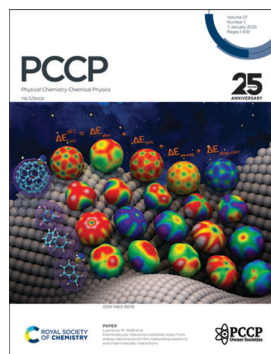


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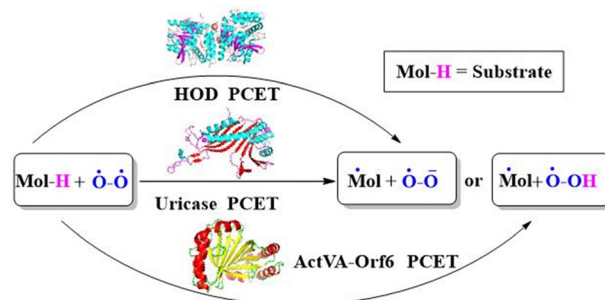
**Inside cover**  
See Mizuki Kimura and Shinkoh Nanbu, pp. 62–76. Image reproduced by permission of Shinkoh Nanbu from *Phys. Chem. Chem. Phys.*, 2025, 27, 62.

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### Unraveling proton-coupled electron transfer in cofactor-free oxidase- and oxygenase-catalyzed oxygen activation: a theoretical view

Qian-Qian Wang, Yan Qiao\* and Donghui Wei\*

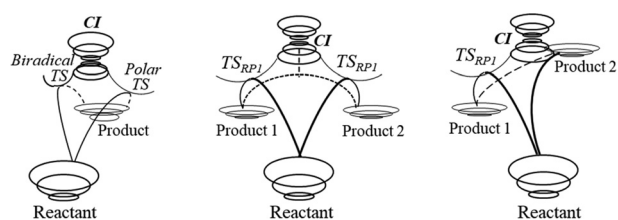


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### Light driven photoswitches: three classes of molecular systems that result in a single photoproduct via a conical intersection and an exothermic reverse reaction

Shmuel Zilberg



Three classes of molecular photoswitches



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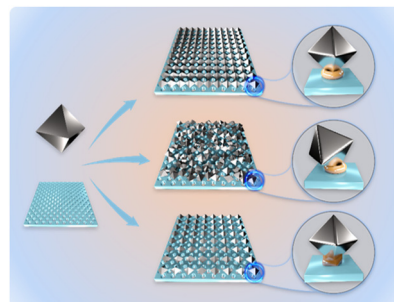


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### Strongly coupled and highly-compacted zirconium aminobenzenedicarboxylate crystal membranes for accelerating carbon dioxide capture

Qi Li,\* Liangmei Luo, Zhiwei Wu, Yufei Cao, Qiyang Guo\* and Yanqing Wang\*

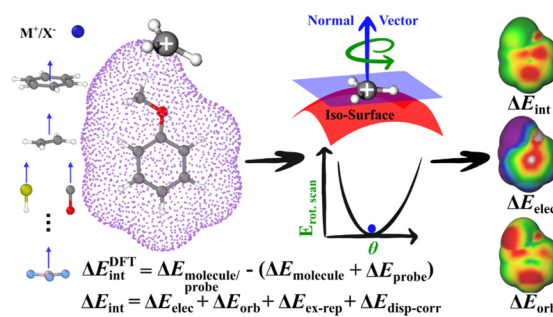


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### Intermolecular interaction potential maps from energy decomposition for interpreting reactivity and intermolecular interactions

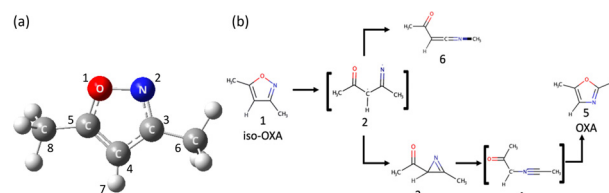
Amin Kiani, Wentong Zhou and Lawrence M. Wolf\*



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### Nonadiabatic *ab initio* chemical reaction dynamics for the photoisomerization reaction of 3,5-dimethylisoxazole via the $S_1$ electronic state

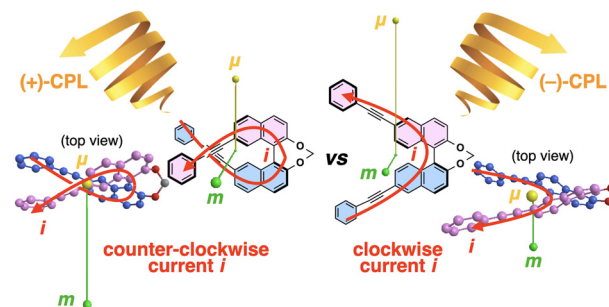
Mizuki Kimura and Shinkoh Nanbu\*



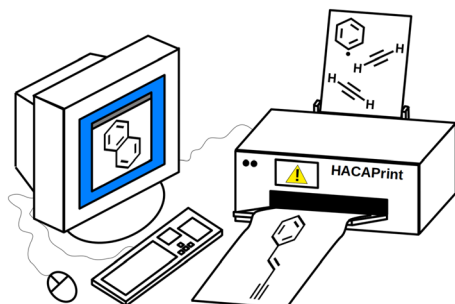
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Ayumi Imayoshi,\* Shinya Fujio, Yuuki Nagaya, Misato Sakai, Atsushi Terazawa, Misa Sakura, Keita Okada, Takahiro Kimoto, Tadashi Mori, Yoshitane Imai, Masahiko Hada and Kazunori Tsubaki\*



