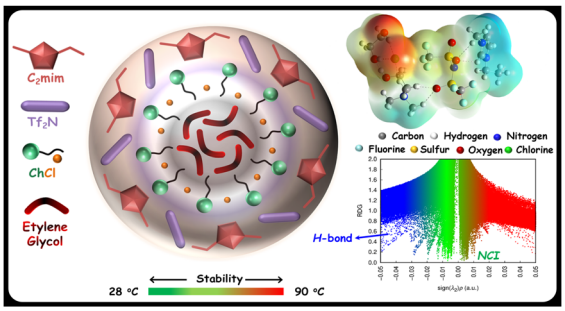


**Surfactant-free microemulsion as a fluid scaffold for the thermal stabilization of lysozyme**

Manvir Kaur, Manpreet Singh, Rajwinder Kaur, Navdeep Kaur, Pratap. K. Pati and Tejwant S. Kang*

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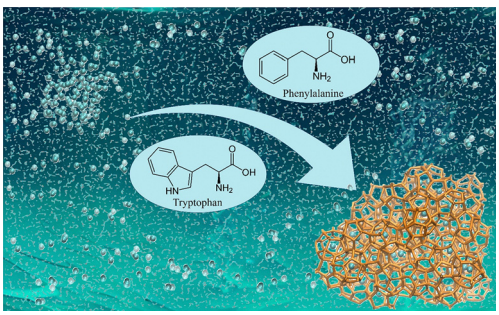


**The nucleation and growth of methane hydrates in the presence of phenylalanine and tryptophan: a comparative molecular dynamics simulation study**

Aashu, Shivam Rawat and C. N. Ramachandran*

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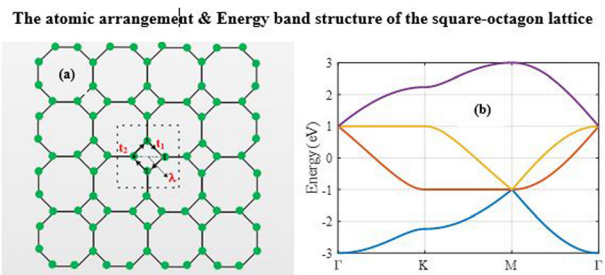


**Exploring the electronic properties and quantum capacitance of the square-octagon lattice for advanced electronic and energy storage applications**

Erfan Norian, Mona Abdi and Bandar Astinchap*

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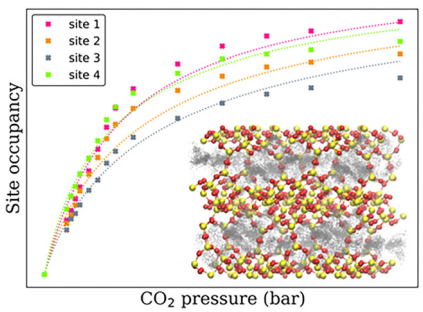


**A comparative study of $CO_2$ adsorption in a series of zeolites**

Loïc Bénariac-Doumal,* Irena Deroche, Habiba Nouali, Jean-Louis Paillaud, Taylan Ors, Andrew N. Fitch and Catherine Dejoie*

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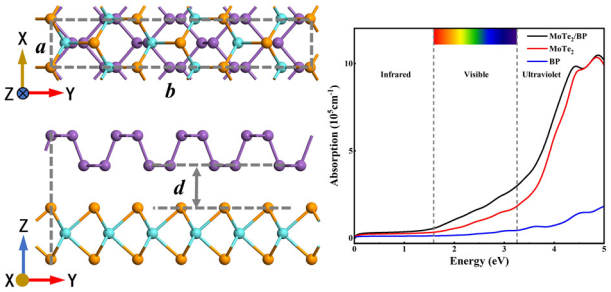
**Tunable electronic and optical properties of the $MoTe_2$/black phosphorene van der Waals heterostructure: a first-principles study**

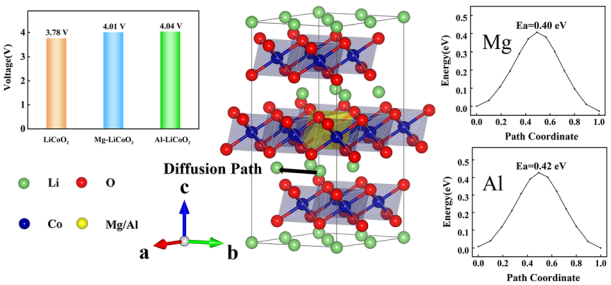
Qing Chu, Bo Peng,* Lei Yuan, Yuming Zhang, Renxu Jia and Lianbi Li




