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See Lawrence M. Wolf et al., pp. 47–61.
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Inside cover

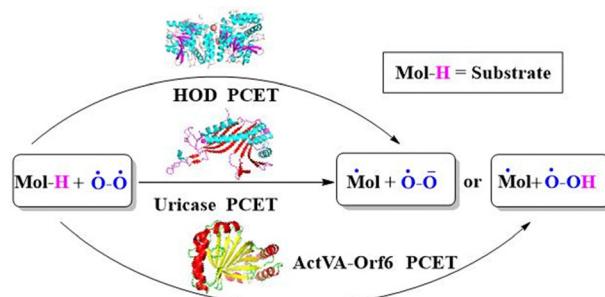
See Mizuki Kimura and Shinkoh Nanbu, pp. 62–76.
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Unraveling proton-coupled electron transfer in cofactor-free oxidase- and oxygenase-catalyzed oxygen activation: a theoretical view

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

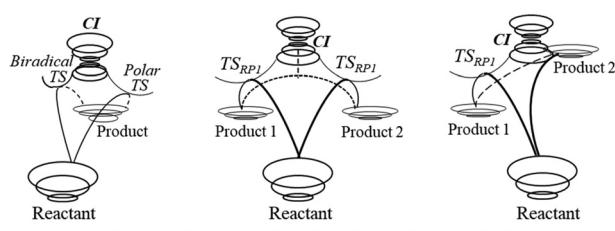


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Light driven photoswitches: three classes of molecular systems that result in a single photoproduct via a conical intersection and an exothermic reverse reaction

Shmuel Zilberg



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Elemental answers



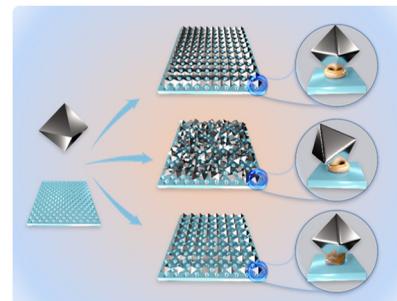
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Strongly coupled and highly-compacted zirconium aminobenzenedicarboxylate crystal membranes for accelerating carbon dioxide capture

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

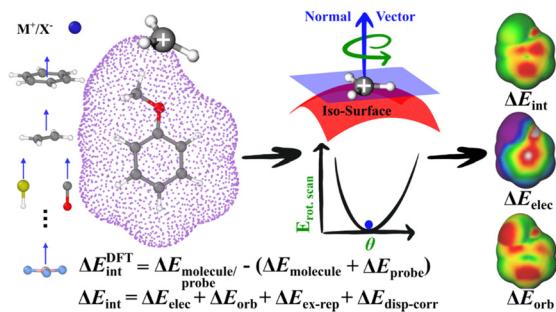


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Intermolecular interaction potential maps from energy decomposition for interpreting reactivity and intermolecular interactions

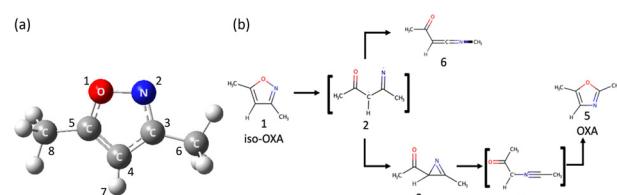
Amin Kiani, Wentong Zhou and Lawrence M. Wolf*



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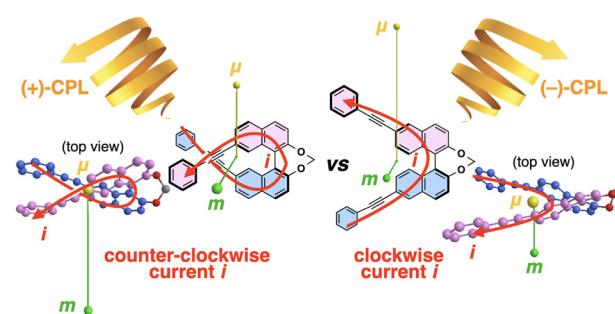
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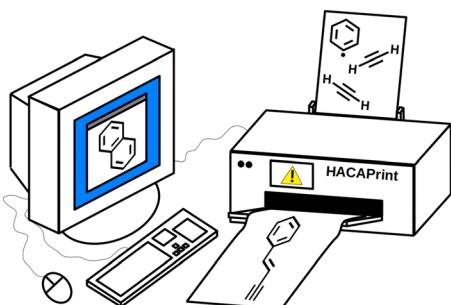
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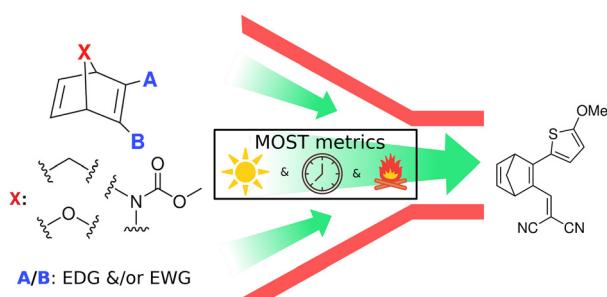
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Patricia D. Kelly,* Jack A. Turner, Oisin J. Shiels, Gabriel da Silva, Stephen J. Blanksby, Berwyck L. J. Poad and Adam J. Trevitt*

