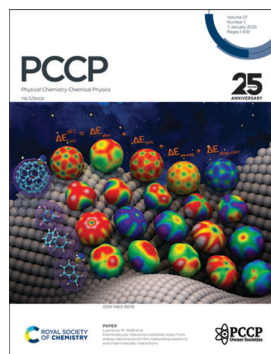


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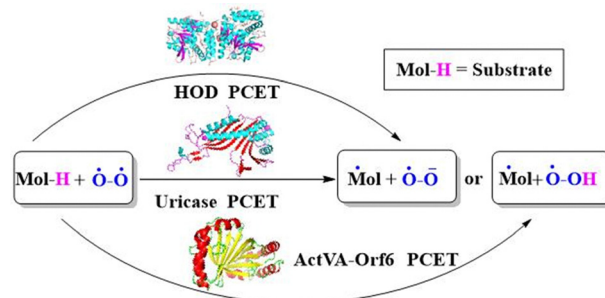
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Unraveling proton-coupled electron transfer in cofactor-free oxidase- and oxygenase-catalyzed oxygen activation: a theoretical view

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

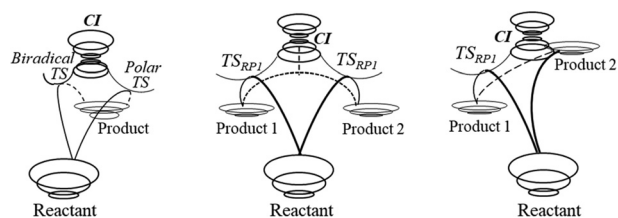


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Light driven photoswitches: three classes of molecular systems that result in a single photoproduct via a conical intersection and an exothermic reverse reaction

Shmuel Zilberg



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Fundamental questions
Elemental answers

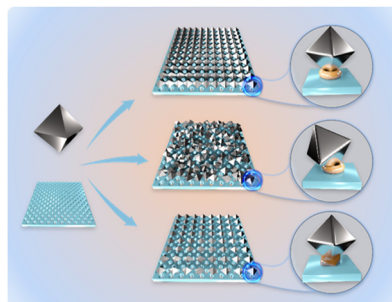


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Strongly coupled and highly-compacted zirconium aminobenzenedicarboxylate crystal membranes for accelerating carbon dioxide capture

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

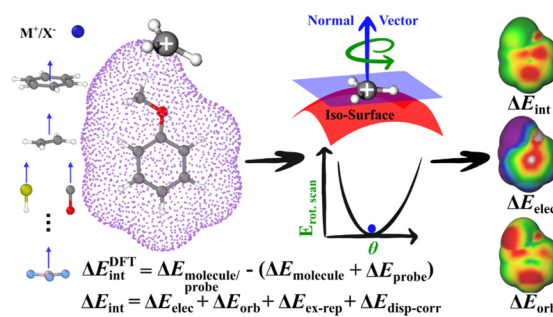


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Intermolecular interaction potential maps from energy decomposition for interpreting reactivity and intermolecular interactions

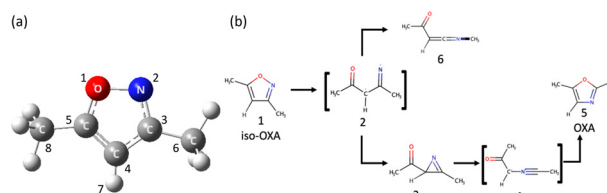
Amin Kiani, Wentong Zhou and Lawrence M. Wolf*



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

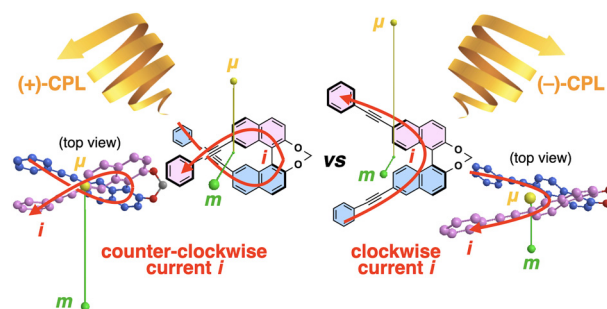
Mizuki Kimura and Shinkoh Nanbu*



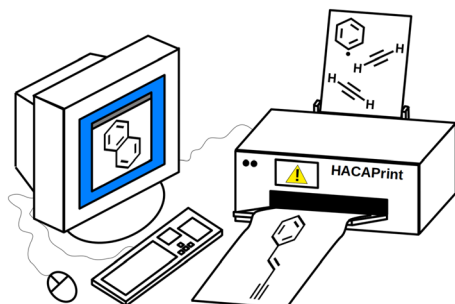
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Ayumi Imayoshi,* Shinya Fujio, Yuuki Nagaya, Misato Sakai, Atsushi Terazawa, Misa Sakura, Keita Okada, Takahiro Kimoto, Tadashi Mori, Yoshitane Imai, Masahiko Hada and Kazunori Tsubaki*



