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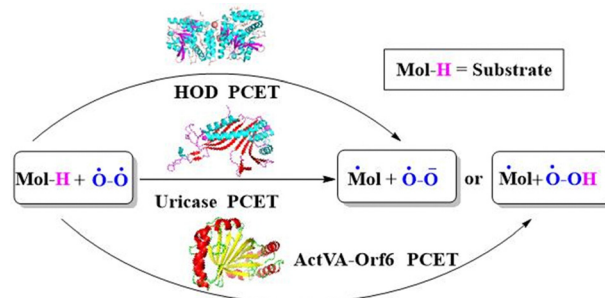
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Unraveling proton-coupled electron transfer in cofactor-free oxidase- and oxygenase-catalyzed oxygen activation: a theoretical view

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

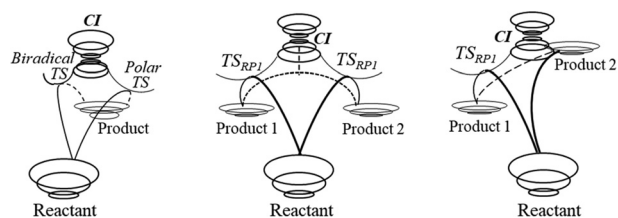


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Light driven photoswitches: three classes of molecular systems that result in a single photoproduct via a conical intersection and an exothermic reverse reaction

Shmuel Zilberg



Three classes of molecular photoswitches



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Fundamental questions
Elemental answers

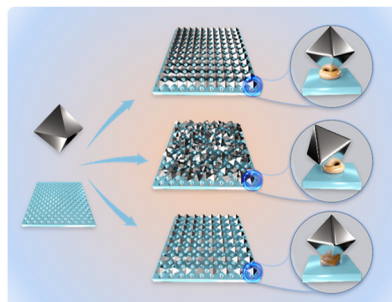


COMMUNICATION

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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*

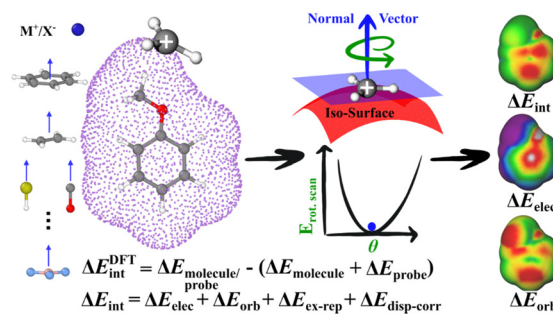


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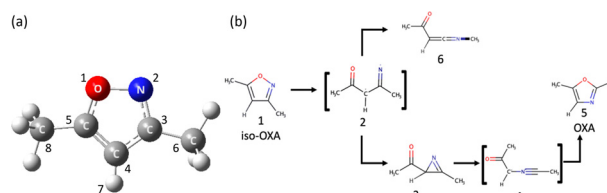
Amin Kiani, Wentong Zhou and Lawrence M. Wolf*



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

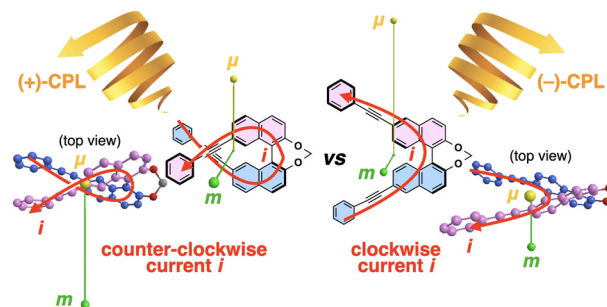
Mizuki Kimura and Shinkoh Nanbu*



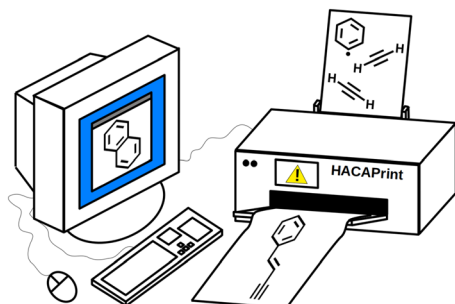
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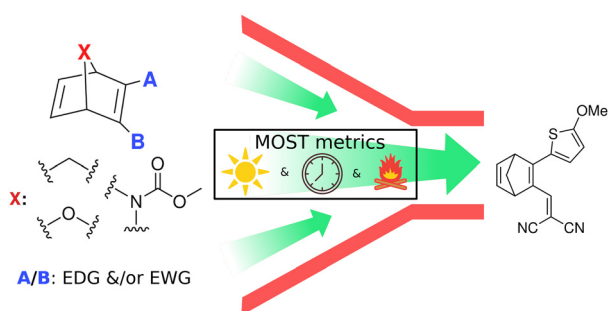
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Patricia D. Kelly,* Jack A. Turner, Oisín J. Shiels, Gabriel da Silva, Stephen J. Blanksby, Berwyck L. J. Poole and Adam J. Trevitt*