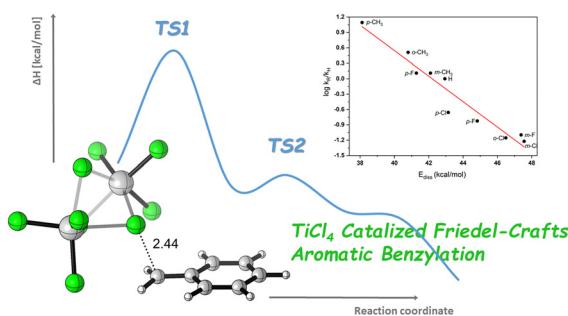
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Nils Oberhof,* Andreas Erbs Hillers-Bendtsen, Oscar Berlin Obel, Karoline Schjelde, Kurt V. Mikkelsen and Andreas Dreuw*

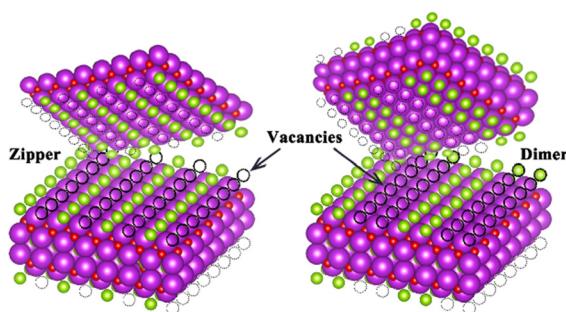
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Freely suspended nematic and smectic films and free-standing smectic filaments in the ferroelectric nematic realm

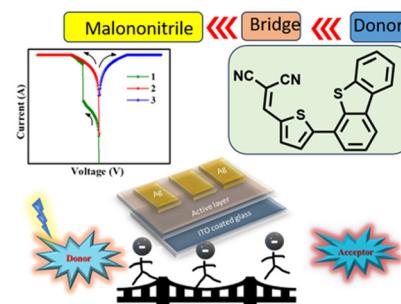
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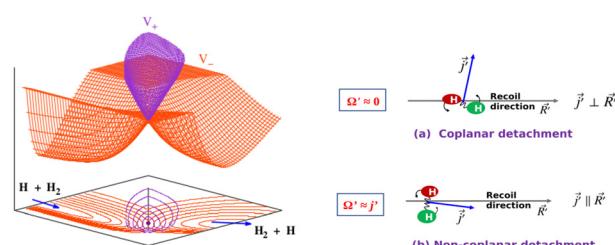
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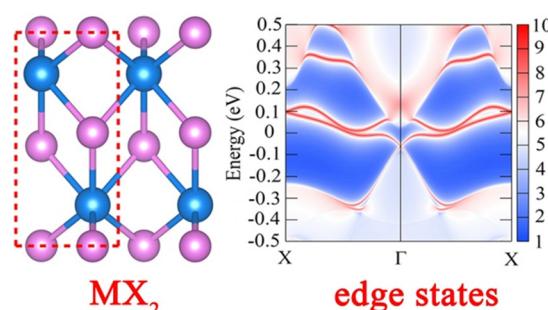
Jayakrushna Sahoo, Sugata Goswami and S. Mahapatra*



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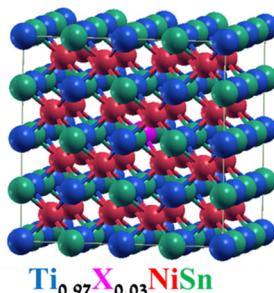
Quantum spin Hall states in MX_2 ($M = Ru, Os$; $X = As, Sb$) monolayers

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



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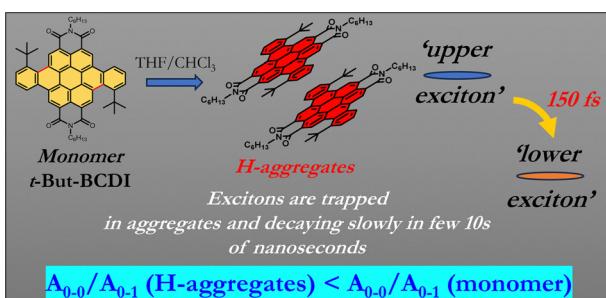
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The effect of acceptor and donor doping on the electronic properties of the half-Heusler TiNiSn