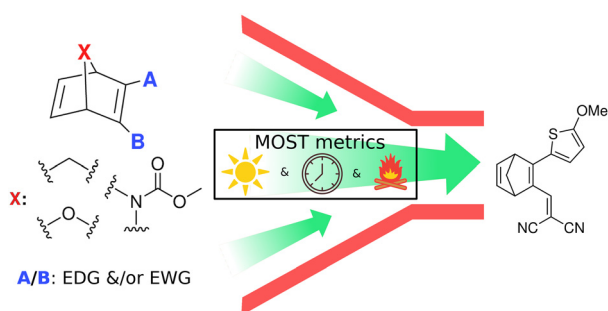
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Don't forget the *trans*: double bond isomerism radical-acetylene growth reactions affect the primary stages of PAH and soot formation

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

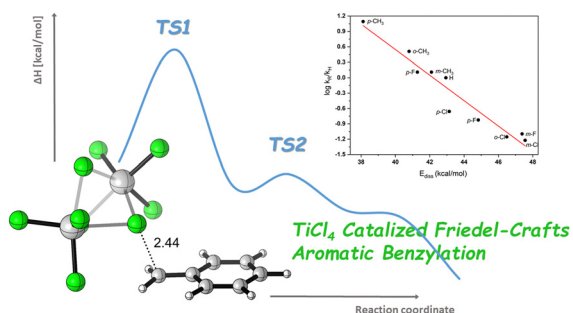
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Searching the chemical space of hetero-atom bridged norbornadienes

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

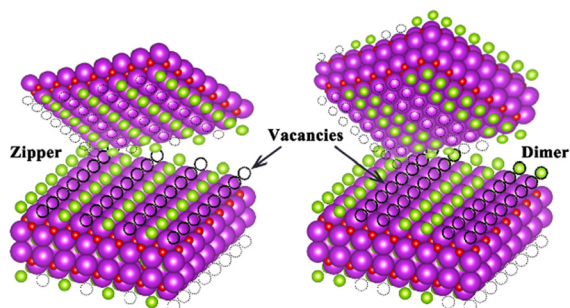
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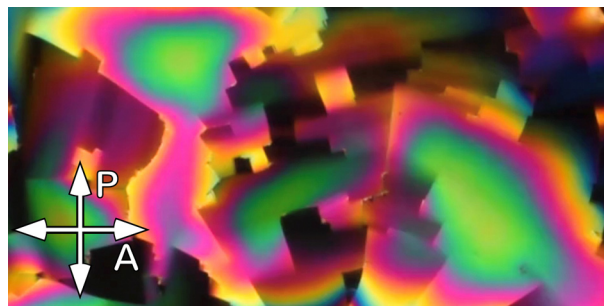
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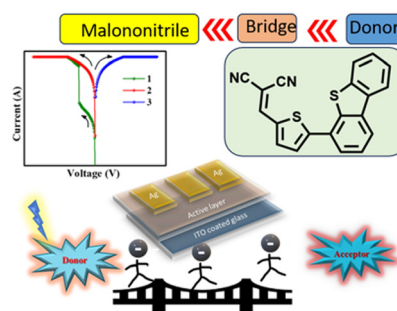
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Exploring the potential of malononitrile functionalized donor–acceptor systems for non-volatile memory device applications

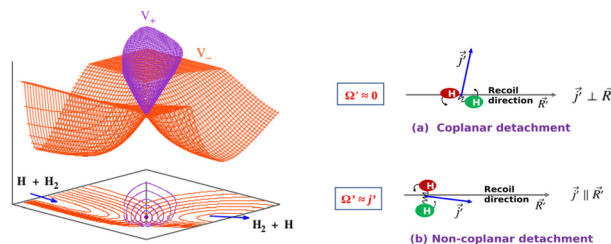
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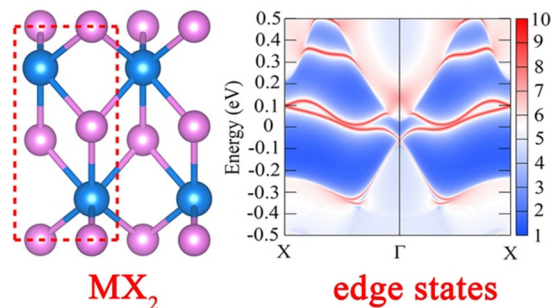
Jayakrushna Sahoo, Sugata Goswami and S. Mahapatra*