10644

**Effect of Mg/Al doping at the Co site on the structural and electrochemical performance of $LiCoO_2$ cathode materials**

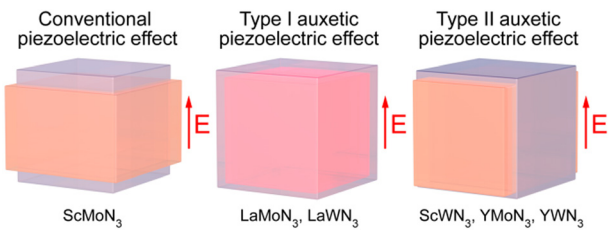
Yubai Li, Zheng Wei, Sumei Wu,* Yao Liang, Xiang Liu, Yang Wen, Weiwei Jiang, Tengfei Lu, Yan Cui and Zhihua Zhang*




10652

**First-principles investigation of auxetic piezoelectric effect in nitride perovskites**

Yanting Peng, Zunyi Deng, Siyu Song, Gang Tang* and Jiawang Hong*

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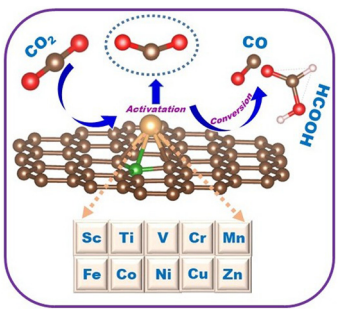
**Transition-metal-embedded boron-doped graphene for reduction of $CO_2$ to HCOOH**

Sudatta Giri, Purushothaman Manivannan and Debolina Misra*



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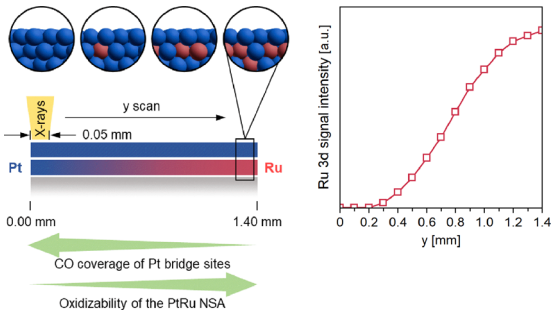


## Effect of the Ru concentration on the CO tolerance and the oxidizability of a composition spread PtRu/Pt(111) near-surface alloy

Valentin Schwaab, Fabian Düll, Phiona Bachmann, Felix Hemauer, Hans-Peter Steinrück and Christian Papp*

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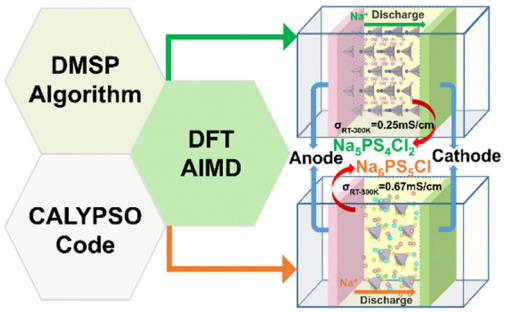


## Design of sodium superionic conductors based on multiple crystal structure prediction methods

Xiangti Zhan, Ziang Ren, Jinsen Zhang, Shihui Zou, Huadong Yuan, Jianmin Luo, Yujing Liu, Jianwei Nai, Peng Shi, Yao Wang* and Xinyong Tao

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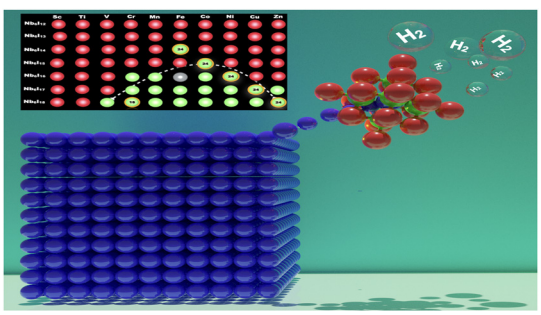