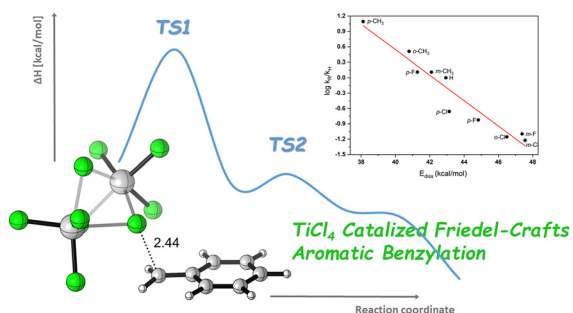
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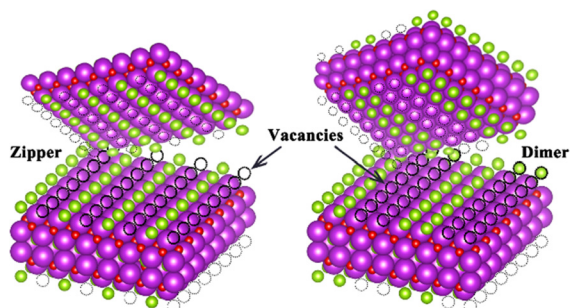
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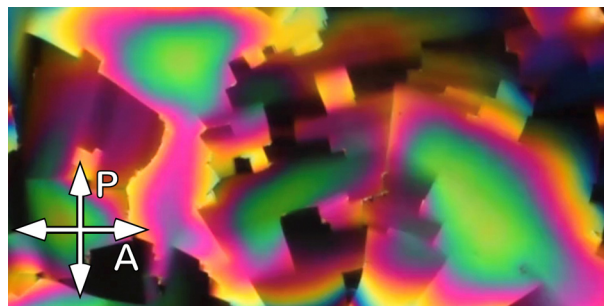
Kai Gao, Yan-Jin Chen, Yang Ou,* Jin-ming Zeng, Chunju Hou and Yi Yang*



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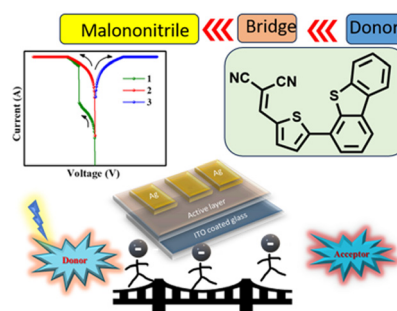
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Exploring the potential of malononitrile functionalized donor-acceptor systems for non-volatile memory device applications

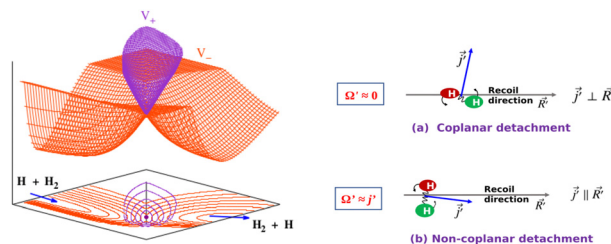
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Unraveling the effect of reagent vibrational excitation on the scattering mechanism of the benchmark $H + H_2 \rightarrow H_2 + H$ hydrogen exchange reaction in the coupled $1^2E'$ ground electronic manifold

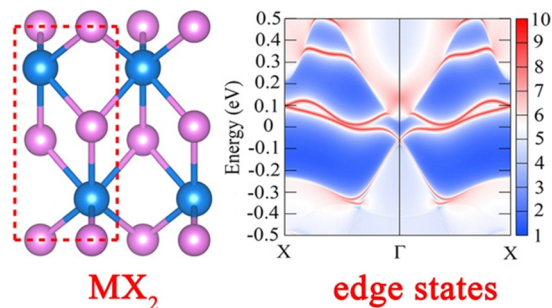
Jayakrushna Sahoo, Sugata Goswami and S. Mahapatra*



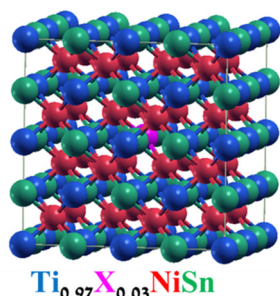
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Quantum spin Hall states in MX_2 ($M = Ru, Os$; $X = As, Sb$) monolayers