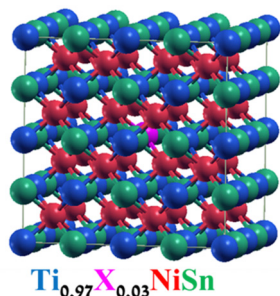
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Quantum spin Hall states in MX_2 ($\text{M} = \text{Ru}, \text{Os}$; $\text{X} = \text{As}, \text{Sb}$) monolayers

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



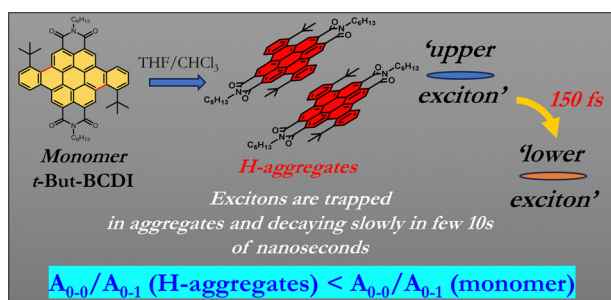
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The effect of acceptor and donor doping on the electronic properties of the half-Heusler TiNiSn

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

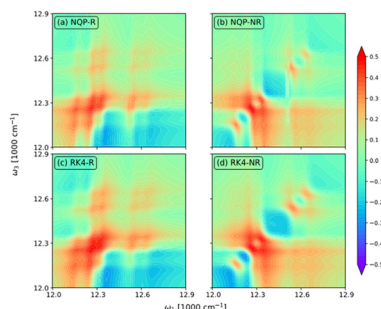
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Unveiling emissive H-aggregates of benzocoronenediimide, their photophysics and ultrafast exciton dynamics

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

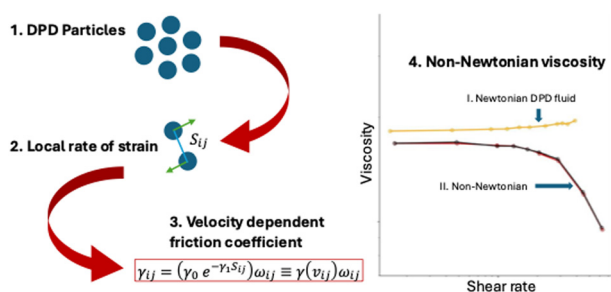
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A non-Markovian neural quantum propagator and its application in the simulation of ultrafast nonlinear spectra

Jiaji Zhang* and Lipeng Chen*

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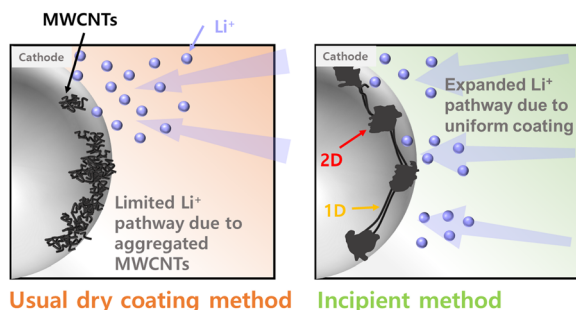
Non-Newtonian dynamics modelled with non-linear transport coefficients at the mesoscale by using dissipative particle dynamics

Ali Naseri, Clara Salueña Perez and Josep Bonet Avalos*



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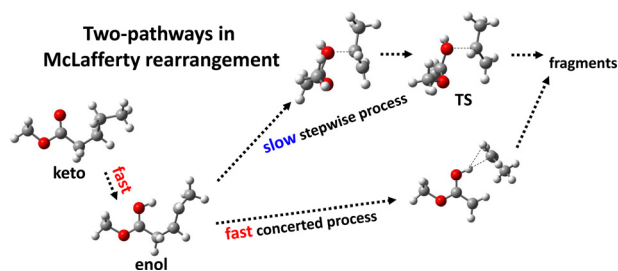
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Superior conductive 1D and 2D network structured carbon-coated Ni-rich $\text{Li}_{1.05}\text{Ni}_{0.88}\text{Co}_{0.08}\text{Mn}_{0.04}\text{O}_2$ as high-ion-diffusion cathodes for lithium-ion batteries