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

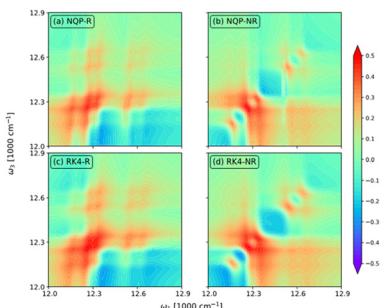
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Unveiling emissive H-aggregates of benzocoronenediimide, their photophysics and ultrafast exciton dynamics

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

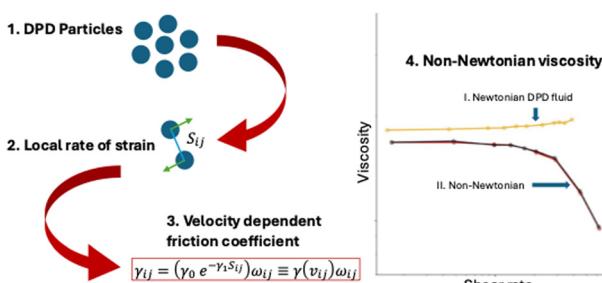
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Non-Newtonian dynamics modelled with non-linear transport coefficients at the mesoscale by using dissipative particle dynamics

Ali Naseri, Clara Salueña Perez and Josep Bonet Avalos*

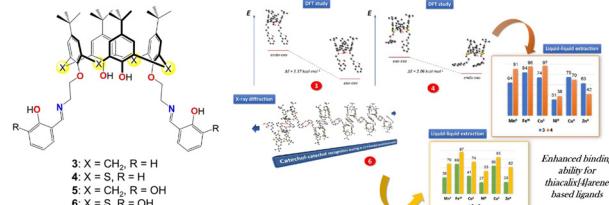


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Interplay between conformational flexibility, intermolecular H-bonding and 3d-metal cation extraction ability in a series of thiocalix[4]arene lower rim disubstituted Schiff base derivatives

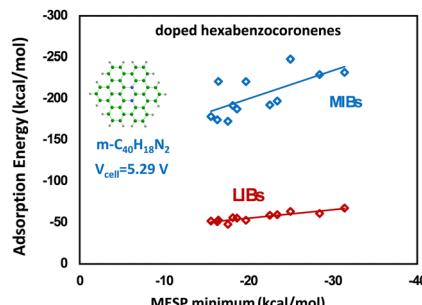
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Doped hexa-peri-hexabenzocoronene as anode materials for lithium- and magnesium-ion batteries

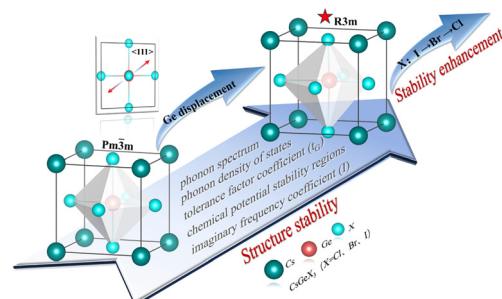
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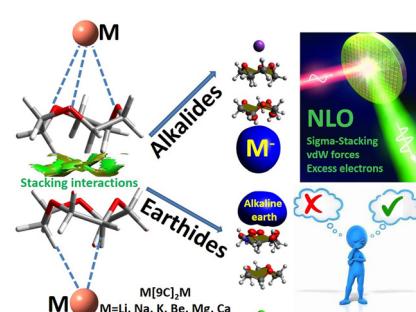
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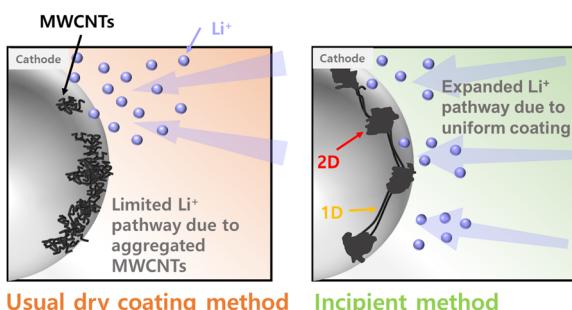
Stacking interactions in stabilizing supramolecular assembly of M[9C]₂M complexes: dynamic stability with remarkable nonlinear optical features

