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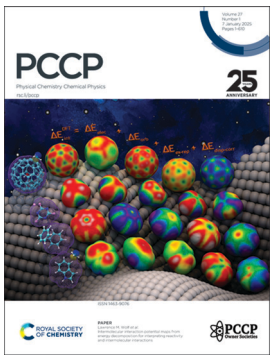

Cover
See Lawrence M. Wolf *et al.*, pp. 47–61.
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Inside cover
See Mizuki Kimura and Shinkoh Nanbu, pp. 62–76.
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REVIEW

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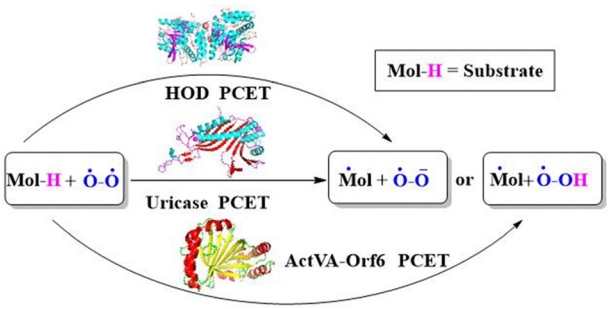
Unraveling proton-coupled electron transfer in cofactor-free oxidase- and oxygenase-catalyzed oxygen activation: a theoretical view

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



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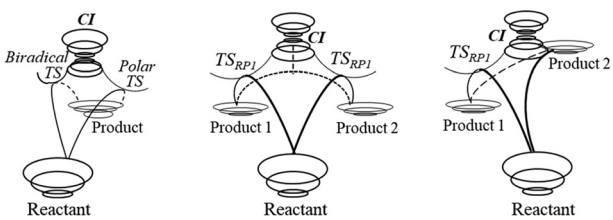
Light driven photoswitches: three classes of molecular systems that result in a single photoproduct *via* a conical intersection and an exothermic reverse reaction

Shmuel Zilberg



Three classes of molecular photoswitches

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COMMUNICATION

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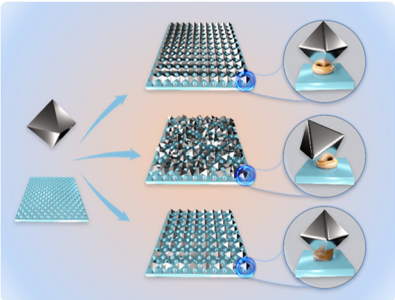
Strongly coupled and highly-compacted zirconium aminobenzenedicarboxylate crystal membranes for accelerating carbon dioxide capture

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



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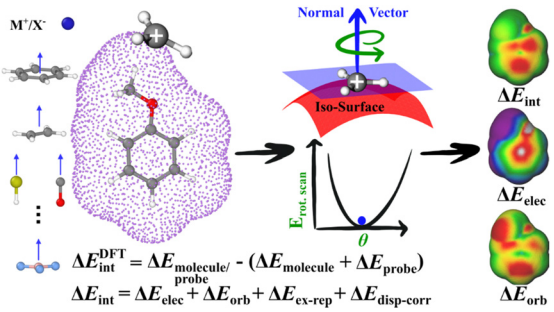
Intermolecular interaction potential maps from energy decomposition for interpreting reactivity and intermolecular interactions

Amin Kiani, Wentong Zhou and Lawrence M. Wolf*



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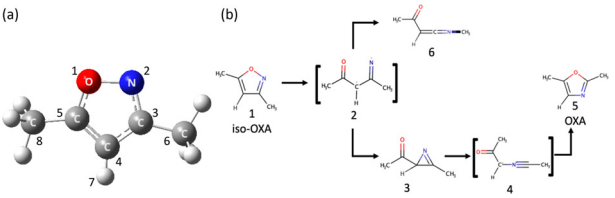
Nonadiabatic *ab initio* chemical reaction dynamics for the photoisomerization reaction of 3,5-dimethylisoxazole *via* the S_1 electronic state

Mizuki Kimura and Shinkoh Nanbu*



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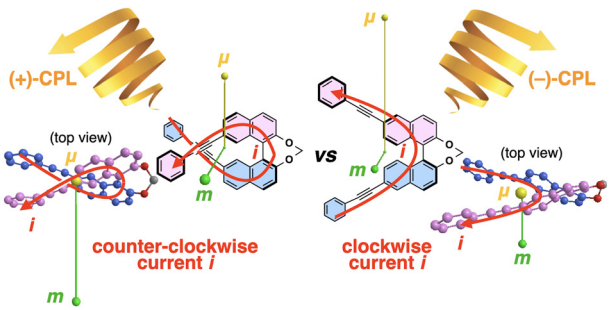
Inversion of circularly polarized luminescence by electric current flow during transition

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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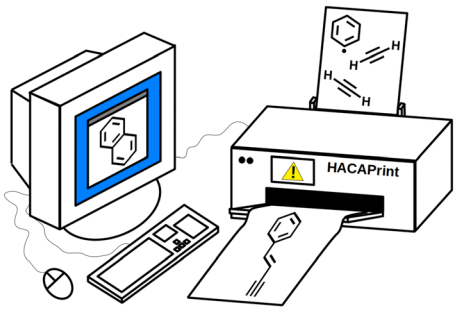

Don't forget the *trans*: double bond isomerism radical-acetylene growth reactions affect the primary stages of PAH and soot formation