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

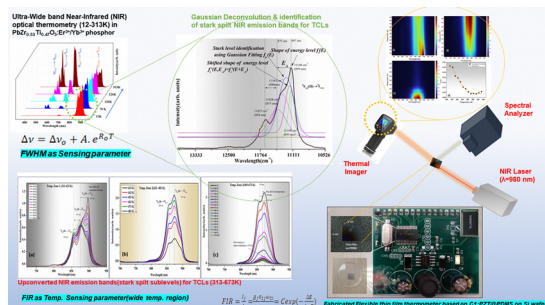
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Comprehensive quantum chemical and mass spectrometric analysis of the McLafferty rearrangement of methyl valerate

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

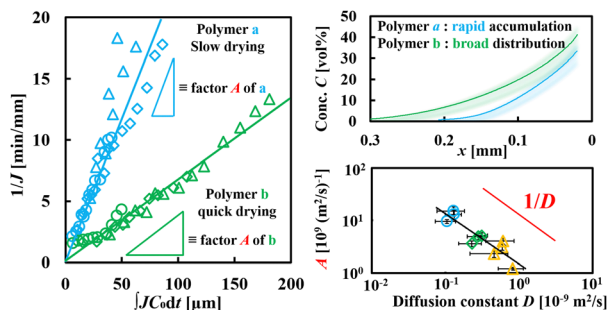
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Ultra-wide band near-infrared (NIR) optical thermometry (12–673 K) performance enhanced by Stark sublevel splitting in Er^{3+} ions near the first biological window in the $\text{PbZr}_{0.53}\text{Ti}_{0.47}\text{O}_3:\text{Er}^{3+}/\text{Yb}^{3+}$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

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

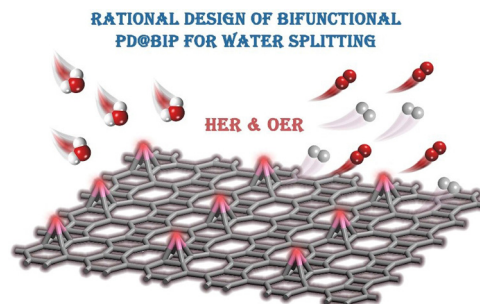
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Single-atom Pd directly anchored on biphenylene: a promising bifunctional electrocatalyst for overall water splitting

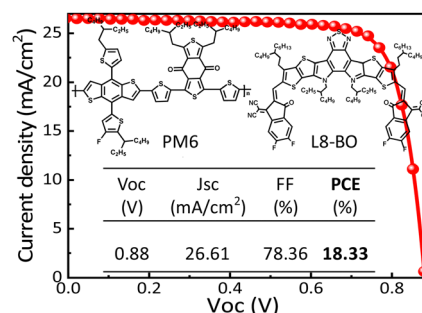
Ting-Ting Wang, Yanan Meng, Hai-Cai Huang, Lei Zhang* and Shi-Bo Cheng*



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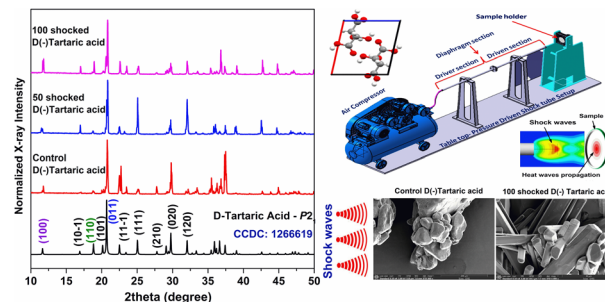
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Acoustic shock wave-induced superheating-assisted dynamic recrystallization – a case study of D-tartaric acid

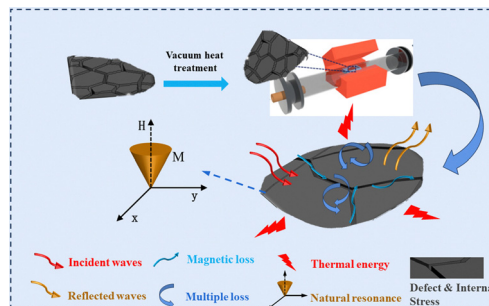
Sivakumar Aswathappa, Lidong Dai,* Sahaya Jude Dhas Sathiyadhas and Raju Suresh Kumar