## Engineering electronic structures of $Nb_6I_x$ superatomic clusters by metal atom incorporation: a first-principles study

Dolan Acharya, Soumyadeep Bhattacharyya, Renna Shakir and J. Karthikeyan*

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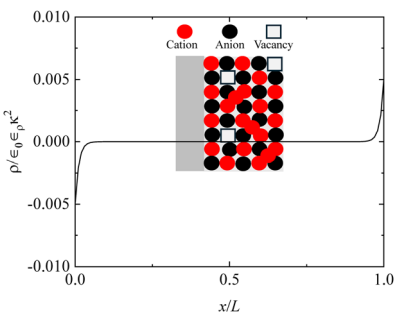


## Electrochemical–mechanical model of the space charge zone at the interface

Fuqian Yang* and Erwin Hüger

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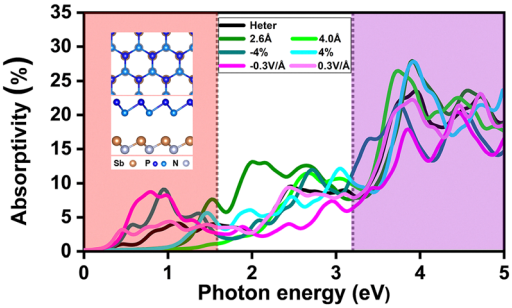
**Band alignment and optoelectronic characteristics of blue phosphorene/SbN van der Waals heterostructures**

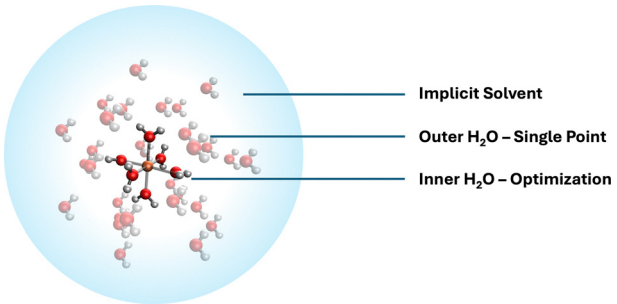
Mengge Li, Yuhua Zhang, Yufei Wang, Weiguang Chen, Liying Zhang* and Yanwei Luo*




10717

**Systematic improvement of redox potential calculation of Fe(III)/Fe(II) complexes using a three-layer micro-solvation model**

Hassan Harb and Rajeev Surendran Assary*

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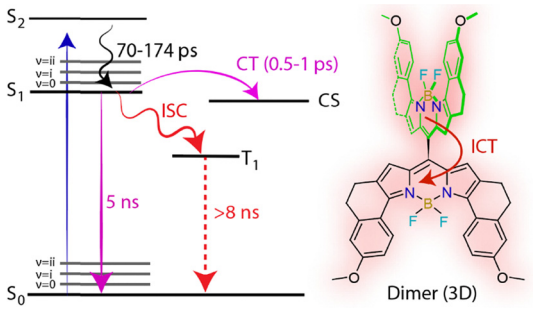
**Symmetry-breaking photoinduced charge transfer state in a near-IR absorbing *meso*-linked BODIPY dimer**

Fariyad Ali, Elizabeth Gehrmann, Tianyi Zhang, Qasim Qayyum Kashif, Robbyn K. Anand, David Lee Phillips* and Arthur H. Winter*

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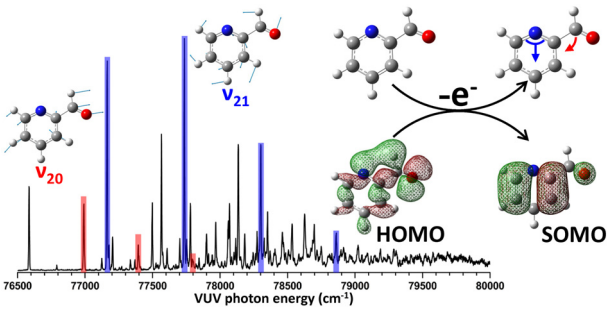
**Deciphering the electronic structure and conformational stability of 2-pyridinecarboxaldehyde**