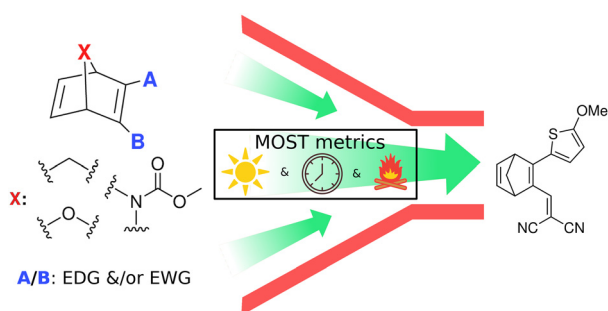
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### Don't forget the *trans*: double bond isomerism radical-acetylene growth reactions affect the primary stages of PAH and soot formation

Patricia D. Kelly,\* Jack A. Turner, Oisín J. Shiels, Gabriel da Silva, Stephen J. Blanksby, Berwyck L. J. Poad and Adam J. Trevitt\*

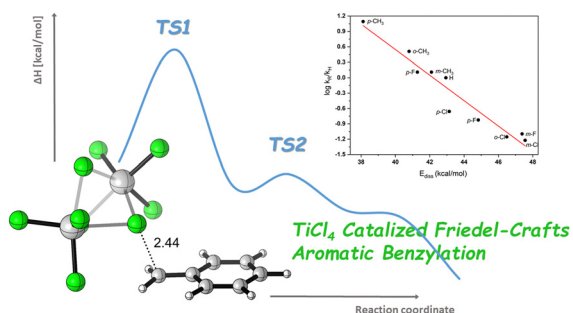
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Nils Oberhof,\* Andreas Erbs Hillers-Bendtsen, Oscar Berlin Obel, Karoline Schjelde, Kurt V. Mikkelsen and Andreas Dreuw\*

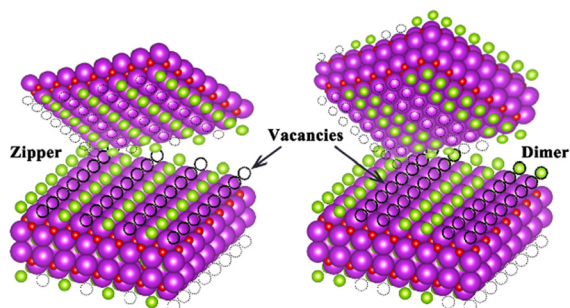
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### Reactivity in Friedel–Crafts aromatic benzylation: the role of the electrophilic reactant

Diana Cheshmedzhieva,\* Ivan Atanasov, Sonia Ilieva, Boris Galabov\* and Henry F. Schaefer III\*

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### Thickness-dependent surface reconstructions in non-van der Waals two-dimensional materials

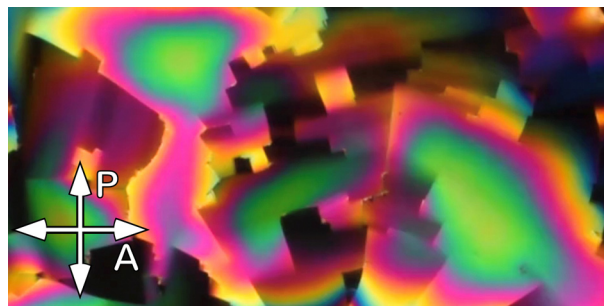
Kai Gao, Yan-Jin Chen, Yang Ou,\* Jin-ming Zeng, Chunju Hou and Yi Yang\*



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### Freely suspended nematic and smectic films and free-standing smectic filaments in the ferroelectric nematic realm

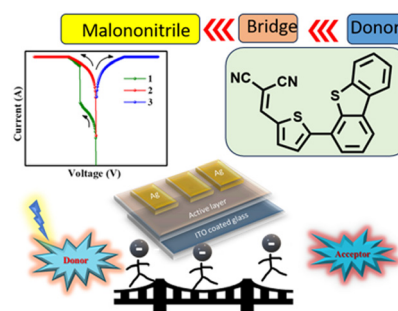
Keith G. Hedlund, Vikina Martinez, Xi Chen, Cheol S. Park, Joseph E. Maclennan,\* Matthew A. Glaser and Noel A. Clark



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### Exploring the potential of malononitrile functionalized donor–acceptor systems for non-volatile memory device applications

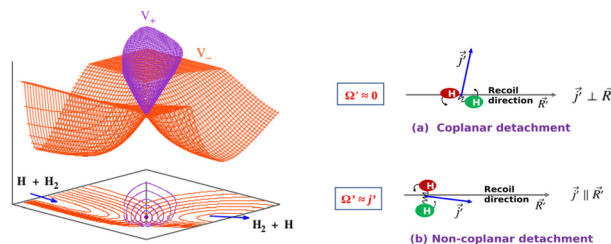
Ramachandran Gokul, Ramesh Gayathri, Predhaneekar Mohamed Imran, Nattamai S. P. Bhuvanesh and Samuthira Nagarajan\*