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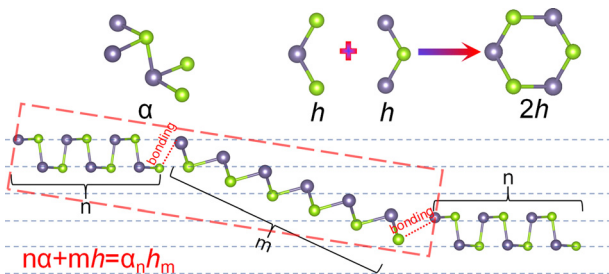
Grain size modulation to optimize the wave-absorbing properties of FeSiCr alloy micropowder

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



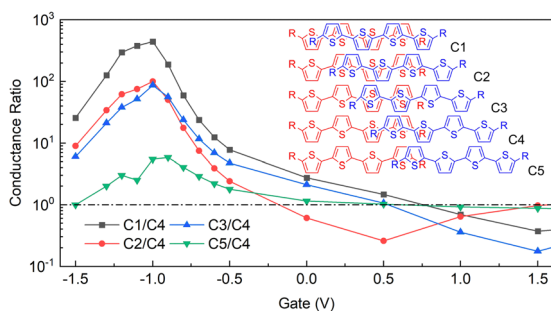
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 **$\alpha_n h_m$ -GeSe: a multifunctional semiconductor combining auxeticity and piezoelectricity**

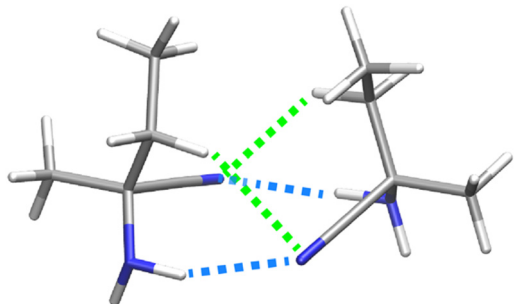
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**A multi-state supramolecular switch realized via a $[\pi \cdot \cdot \pi]$ dimer**

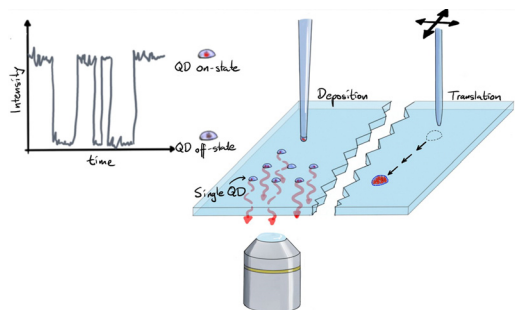
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**Enantioselective interactions of aminonitrile dimers**

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**

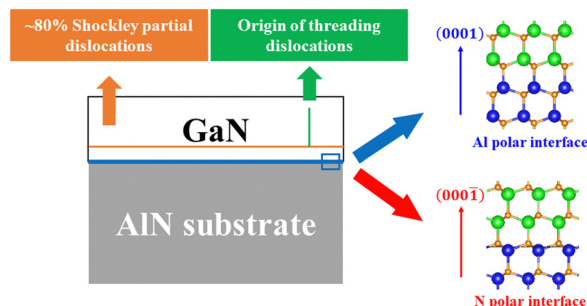
Maciej Biały, Martyna Jankowska, Karolina Sulowska, Marcin Szalkowski, Joanna Niedziółka-Jonsson* and Sebastian Maćkowski*



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

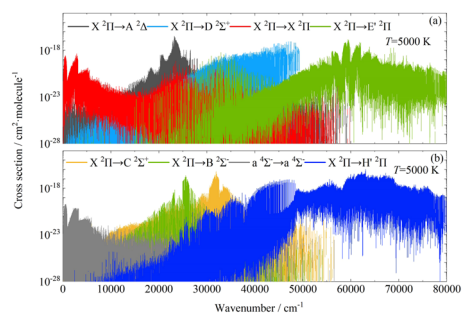
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An *ab initio* study of the rovibronic spectra of CH