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



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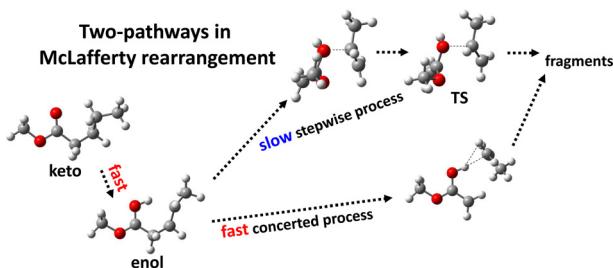
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Superior conductive 1D and 2D network structured carbon-coated Ni-rich $\text{Li}_{1.05}\text{Ni}_{0.88}\text{Co}_{0.08}\text{Mn}_{0.04}\text{O}_2$ as high-ion-diffusion cathodes for lithium-ion batteries

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

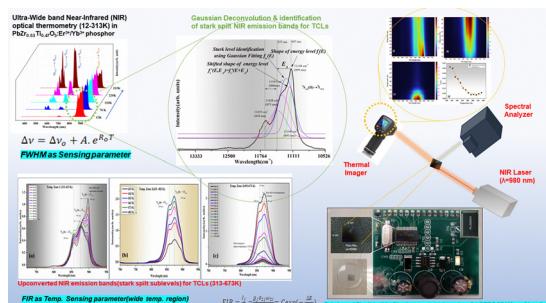
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Comprehensive quantum chemical and mass spectrometric analysis of the McLafferty rearrangement of methyl valerate

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

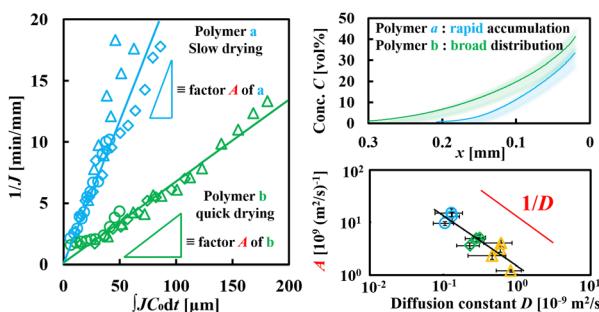
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Ultra-wide band near-infrared (NIR) optical thermometry (12–673 K) performance enhanced by Stark sublevel splitting in Er^{3+} ions near the first biological window in the $\text{PbZr}_{0.53}\text{Ti}_{0.47}\text{O}_3:\text{Er}^{3+}/\text{Yb}^{3+}$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

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Masahiko Tanaka and Susumu Inasawa*

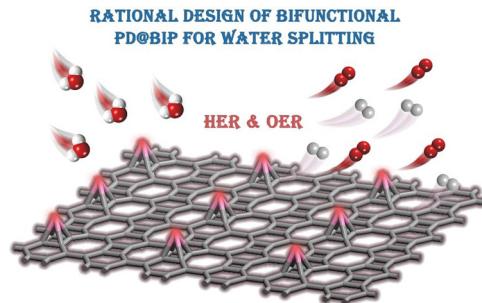


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Single-atom Pd directly anchored on biphenylene: a promising bifunctional electrocatalyst for overall water splitting

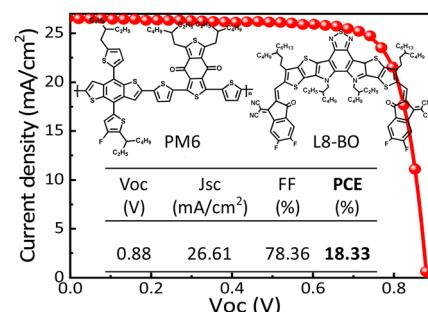
Ting-Ting Wang, Yanan Meng, Hai-Cai Huang,
Lei Zhang* and Shi-Bo Cheng*



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Optimization of active layers for efficient binary organic solar cells

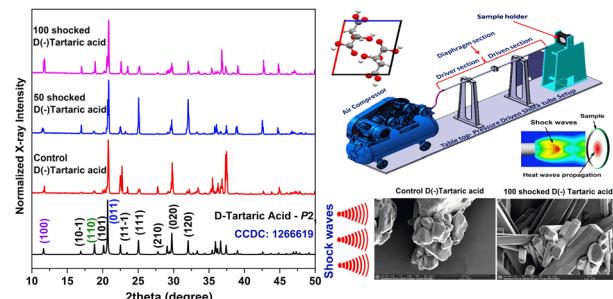
Yunjie Li, Beining Wang, Lijun Chen, Yaqian Yuan,
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Acoustic shock wave-induced superheating-assisted dynamic recrystallization – a case study of D-tartaric acid