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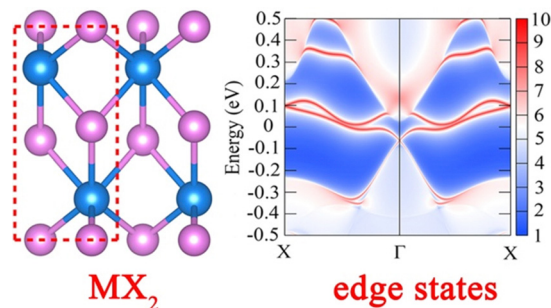
Jayakrushna Sahoo, Sugata Goswami and S. Mahapatra\*



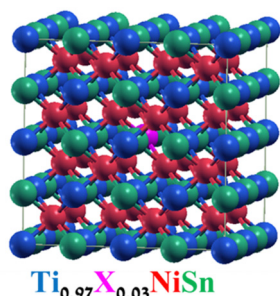
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### Quantum spin Hall states in $\text{MX}_2$ ( $\text{M} = \text{Ru}, \text{Os}$ ; $\text{X} = \text{As}, \text{Sb}$ ) monolayers

Tao Jing,\* Dongmei Liang, Yongchen Xiong, Jun Zhang, Yongjin Hu, Qin Zhang, Dongyan Lv, Zhi He and Mingsen Deng\*



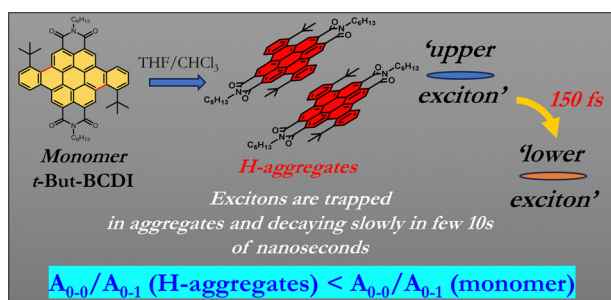
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### The effect of acceptor and donor doping on the electronic properties of the half-Heusler TiNiSn

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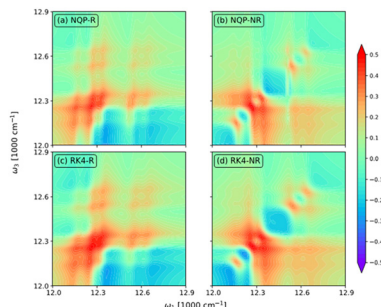
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### Unveiling emissive H-aggregates of benzocoronenediimide, their photophysics and ultrafast exciton dynamics

Swati J. N. Dixit, Rajib Ghosh\* and Neeraj Agarwal\*

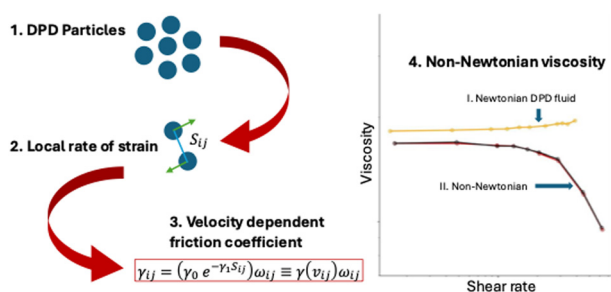
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Jiaji Zhang\* and Lipeng Chen\*

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### Non-Newtonian dynamics modelled with non-linear transport coefficients at the mesoscale by using dissipative particle dynamics

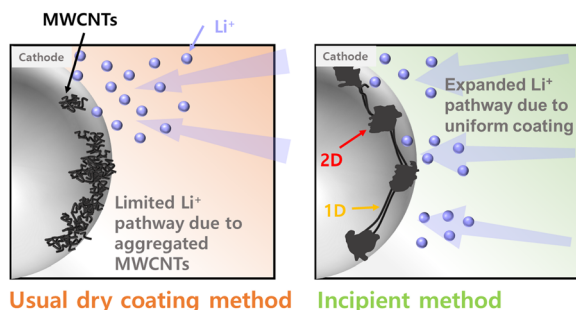
Ali Naseri, Clara Salueña Perez and Josep Bonet Avalos\*





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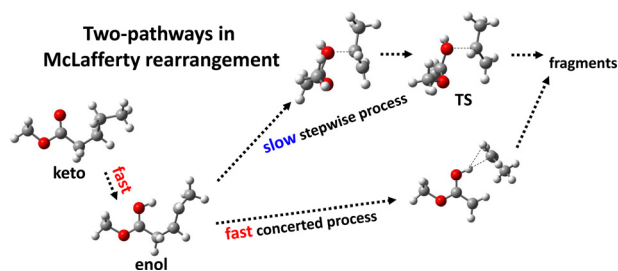
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### Superior conductive 1D and 2D network structured carbon-coated Ni-rich $\text{Li}_{1.05}\text{Ni}_{0.88}\text{Co}_{0.08}\text{Mn}_{0.04}\text{O}_2$ as high-ion-diffusion cathodes for lithium-ion batteries

Sungmin Na, Junwoo Park, Hyunjin An, Seonhwa Lee, Byongyong Yu\* and Kwangjin Park\*