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



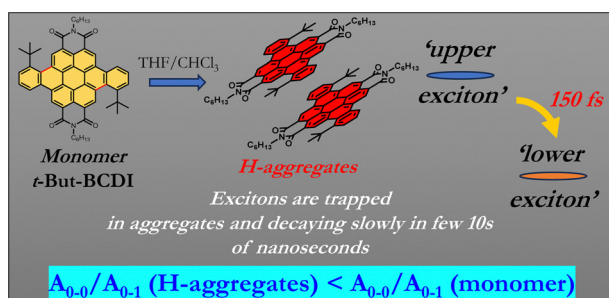
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The effect of acceptor and donor doping on the electronic properties of the half-Heusler TiNiSn

Ronit Eshel,* David Fuks, Yaniv Gelbstein and Daniel Rabin

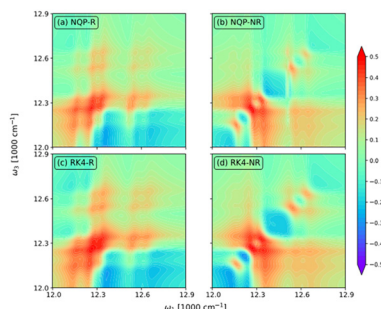
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Unveiling emissive H-aggregates of benzocoronenediimide, their photophysics and ultrafast exciton dynamics

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

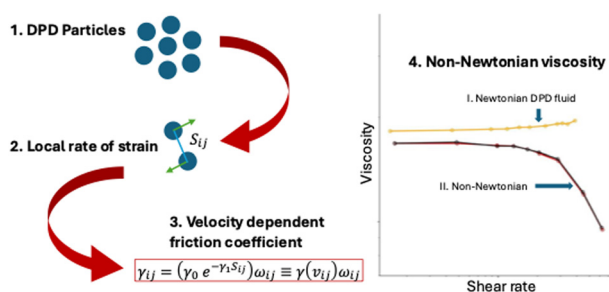
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Jiaji Zhang* and Lipeng Chen*

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

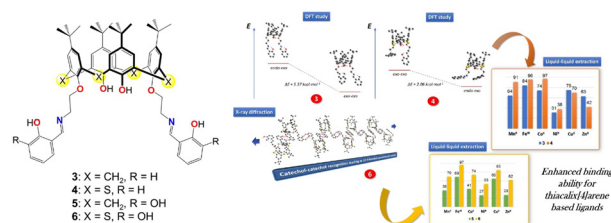
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Interplay between conformational flexibility, intermolecular H-bonding and 3d-metal cation extraction ability in a series of thiacalix[4]arene lower rim disubstituted Schiff base derivatives

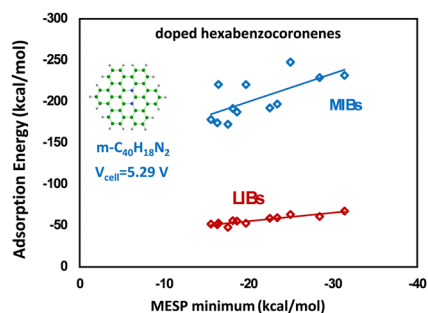
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Doped hexa-*peri*-hexabenzocoronene as anode materials for lithium- and magnesium-ion batteries

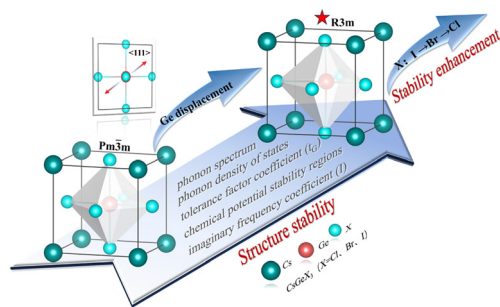
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The stability of CsGeX₃ (X = I, Br, Cl) selectively tuned by the crystal structures and halide ions as inferred from the calculated phonon spectrum

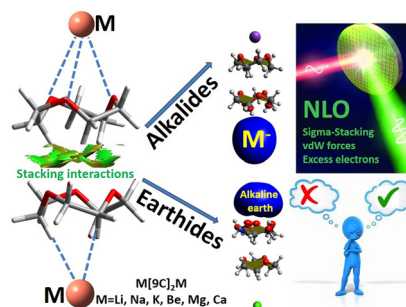
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Xin Xu, Yujia Gao, Zhuxia Wu, Haiyan Li, Fei Yuan,
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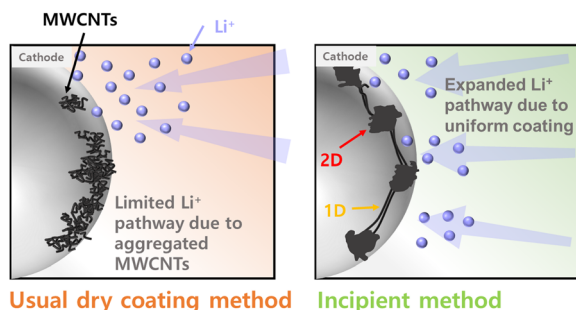
Stacking interactions in stabilizing supramolecular assembly of M[9C]2M complexes: dynamic stability with remarkable nonlinear optical features