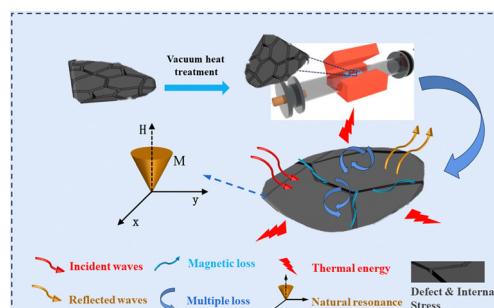
Sivakumar Aswathappa, Lidong Dai,*
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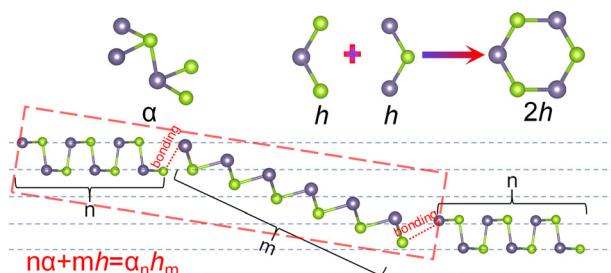
Grain size modulation to optimize the wave-absorbing properties of FeSiCr alloy micropowder

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



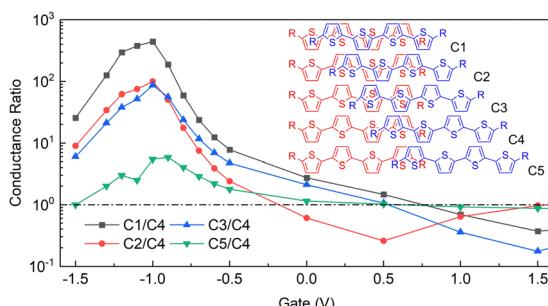
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 $\alpha_n h_m$ -GeSe: a multifunctional semiconductor combining auxeticity and piezoelectricity

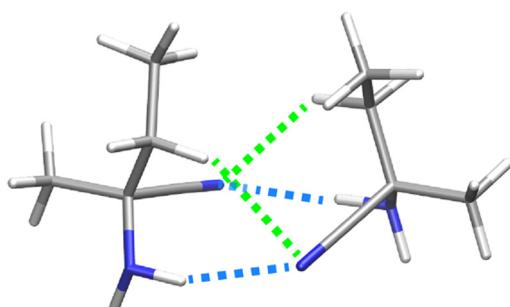
Jiajun Zhu, Heyun Zhao and Wanbiao Hu*

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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

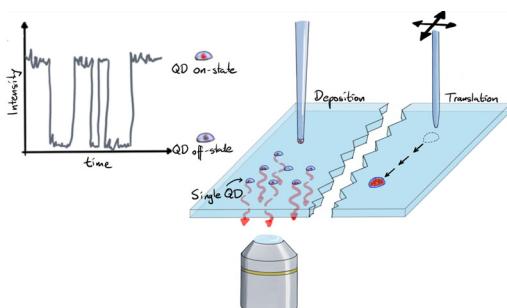
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Enantioselective interactions of aminonitrile dimers

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

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

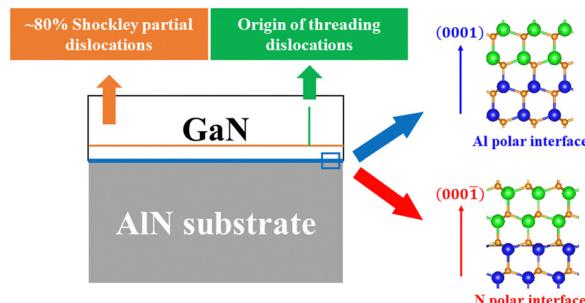


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The effect of interface polarity on the basal dislocations at the GaN/AlN interface

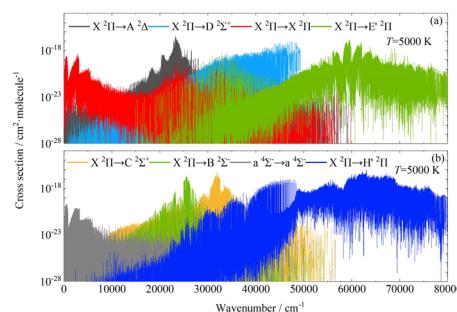
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An *ab initio* study of the rovibronic spectra of CH

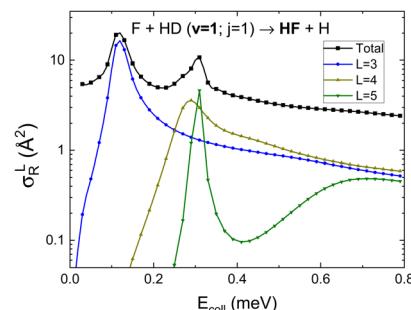
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The F + HD ($v = 0, 1; j = 1$) reaction: angular momentum correlations in the low (<1 meV) collision energy regime