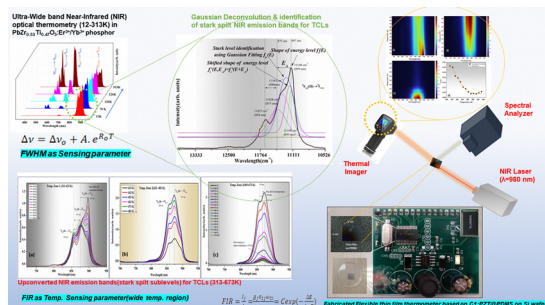
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### Comprehensive quantum chemical and mass spectrometric analysis of the McLafferty rearrangement of methyl valerate

Mitsuo Takayama,\* Masahiro Hashimoto, Keijiro Ohshimo, Fuminori Misaizu, Masaaki Ubukata and Kenji Nagatomo

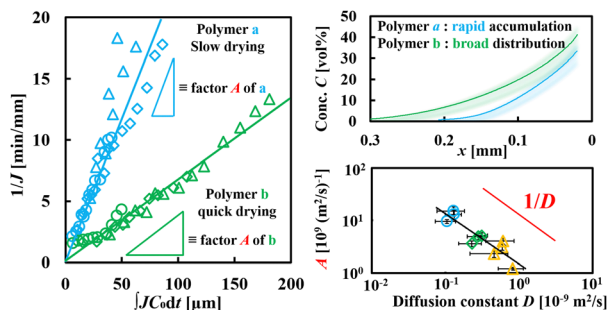
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### Ultra-wide band near-infrared (NIR) optical thermometry (12–673 K) performance enhanced by Stark sublevel splitting in $\text{Er}^{3+}$ ions near the first biological window in the $\text{PbZr}_{0.53}\text{Ti}_{0.47}\text{O}_3:\text{Er}^{3+}/\text{Yb}^{3+}$ phosphor

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### How does the polymer type affect the rate of water evaporation from polymer solutions?

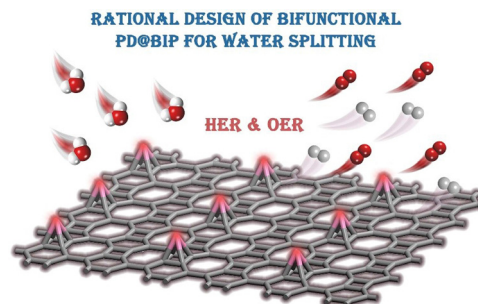
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### Single-atom Pd directly anchored on biphenylene: a promising bifunctional electrocatalyst for overall water splitting

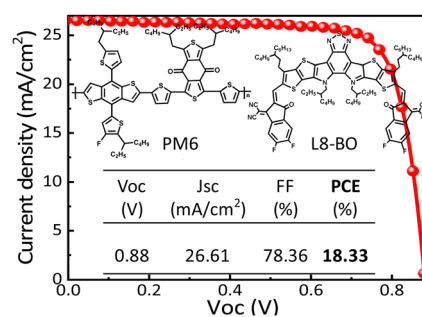
Ting-Ting Wang, Yanan Meng, Hai-Cai Huang, Lei Zhang\* and Shi-Bo Cheng\*



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### Optimization of active layers for efficient binary organic solar cells

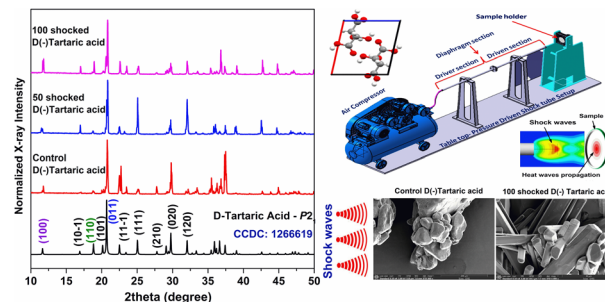
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### Acoustic shock wave-induced superheating-assisted dynamic recrystallization – a case study of D-tartaric acid

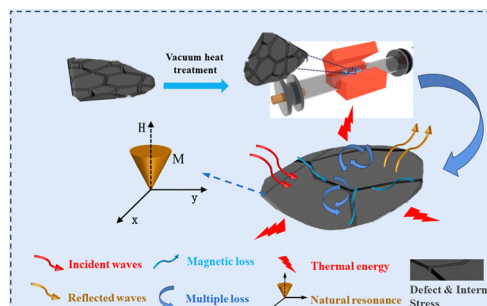
Sivakumar Aswathappa, Lidong Dai,\* Sahaya Jude Dhas Sathiyadhas and Raju Suresh Kumar



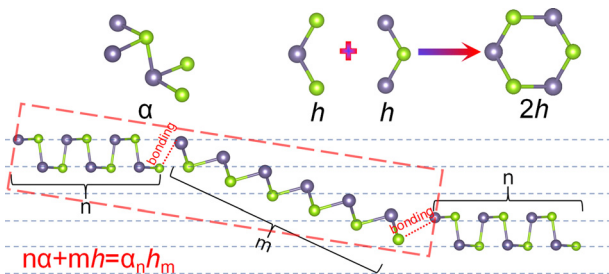
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### Grain size modulation to optimize the wave-absorbing properties of FeSiCr alloy micropowder

Weiwei Dong, Wenmiao Zhang, Lei Wang,\* Sajjad Ur Rehman, Yifeng Hu, Haiping Zou,\* Tongxiang Liang, Changcai Chen and Jianping Zou