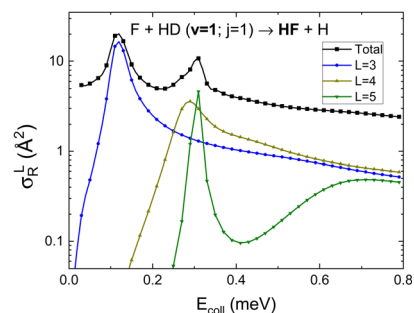
Zhenlu Hou and Linhua Liu*



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

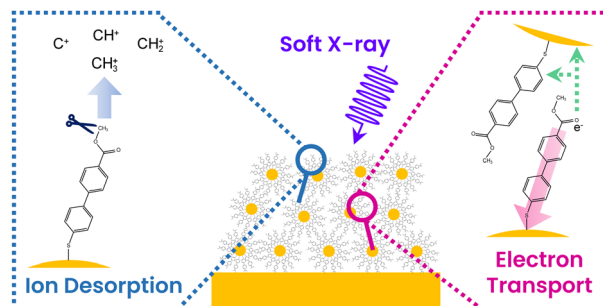
V. Sáez-Rábanos,* G. Sáez-Cano, J. E. Verdasco, F. J. Aoiz and V. J. Herrero



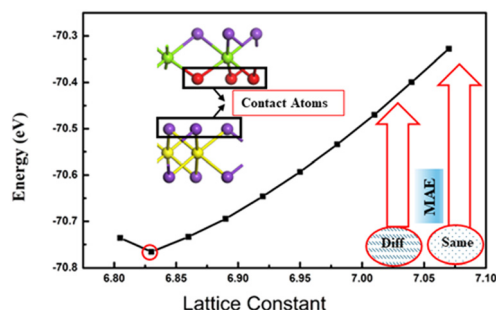
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Comparative study of electron transport through aromatic molecules on gold nanoparticles: insights from soft X-ray spectroscopy of condensed nanoparticle films versus flat monolayer films

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



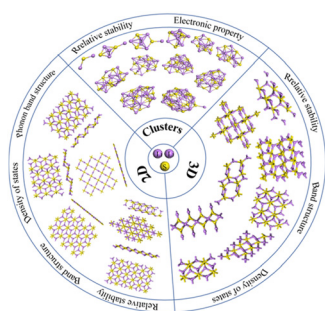
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Pressure-driven magnetic phase change in the $\text{CrI}_3/\text{Br}_3\text{Cr}_2\text{I}_3$ heterostructure

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

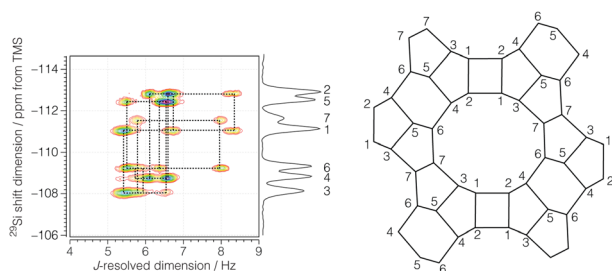
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Structure and property exploration of two-dimensional, bulk, and cluster lithium sulfide using the IM²ODE method

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

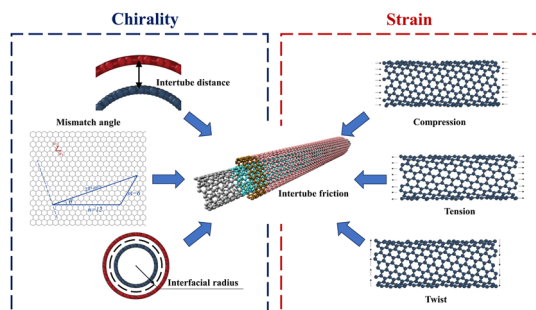
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Refining siliceous zeolite framework structures with ^{29}Si 2D J -resolved NMR spectroscopy

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

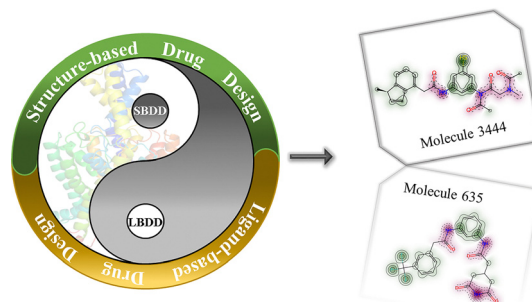
Yi Cai, Jianzhang Huang,* Shuang Gan, Yingjing Liang, Kejing Wang and Qiang Han