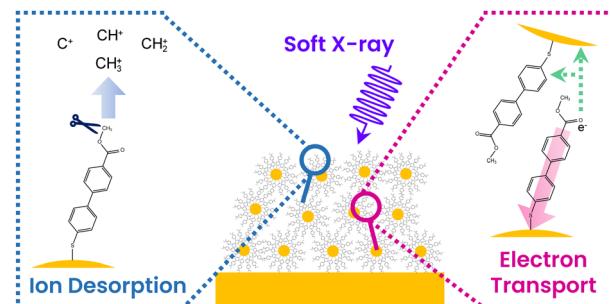
V. Sáez-Rábanos,* G. Sáez-Cano, J. E. Verdasco, F. J. Aoiz and V. J. Herrero



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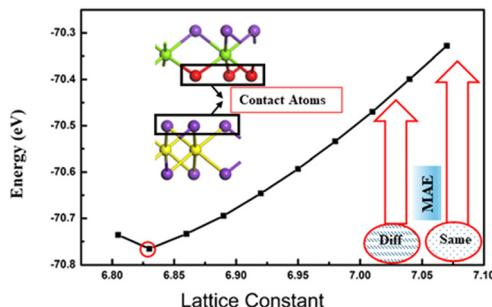
Comparative study of electron transport through aromatic molecules on gold nanoparticles: insights from soft X-ray spectroscopy of condensed nanoparticle films *versus* flat monolayer films

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



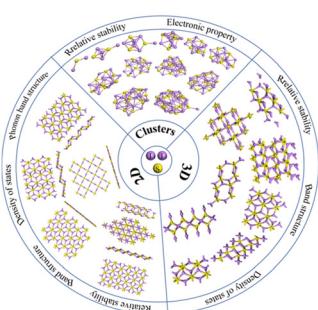
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**Pressure-driven magnetic phase change in the $\text{CrI}_3/\text{Br}_3\text{Cr}_2\text{I}_3$ heterostructure**

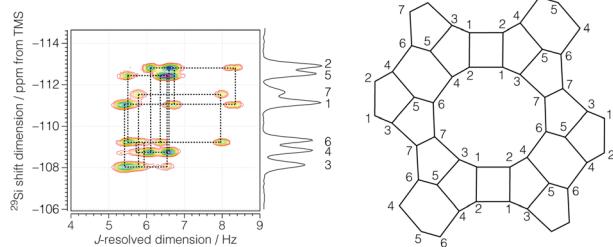
Fazle Subhan, Luqman Ali, Razia Aman, Ailing Chen, Bo Peng, Yanguang Zhou,* Zhenzhen Qin* and Guangzhao Qin*

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

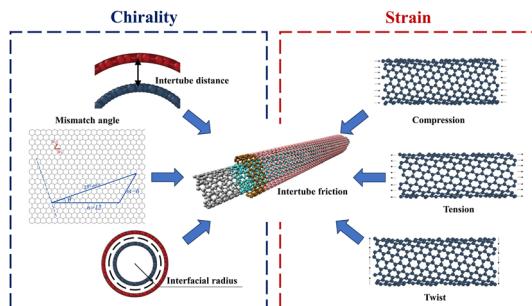
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**Refining siliceous zeolite framework structures with ²⁹Si 2D J-resolved NMR spectroscopy**

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

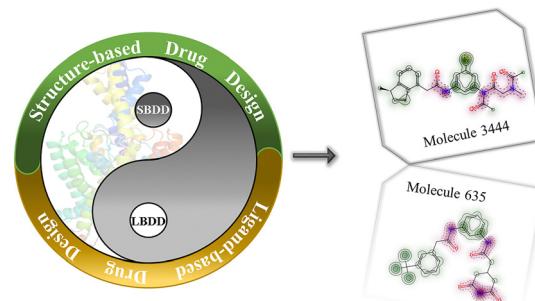
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**Mechanisms of interlayer friction in low-dimensional homogeneous thin-wall shell structures and its strain effect**

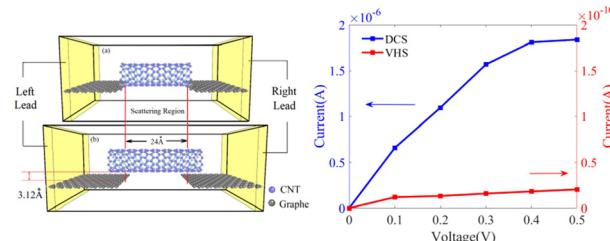
Yi Cai, Jianzhang Huang,* Shuang Gan, Yingjing Liang, Kejing Wang and Qiang Han