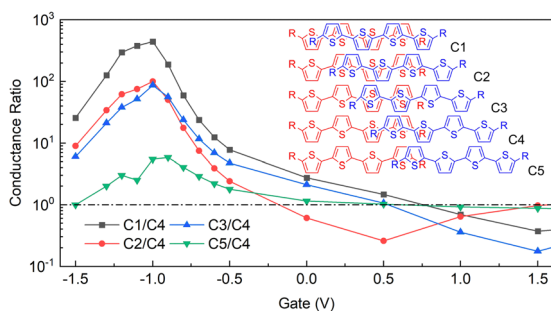
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### $\alpha_n h_m$ -GeSe: a multifunctional semiconductor combining auxeticity and piezoelectricity

Jiajun Zhu, Heyun Zhao and Wanbiao Hu\*

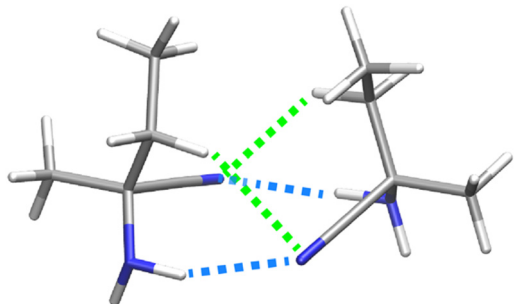
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### A multi-state supramolecular switch realized via a $[\pi \cdots \pi]$ dimer

Hua Hao,\* Honghao Li, Ting Jia and Xiaohong Zheng

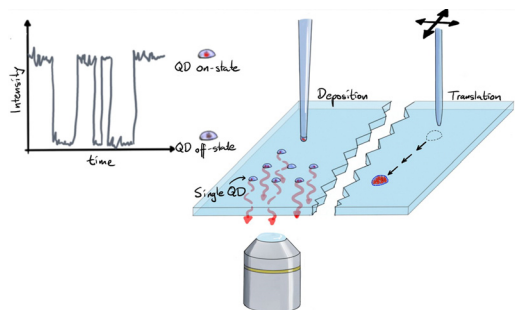
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### Enantioselective interactions of aminonitrile dimers

Natsuki Watanabe, Yu Komatsu, Koichi Miyagawa, Yuta Hori, Yasuteru Shigeta and Mitsuo Shoji\*

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### Controlled encapsulation of colloidal semiconductor quantum dots in a microdroplet

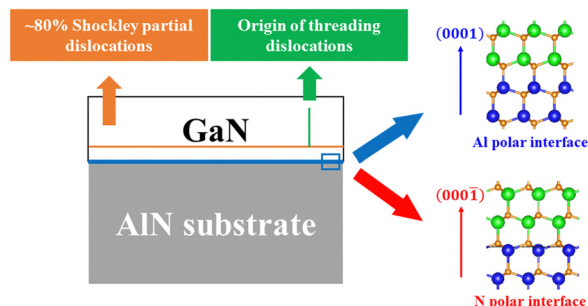
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### The effect of interface polarity on the basal dislocations at the GaN/AlN interface

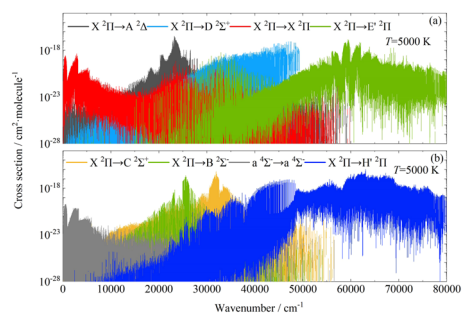
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### An *ab initio* study of the rovibronic spectra of CH

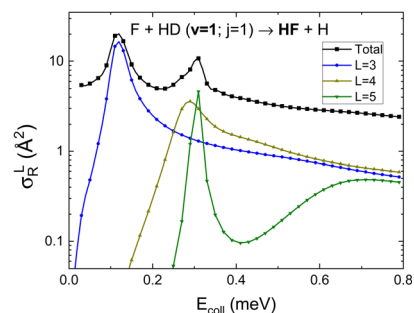
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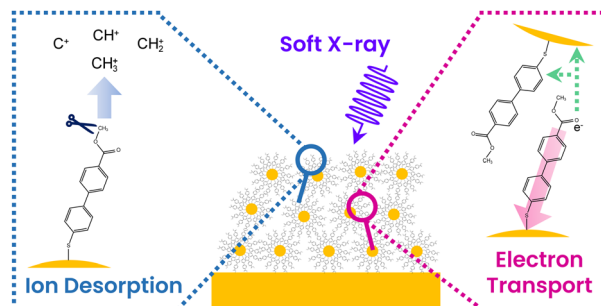
V. Sáez-Rábanos,\* G. Sáez-Cano, J. E. Verdasco, F. J. Aoiz and V. J. Herrero



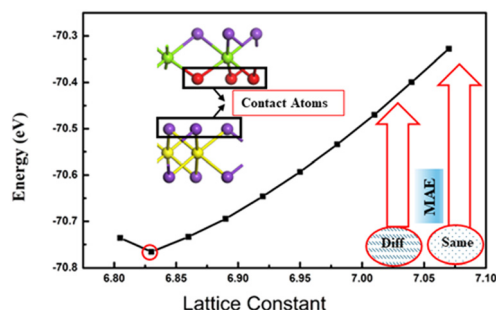
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### Comparative study of electron transport through aromatic molecules on gold nanoparticles: insights from soft X-ray spectroscopy of condensed nanoparticle films versus flat monolayer films