Atazaz Ahsin,* Aamna Qamar, Sadegh Kaviani and
V. Vetrivelan



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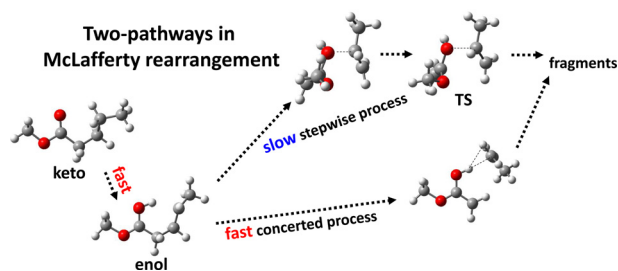
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Superior conductive 1D and 2D network structured carbon-coated Ni-rich $\text{Li}_{1.05}\text{Ni}_{0.88}\text{Co}_{0.08}\text{Mn}_{0.04}\text{O}_2$ as high-ion-diffusion cathodes for lithium-ion batteries

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

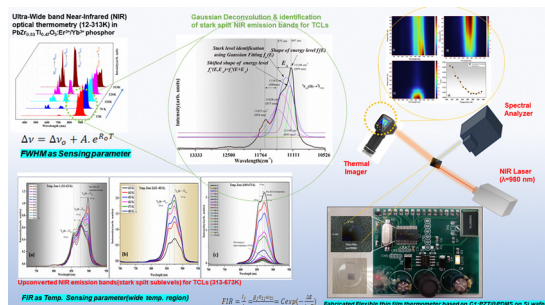
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Comprehensive quantum chemical and mass spectrometric analysis of the McLafferty rearrangement of methyl valerate

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

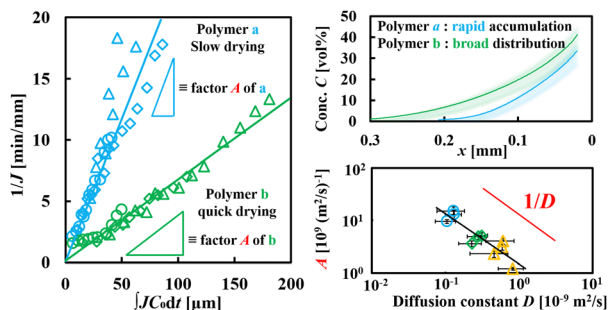
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Ultra-wide band near-infrared (NIR) optical thermometry (12–673 K) performance enhanced by Stark sublevel splitting in Er^{3+} ions near the first biological window in the $\text{PbZr}_{0.53}\text{Ti}_{0.47}\text{O}_3:\text{Er}^{3+}/\text{Yb}^{3+}$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

Prasenjit Prasad Sukul,* Yadendra Singh and Hendrik Swart

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

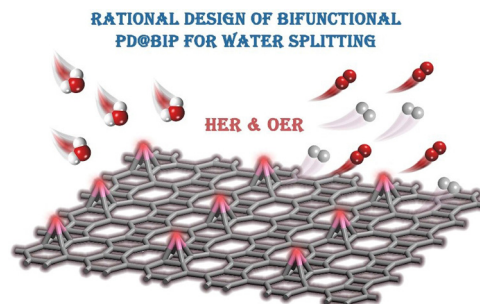
Masahiko Tanaka and Susumu Inasawa*



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

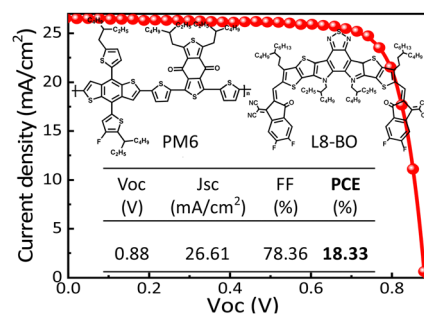
Ting-Ting Wang, Yanan Meng, Hai-Cai Huang, Lei Zhang* and Shi-Bo Cheng*



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Optimization of active layers for efficient binary organic solar cells

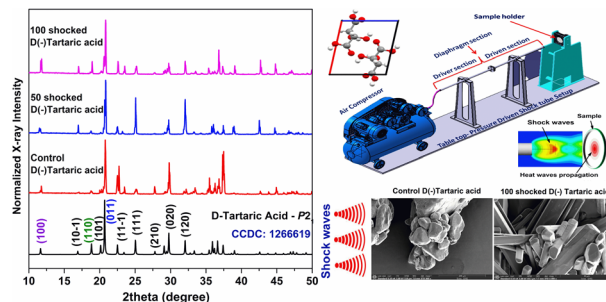
Yunjie Li, Beining Wang, Lijun Chen, Yaqian Yuan, Jianfei Fu, Chong Geng, Junmin Wan* and Hai-Qiao Wang*