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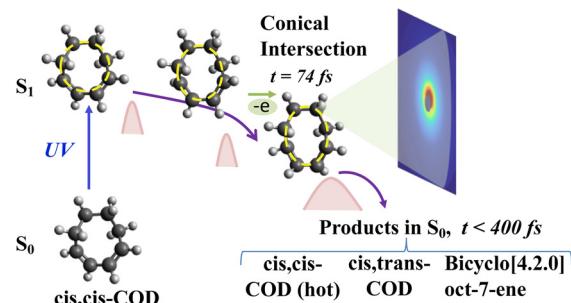
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Design of bisamide inhibitors of the TASK-1 potassium channel *in silico*Lu Liu, Jixiang Liu, Liang Chen, Risong Na,
Lianjuan Yang, Xiaoping Liu and Xi Zhao*

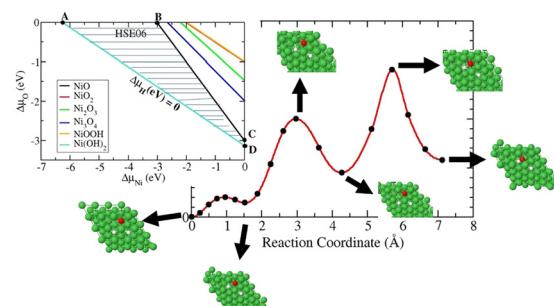
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Low contact resistance in carbon nanotube devices: metal-induced gap statesBo Zhang, Xiaojie Liu,* Huan Wang,* Lifeng Feng* and
Haitao Yin*

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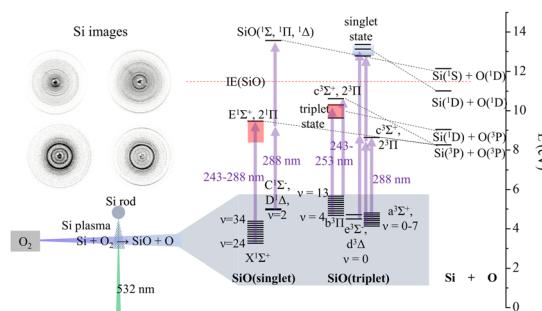
Ultrafast structural dynamics of UV photoexcited *cis,cis*-1,3-cyclooctadiene observed with time-resolved electron diffractionS. B. Muvva,* Y. Liu, P. Chakraborty, J. P. F. Nunes,
A. R. Attar, S. Bhattacharyya, K. Borne, E. G. Champenois,
N. Goff, K. Hegazy, M. C. Hoffmann, F. Ji, M.-F. Lin,
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J. 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 storageDe Nyago Tafen, Hari P. Paudel, David J. Senor,
Andrew M. Casella and Yuhua Duan*

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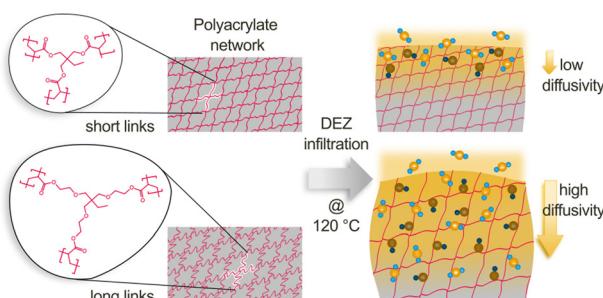
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Unveiling ultraviolet photodissociation dynamics of SiO from a laser-ablated supersonic beam with time-sliced ion velocity imaging

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

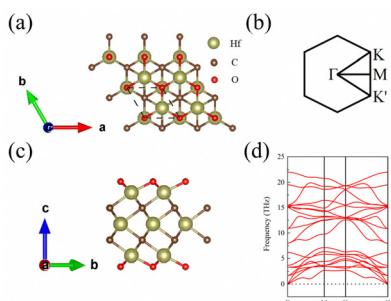
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Effects of polymer network flexibility on the kinetics of DEZ vapor phase infiltration into photo-polymerized polyacrylates

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

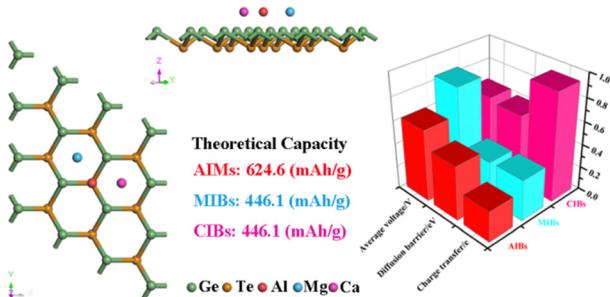
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Valley splitting of monolayer Hf₃C₂O₂ by the spin-orbit coupling effect: first principles calculations using the HSE06 methods

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*

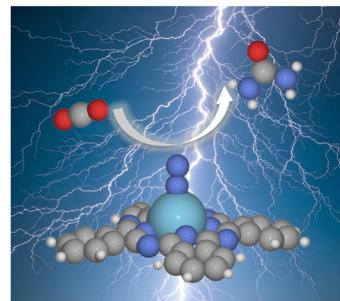


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Are transition metal phthalocyanines active for urea synthesis via electrocatalytic coupling of CO₂ and N₂?