Shogo Tendo, Akinobu Niozu, Kakuto Yoshioka, Masataka Tabuse, Jun-ichi Adachi, Hirokazu Tanaka and Shin-ichi Wada\*



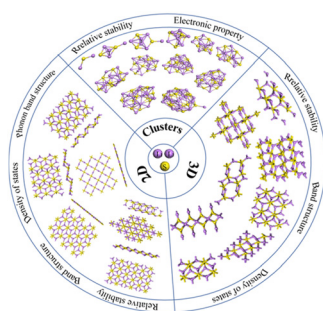
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### Pressure-driven magnetic phase change in the $\text{CrI}_3/\text{Br}_3\text{Cr}_2\text{I}_3$ heterostructure

Fazle Subhan, Luqman Ali, Razia Aman, Ailing Chen, Bo Peng, Yanguang Zhou,\* Zhenzhen Qin\* and Guangzhao Qin\*

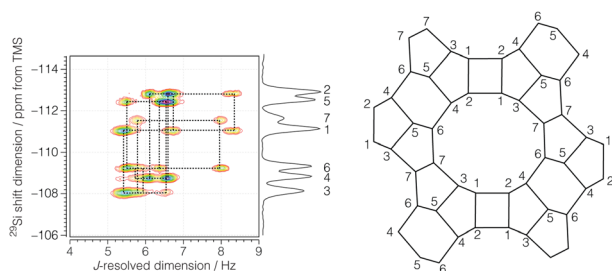
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### Structure and property exploration of two-dimensional, bulk, and cluster lithium sulfide using the IM<sup>2</sup>ODE method

Danling Wang, Chenqi Bai, Jian Cao, Yu Wang, Zian Chen, Lei Wang, Lina Xu,\* Hongping Xiao, Yueyu Zhang\* and Guoyong Fang\*

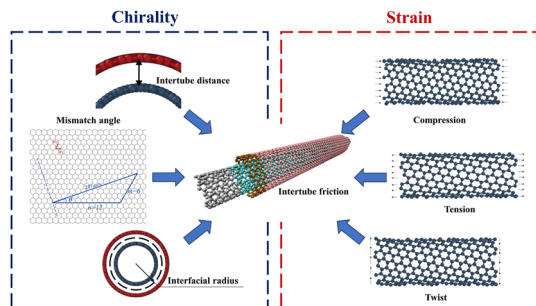
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### Refining siliceous zeolite framework structures with <sup>29</sup>Si 2D J-resolved NMR spectroscopy

Deepansh J. Srivastava, Maxwell C. Venetos, Lexi McCarthy-Carney, Jay H. Baltisberger, Philip J. Grandinetti\* and Darren Brouwer

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### Mechanisms of interlayer friction in low-dimensional homogeneous thin-wall shell structures and its strain effect

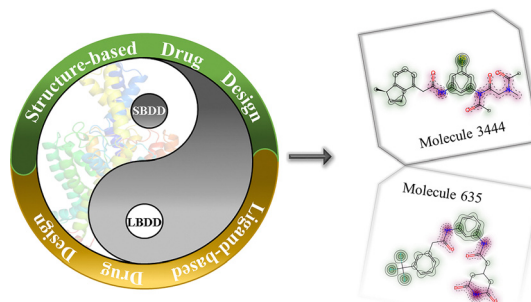
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### Design of bisamide inhibitors of the TASK-1 potassium channel *in silico*

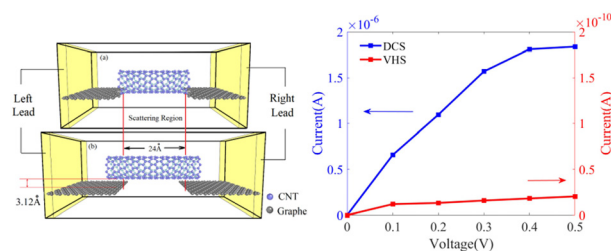
Lu Liu, Jixiang Liu, Liang Chen, Risong Na, Lianjuan Yang, Xiaoping Liu and Xi Zhao\*



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### Low contact resistance in carbon nanotube devices: metal-induced gap states

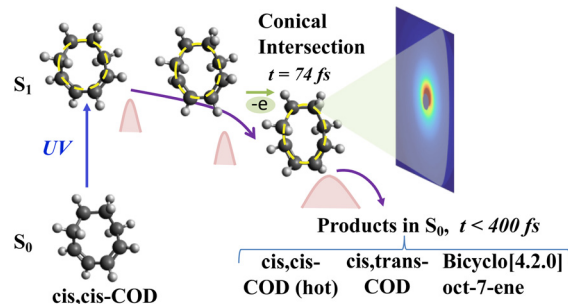
Bo Zhang, Xiaojie Liu,\* Huan Wang,\* Lifeng Feng\* and Haitao Yin\*



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### Ultrafast structural dynamics of UV photoexcited *cis,cis*-1,3-cyclooctadiene observed with time-resolved electron diffraction