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

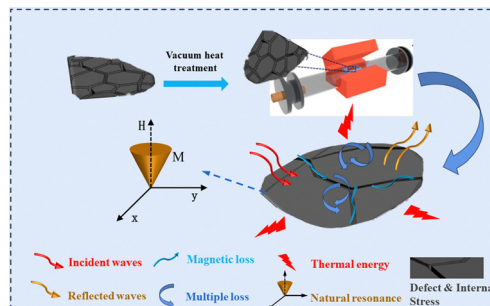
Sivakumar Aswathappa, Lidong Dai,* Sahaya Jude Dhas Sathiyadhas and Raju Suresh Kumar



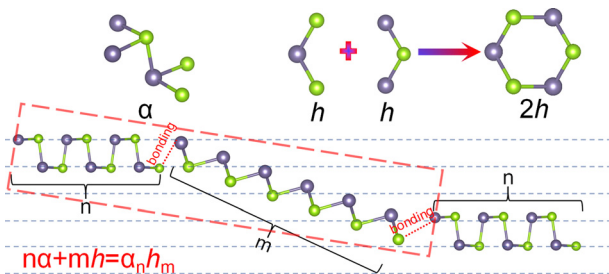
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Grain size modulation to optimize the wave-absorbing properties of FeSiCr alloy micropowder

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



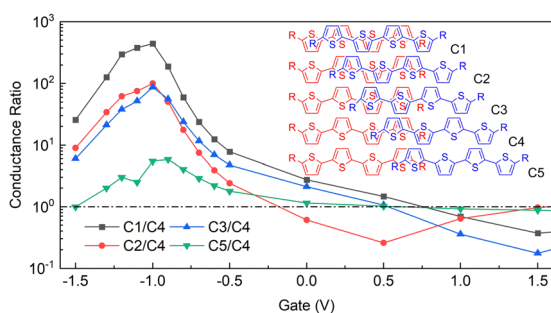
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$\alpha_n h_m$ -GeSe: a multifunctional semiconductor combining auxeticity and piezoelectricity

Jiajun Zhu, Heyun Zhao and Wanbiao Hu*

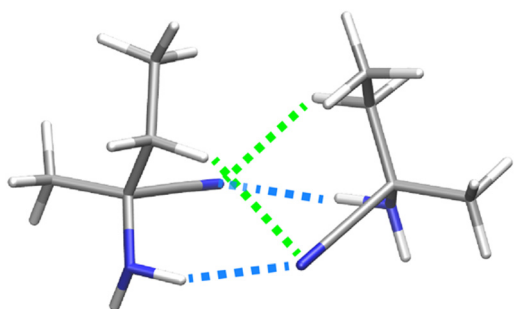
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A multi-state supramolecular switch realized via a $[\pi \cdots \pi]$ dimer

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

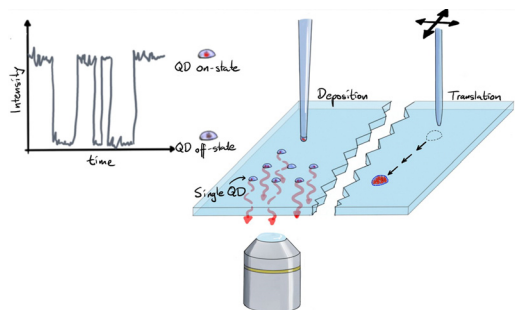
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Enantioselective interactions of aminonitrile dimers

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

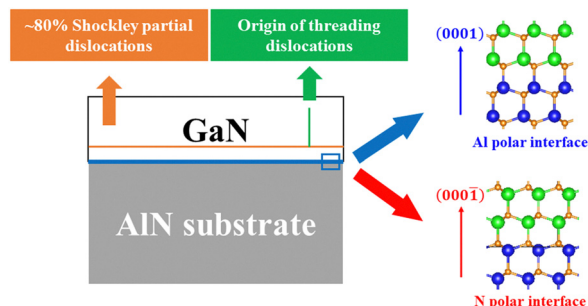
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The effect of interface polarity on the basal dislocations at the GaN/AlN interface

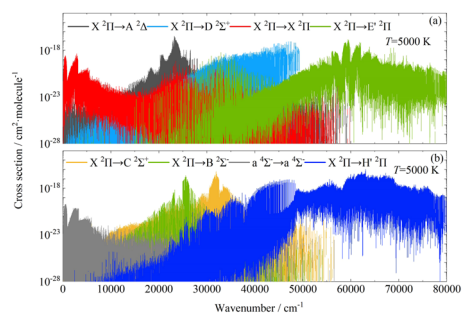
Yuming Yang, Xuemei Zhang, Mi Qin, Jun Liu, Chuanguo Zhang, Zhixin Hui, Yonggang Li, Zhi Zeng and Yongsheng Zhang*