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

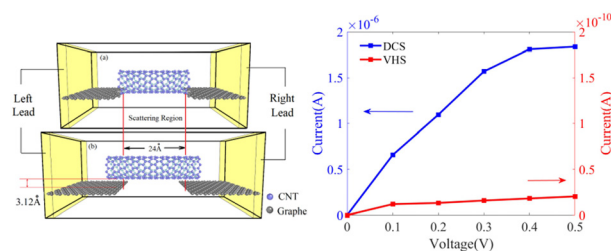
Lu Liu, Jixiang Liu, Liang Chen, Risong Na, Lianjuan Yang, Xiaoping Liu and Xi Zhao*



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

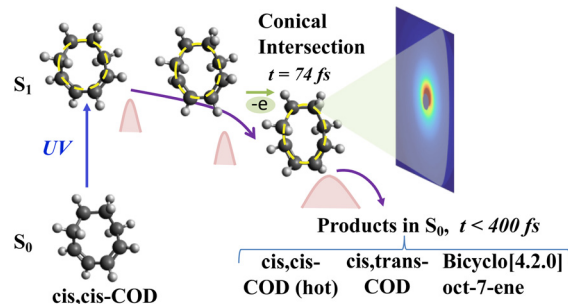
Bo Zhang, Xiaojie Liu,* Huan Wang,* Lifeng Feng* and Haitao Yin*



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

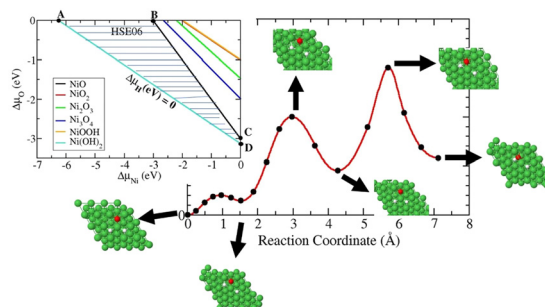
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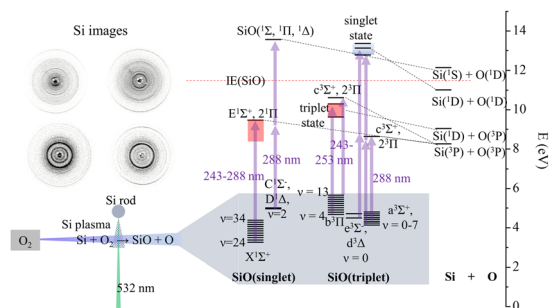
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First principles density functional theory study of tritium species adsorption on Ni(111) surface and diffusion in nickel-sublayer for tritium storage

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



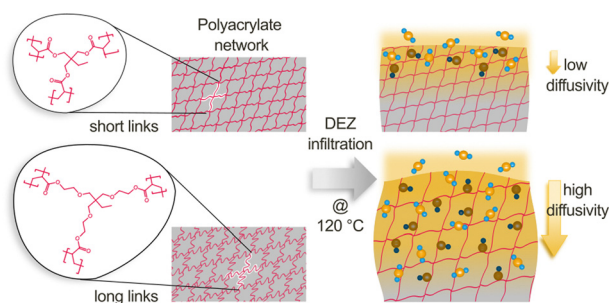
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Unveiling ultraviolet photodissociation dynamics of SiO from a laser-ablated supersonic beam with time-sliced ion velocity imaging

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

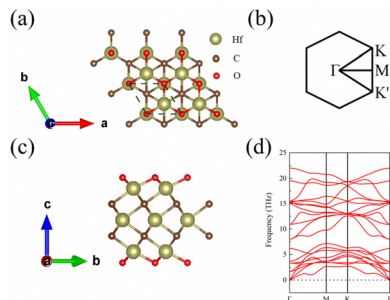
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Effects of polymer network flexibility on the kinetics of DEZ vapor phase infiltration into photo-polymerized polyacrylates

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

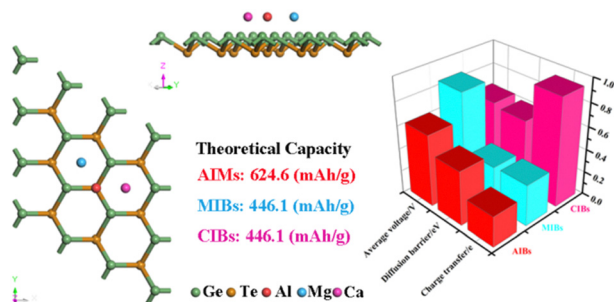
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Valley splitting of monolayer $\text{Hf}_3\text{C}_2\text{O}_2$ by the spin-orbit coupling effect: first principles calculations using the HSE06 methods

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*

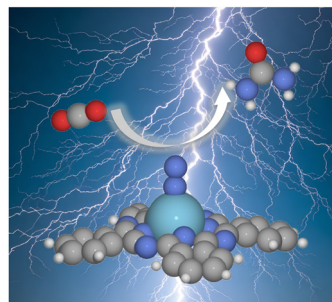


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Are transition metal phthalocyanines active for urea synthesis via electrocatalytic coupling of CO₂ and N₂?