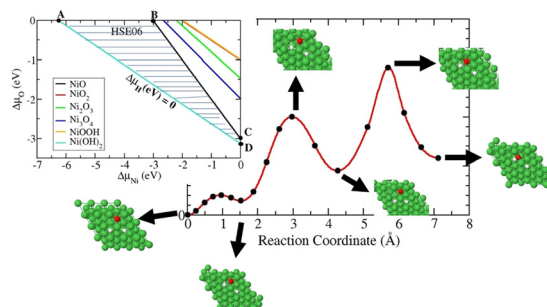
S. B. Muwa,\* Y. Liu, P. Chakraborty, J. P. F. Nunes, A. R. Attar, S. Bhattacharyya, K. Borne, E. G. Champenois, N. Goff, K. Hegazy, M. C. Hoffmann, F. Ji, M.-F. Lin, D. Luo, L. Ma, A. Odate, S. Pathak, D. Rolles, A. Rudenko, S. K. Saha, X. Shen, X. Wang, M. R. Ware, S. Weathersby, P. M. Weber, K. J. Wilkin, T. J. A. Wolf, Y. Xiong, X. Xu, J. Yang, S. Matsika, T. Weinacht and M. Centurion\*



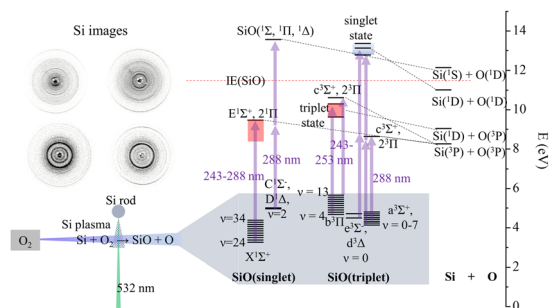
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### First principles density functional theory study of tritium species adsorption on Ni(111) surface and diffusion in nickel-sublayer for tritium storage

De Nyago Tafen, Hari P. Paudel, David J. Senor, Andrew M. Casella and Yuhua Duan\*



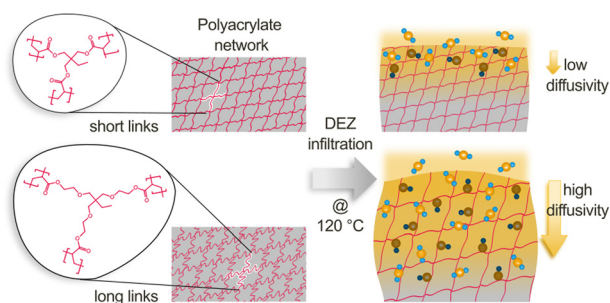
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### Unveiling ultraviolet photodissociation dynamics of SiO from a laser-ablated supersonic beam with time-sliced ion velocity imaging

Yujie Ma, Fangfang Li, Dong Yan, Ang Xu, Ti Zhou, Jiaxing Liu and Fengyan Wang\*

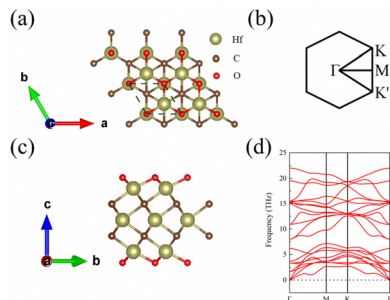
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### Effects of polymer network flexibility on the kinetics of DEZ vapor phase infiltration into photo-polymerized polyacrylates

Lisanne Demelius, Anna Maria Coclite and Mark D. Losego\*

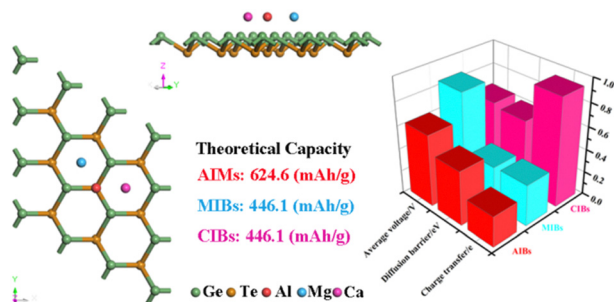
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### Valley splitting of monolayer $\text{Hf}_3\text{C}_2\text{O}_2$ by the spin-orbit coupling effect: first principles calculations using the HSE06 methods

Shiqian Qiao, Yang Zhang, Shasha Li, Lujun Wei, Hong Wu and Feng Li\*

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### First principles study on monolayer GeTe as an anode material for multivalent ion batteries

Junjie Chen,\* Zhiyu Zhou and Ruidan Zhang\*

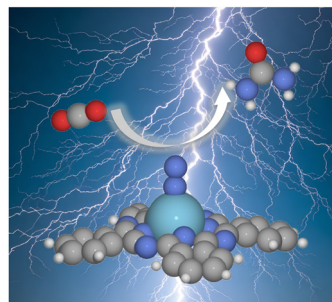


## RESEARCH PAPERS

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### Are transition metal phthalocyanines active for urea synthesis via electrocatalytic coupling of CO<sub>2</sub> and N<sub>2</sub>?