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

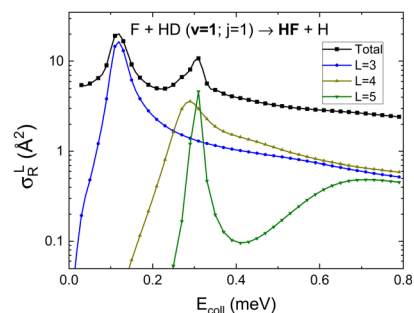
Zhenlu Hou and Linhua Liu*



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The F + HD ($\nu = 0, 1; j = 1$) reaction: angular momentum correlations in the low (< 1 meV) collision energy regime

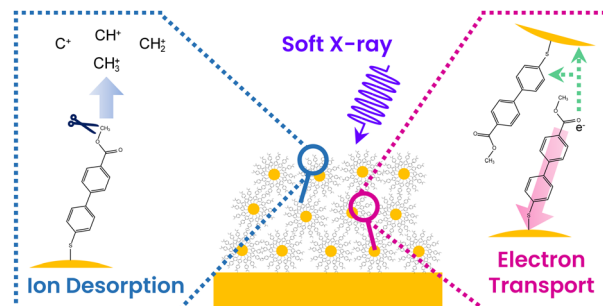
V. Sáez-Rábanos,* G. Sáez-Cano, J. E. Verdasco, F. J. Aoiz and V. J. Herrero



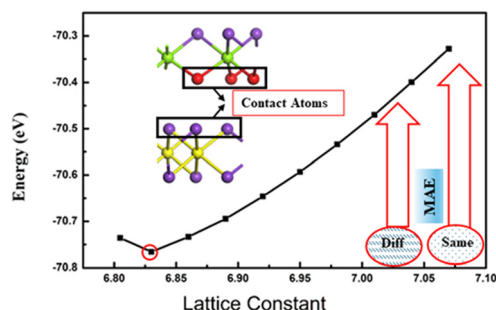
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Comparative study of electron transport through aromatic molecules on gold nanoparticles: insights from soft X-ray spectroscopy of condensed nanoparticle films versus flat monolayer films

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



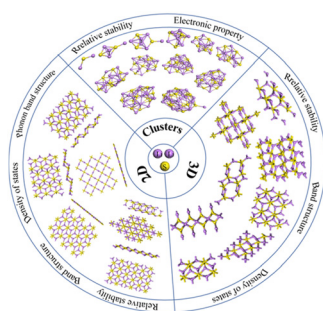
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Pressure-driven magnetic phase change in the $\text{CrI}_3/\text{Br}_3\text{Cr}_2\text{I}_3$ heterostructure

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

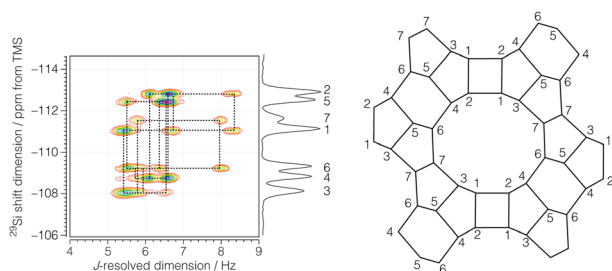
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Structure and property exploration of two-dimensional, bulk, and cluster lithium sulfide using the IM²ODE method

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

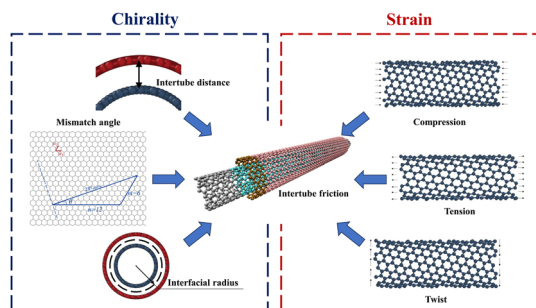
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Refining siliceous zeolite framework structures with ^{29}Si 2D J -resolved NMR spectroscopy

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

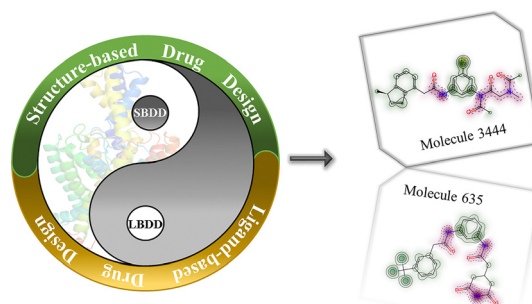
Yi Cai, Jianzhang Huang,* Shuang Gan, Yingjing Liang, Kejing Wang and Qiang Han