Hyojung Kim, Sung Man Park and Chan Ho Kwon*



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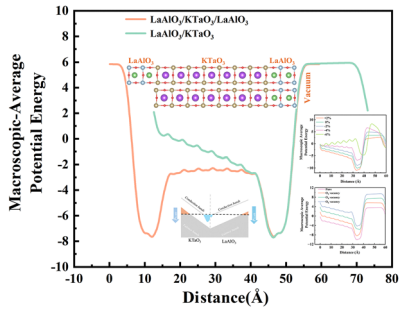
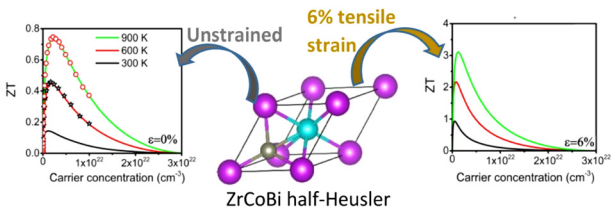



**Two-dimensional n/p type carriers at the interface of $LaAlO_3/KTaO_3$ heterostructures**

Yirong Geng, Zuhui Hu, Chang Liu, Ruiling Gao, Hui Zhang,* Le Fang* and Wei Ren*

10758




**Strain trailing band engineering and phonon transport of high *ZT* ZrCoBi half-Heusler alloy: a mechanistic understanding from first principles**

Suman Mahakal, Avijit Jana, Subrata Jana* and Prasanjit Samal

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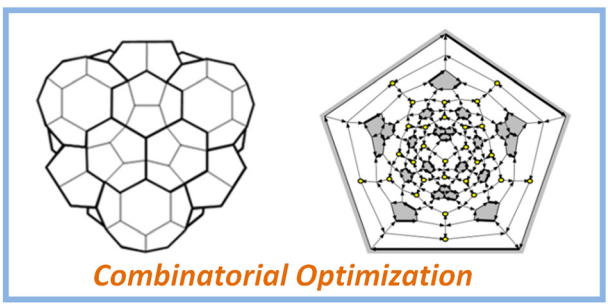


**Stability of multi-cage water structures**

Mikhail V. Kirov

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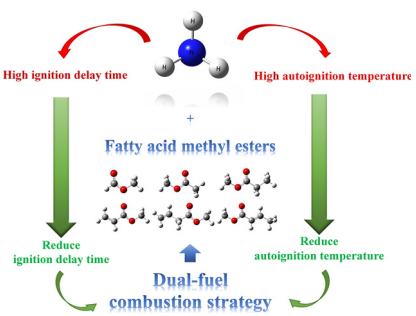


**Implications of amino cross-reactions for the ignition characteristics of ammonia-blended typical small saturated and unsaturated fatty acid methyl esters**

Haixing Deng, Sihao Wang, Li Fu and Hongbo Ning*

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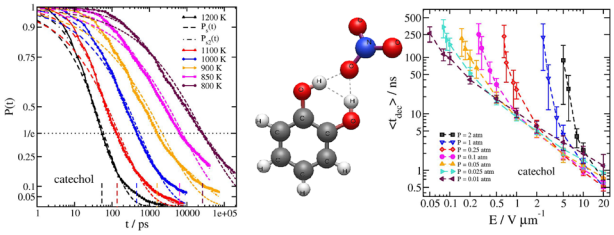
**Molecular dynamics simulations of atmospherically relevant molecular clusters: a case study of nitrate ion complexes**

Christopher David Daub,* Theo Kurtén and Matti Rissanen

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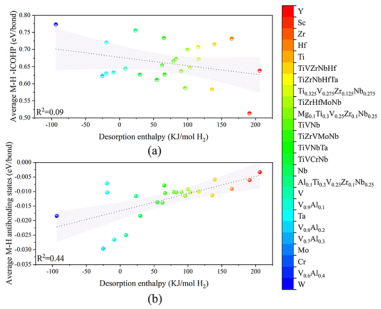
**The effects of Al on the hydrogen storage properties of V from first-principles calculations**

Jutao Hu,* Xiaoqing Li and Stephan Schönecker*

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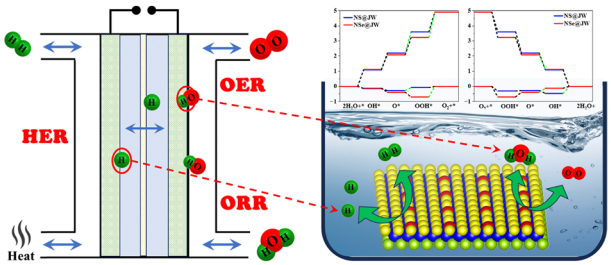
**Delineating the multifunctional performance of Janus WSSe with nonmetals in water splitting and hydrogen fuel cell applications *via* first-principles calculations**