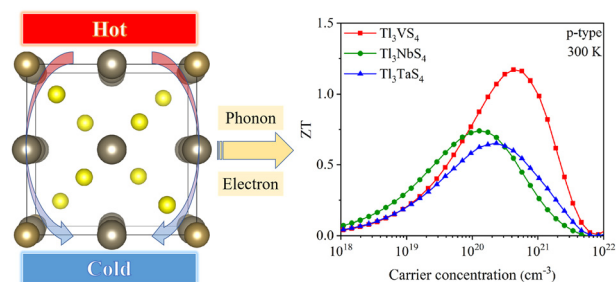
Yungan Huang, Ting Fan and Yongfei Ji\*



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### Potential thermoelectric material Ti<sub>3</sub>XS<sub>4</sub> (X = V, Nb, Ta) with ultralow lattice thermal conductivity

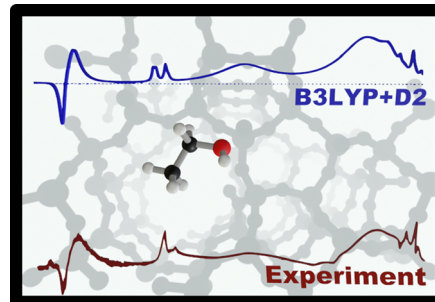
Xiefei Song,\* Guangzhao Wang, Wenzhong Li, Siyu Gan, Yan Cai, Dianxu Ma, Yuhui Luo, Yao He\* and Ning Wang\*



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### Assignment of IR spectra of ethanol at Brønsted sites of H-ZSM-5 to monomer adsorption using a Fermi resonance model

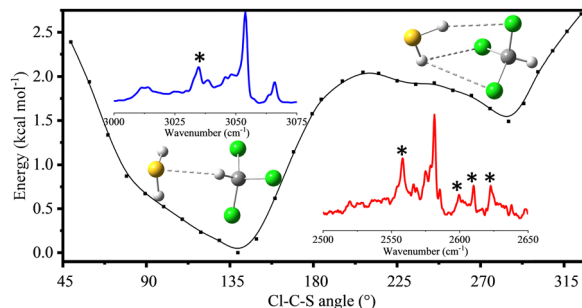
Dipanshu Kumar, Joachim Sauer, Alessia Airi,\* Silvia Bordiga and Daria Ruth Galimberti\*



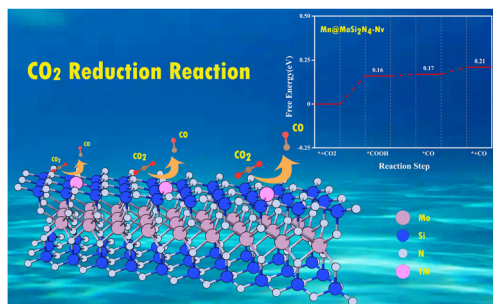
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### Competition between C–H···S and S–H···Cl H-bonds in a CHCl<sub>3</sub>–H<sub>2</sub>S complex: a combined matrix isolation IR spectroscopic and quantum chemical investigation

Binod Kumar Oram, Monu, Ankita Kothari and Biman Bandyopadhyay\*



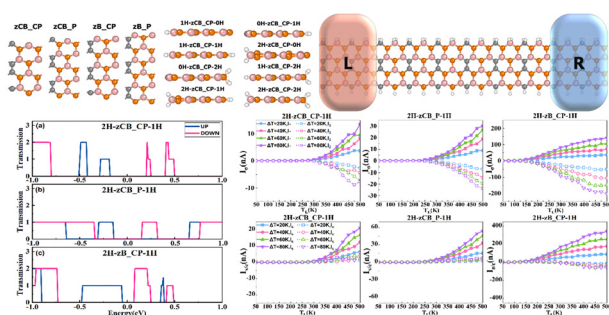
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### Theoretical investigations of transition metal atom-doped $\text{MoSi}_2\text{N}_4$ monolayers as catalysts for electrochemical $\text{CO}_2$ reduction reactions

Guoqiang Ding, Yiwen Gao, Hetong Zhang, Na Yang, Xiaobin Niu\* and Jianwei Wang\*

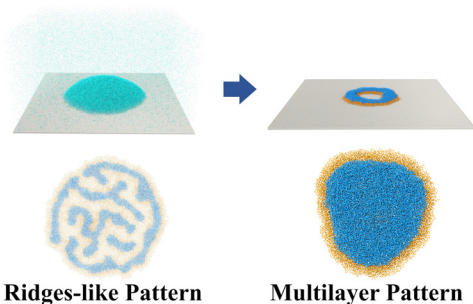
589



### Pure spin currents induced by asymmetric H-passivation in $\text{B}_3\text{C}_2\text{P}_3$ nanoribbons

Jing-Jing He, Jia-Bei Dong, Ling-Xiao Liu, Qin-Yue Cao, Jun-Yi Gu, Ying Zhang, Min Hua, Jia-Ren Yuan\* and Xiao-Hong Yan\*

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### Influence of polymer chain length and concentration on the deposition patterns of linear diblock copolymer solution nanodroplets

Han-Wen Pei, Jun Zhang and Zhao-Yan Sun\*

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### Expression of concern: Localized electropolymerization on oxidized boron-doped diamond electrodes modified with pyrrolyl units

Paolo Actis, Mael Manesse, Carolina Nunes-Kirchner, Gunther Wittstock, Yannick Coffinier, Rabah Boukherroub and Sabine Szunerits\*



## CORRECTION

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**Correction: Density functional theory study of crown ether–magnesium complexes: from a solvated ion to an ion trap**

Katarina Čeranić, Branislav Milovanović and Milena Petković\*