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

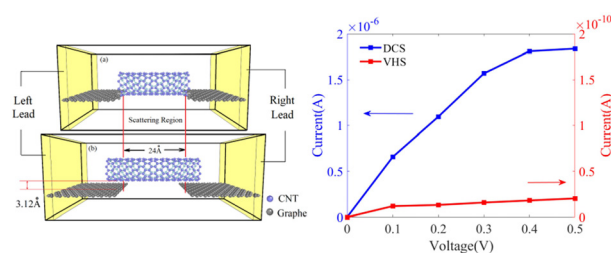
Lu Liu, Jixiang Liu, Liang Chen, Risong Na, Lianjuan Yang, Xiaoping Liu and Xi Zhao*



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

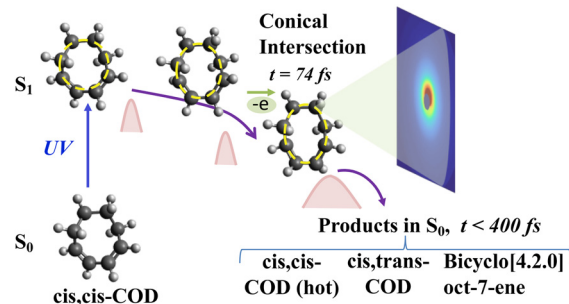
Bo Zhang, Xiaojie Liu,* Huan Wang,* Lifeng Feng* and Haitao Yin*



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

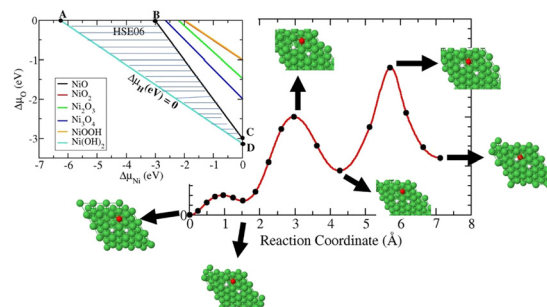
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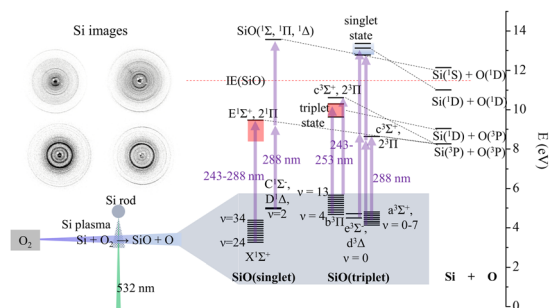
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First principles density functional theory study of tritium species adsorption on Ni(111) surface and diffusion in nickel-sublayer for tritium storage

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



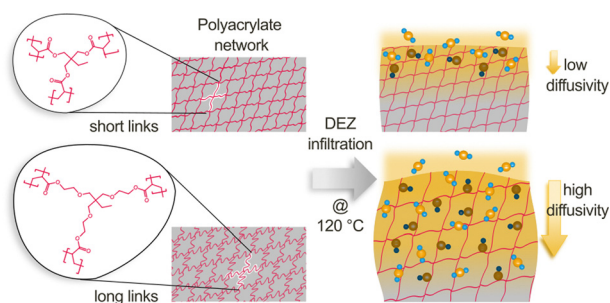
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Unveiling ultraviolet photodissociation dynamics of SiO from a laser-ablated supersonic beam with time-sliced ion velocity imaging

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

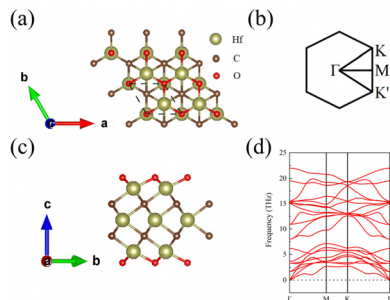
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Effects of polymer network flexibility on the kinetics of DEZ vapor phase infiltration into photo-polymerized polyacrylates

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

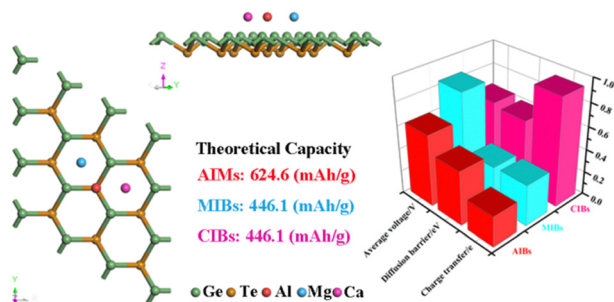
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Valley splitting of monolayer $\text{Hf}_3\text{C}_2\text{O}_2$ by the spin-orbit coupling effect: first principles calculations using the HSE06 methods

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*

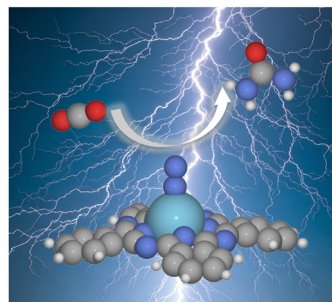


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Are transition metal phthalocyanines active for urea synthesis via electrocatalytic coupling of CO₂ and N₂?