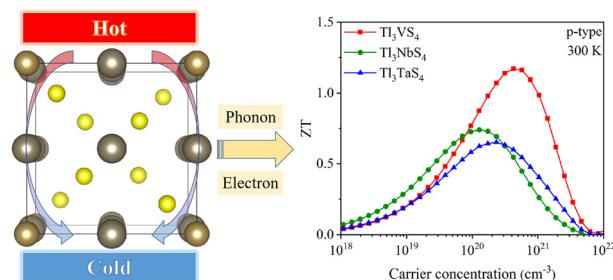
Yungan Huang, Ting Fan and Yongfei Ji*



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Potential thermoelectric material Tl₃XS₄ (X = V, Nb, Ta) with ultralow lattice thermal conductivity

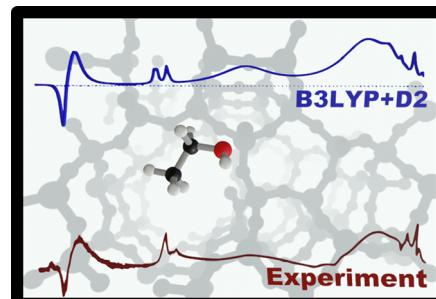
Xiefei Song,* Guangzhao Wang, Wenzhong Li, Siyu Gan, Yan Cai, Dianxu Ma, Yuhui Luo, Yao He* and Ning Wang*



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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

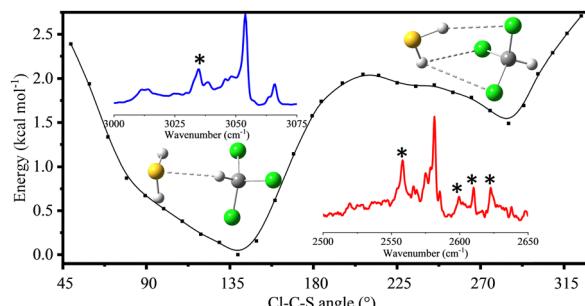
Dipanshu Kumar, Joachim Sauer, Alessia Airi,* Silvia Bordiga and Daria Ruth Galimberti*



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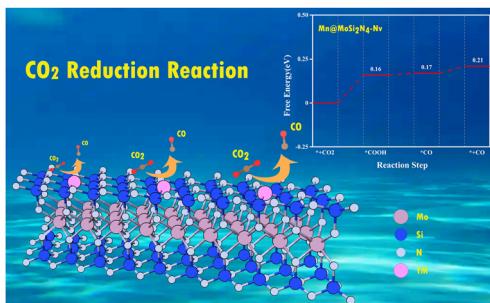
Competition between C–H···S and S–H···Cl H-bonds in a CHCl₃–H₂S complex: a combined matrix isolation IR spectroscopic and quantum chemical investigation

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



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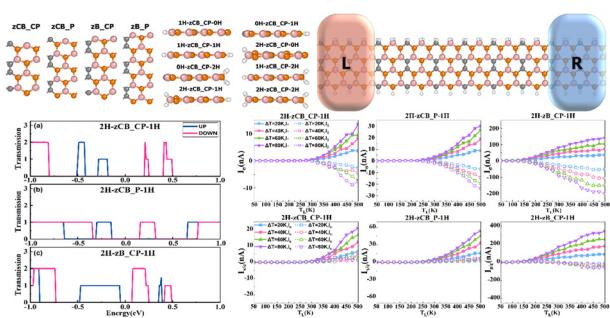
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Theoretical investigations of transition metal atom-doped MoSi₂N₄ monolayers as catalysts for electrochemical CO₂ reduction reactions

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

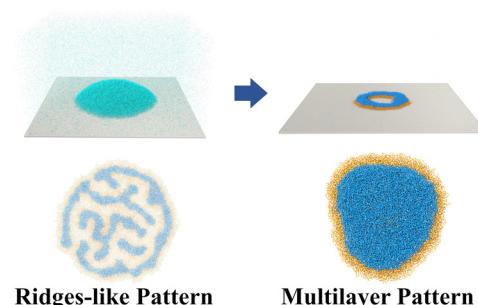
589



Pure spin currents induced by asymmetric H-passivation in B₃C₂P₃ 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*

EXPRESSION OF CONCERN

606

Expression of concern: Localized electropolymerization on oxidized boron-doped diamond electrodes modified with pyrrol 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 Ćeranić, Branislav Milovanović and Milena Petković*