Deepak Arumugam, Divyakaaviri Subramani, Shamini Pazhani Beena and Shankar Ramasamy*

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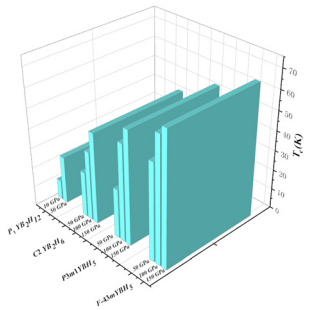
**Pressure-induced superconductivity in ternary yttrium borohydride systems**

Wen-Hua Yang,* Hui-Juan Sun, Xia Wang, Yue-Hang Dong, Wei Zhang, Wen-Cai Lu, K. M. Ho and C. Z. Wang*



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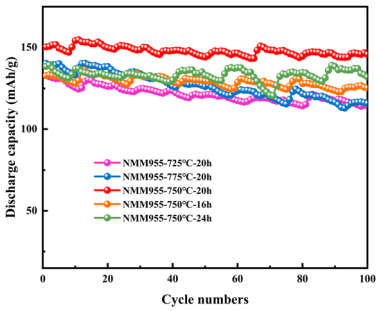
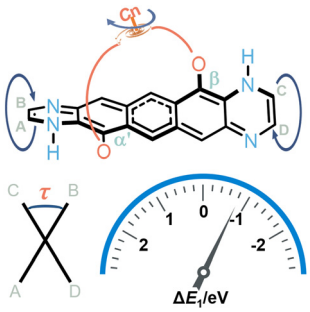



**Cobalt-free cathode material $LiNi_{0.9}Mn_{0.05}Mg_{0.05}O_2$ with high cycle stability synthesized *via* the homogeneous co-precipitation method**

Jiatai Wang,* Xi Wen, Yan Tan and Yuanyuan Li

10858




**Reducing the excessive exoergicity through a helically locked tether-driven approach for high-efficiency singlet fission chromophores**

Qing Li, Lingyi Meng,* Luyao Liu, Ziang Nan, Zhu Zhuo, Wei Wang and Yougui Huang*

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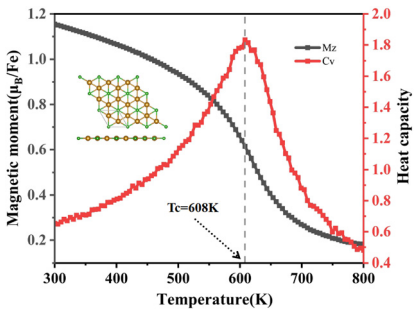


**A planar $Fe_2B$ monolayer with room temperature antiferromagnetism**

Wanting Han, Xu Yan, Ying Liu, Han Fu, Mingyang Sun, Xinrong Li, Dandan Wang, Lihua Yang* and Xin Qu*

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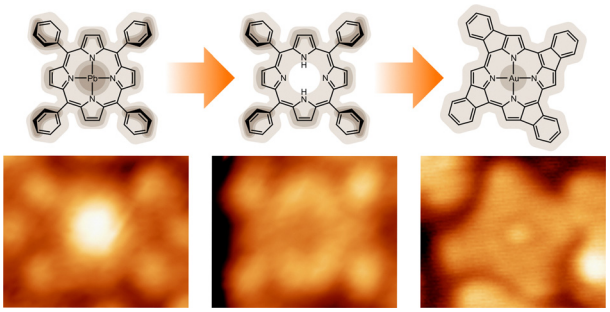

**On-surface chemistry of Pb(II) tetraphenylporphyrin on Au(111): reversible metalation, thermal degradation, and formation of a covalent organic framework**

Jan Herritsch, Cong Guo, Lukas J. Heuplick, Mark Hutter, Qitang Fan, Florian Münster, Stefan R. Kachel, Malte Zugermeier and J. Michael Gottfried*

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# A general, robust framework for determining the key species that forewarns sudden transitions in biological circuits

Dinesh Kashyap, Taranjot Kaur, Partha Sharathi Dutta and Sudipta Kumar Sinha*