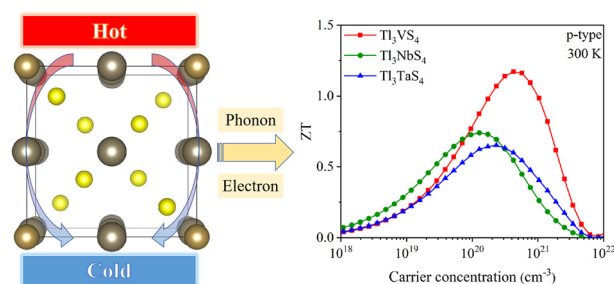
Yungan Huang, Ting Fan and Yongfei Ji*



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

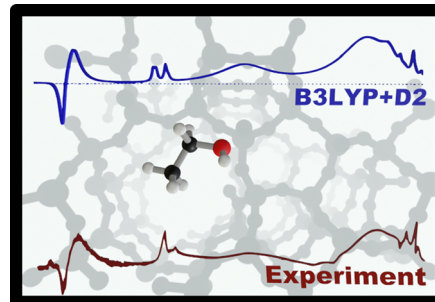
Xiefei Song,* Guangzhao Wang, Wenzhong Li, Siyu Gan, Yan Cai, Dianxu Ma, Yuhui Luo, Yao He* and Ning Wang*



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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

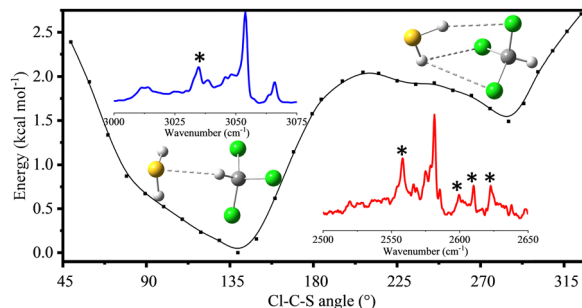
Dipanshu Kumar, Joachim Sauer, Alessia Airi,* Silvia Bordiga and Daria Ruth Galimberti*



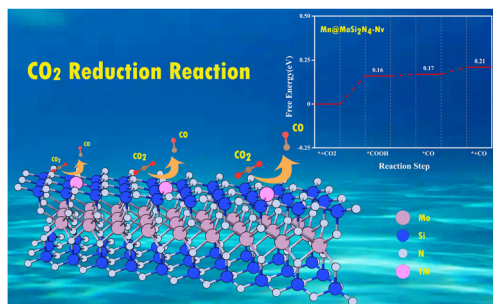
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Competition between C–H···S and S–H···Cl H-bonds in a CHCl₃–H₂S complex: a combined matrix isolation IR spectroscopic and quantum chemical investigation

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



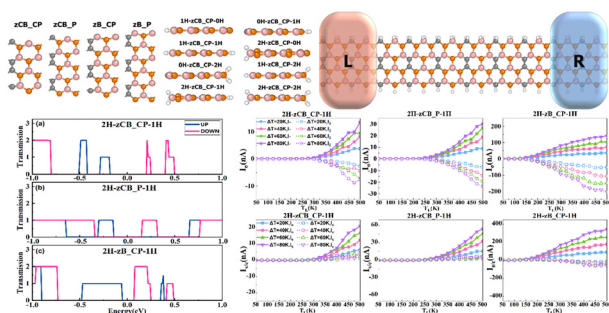
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Theoretical investigations of transition metal atom-doped MoSi_2N_4 monolayers as catalysts for electrochemical CO_2 reduction reactions

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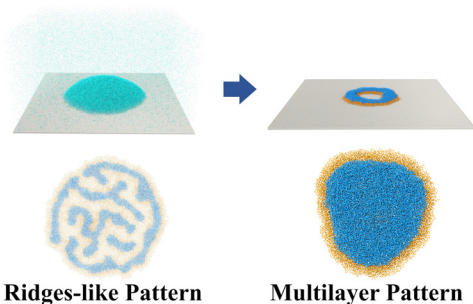
589



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*