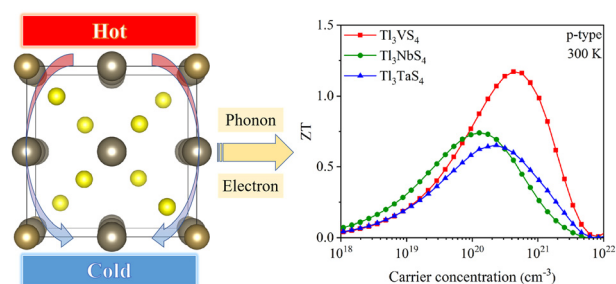
Yungan Huang, Ting Fan and Yongfei Ji*



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Potential thermoelectric material Ti₃XS₄ (X = V, Nb, Ta) with ultralow lattice thermal conductivity

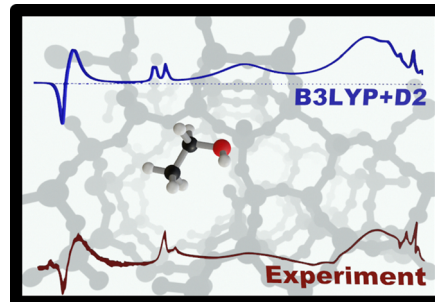
Xiefei Song,* Guangzhao Wang, Wenzhong Li, Siyu Gan, Yan Cai, Dianxu Ma, Yuhui Luo, Yao He* and Ning Wang*



550

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

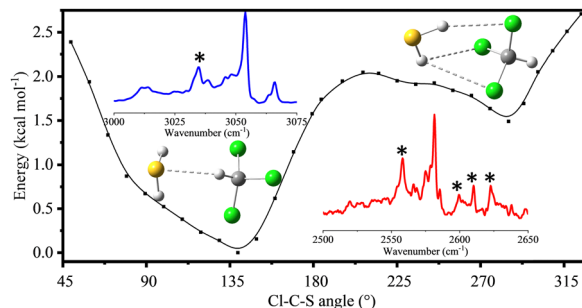
Dipanshu Kumar, Joachim Sauer, Alessia Airi,* Silvia Bordiga and Daria Ruth Galimberti*



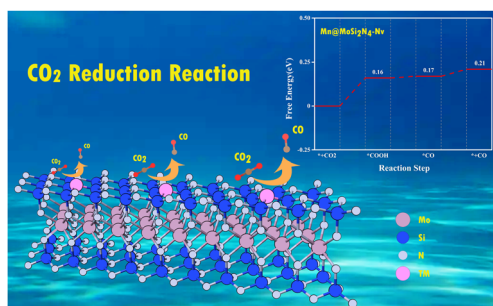
564

Competition between C–H···S and S–H···Cl H-bonds in a CHCl₃–H₂S complex: a combined matrix isolation IR spectroscopic and quantum chemical investigation

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



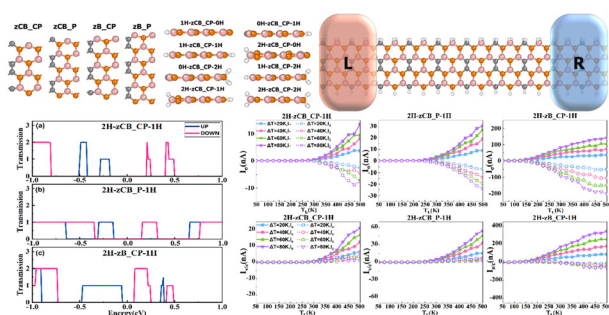
577



Theoretical investigations of transition metal atom-doped MoSi_2N_4 monolayers as catalysts for electrochemical CO_2 reduction reactions

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

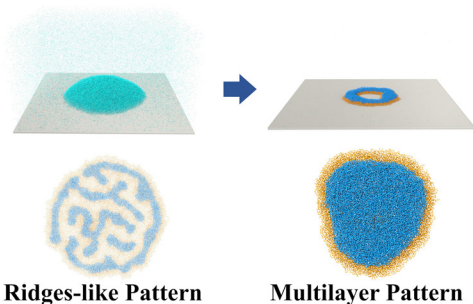
589



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*

596



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*

606

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*