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

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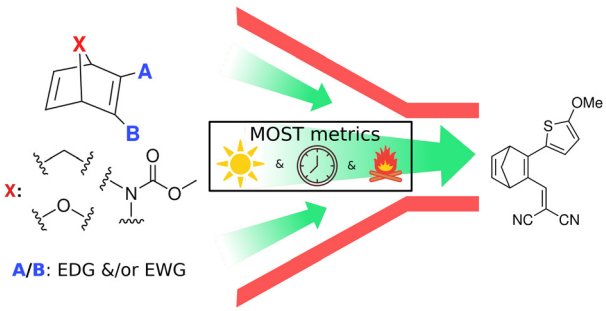

Searching the chemical space of hetero-atom bridged norbornadienes

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

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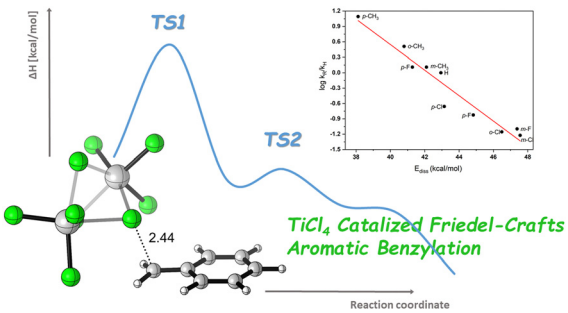

Reactivity in Friedel–Crafts aromatic benzylation: the role of the electrophilic reactant

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

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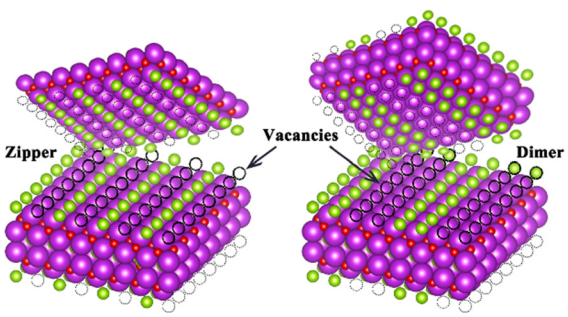

Thickness-dependent surface reconstructions in non-van der Waals two-dimensional materials

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

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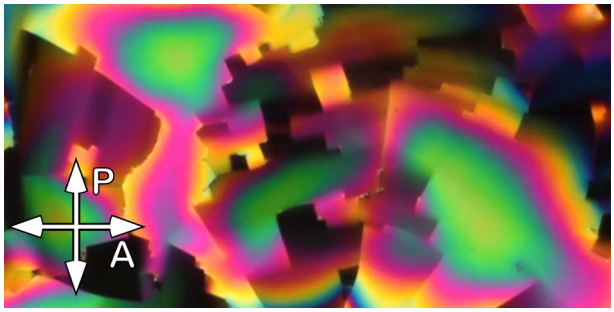
Freely suspended nematic and smectic films and free-standing smectic filaments in the ferroelectric nematic realm

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



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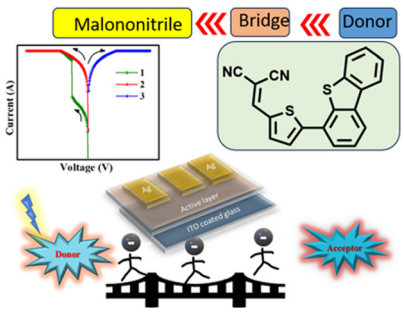
Exploring the potential of malononitrile functionalized donor–acceptor systems for non-volatile memory device applications

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



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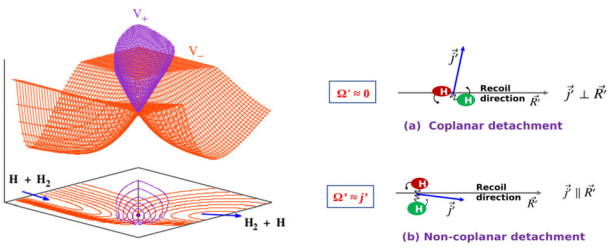
Unraveling the effect of reagent vibrational excitation on the scattering mechanism of the benchmark H + H_2 → H_2 + H hydrogen exchange reaction in the coupled $1^2E'$ ground electronic manifold

Jayakrushna Sahoo, Sugata Goswami and S. Mahapatra*



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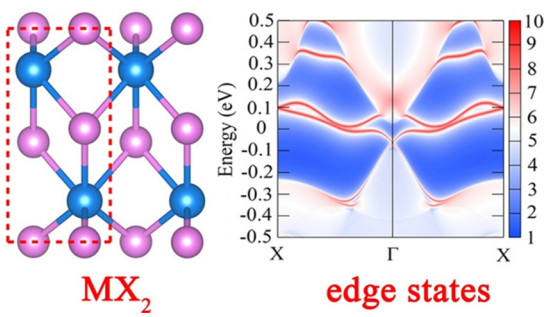
Quantum spin Hall states in MX_2 (M = Ru, Os; X = As, Sb) monolayers

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



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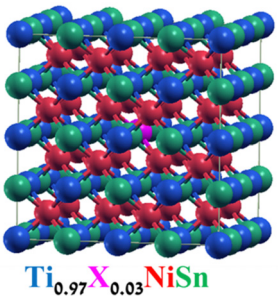

The effect of acceptor and donor doping on the electronic properties of the half-Heusler TiNiSn

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

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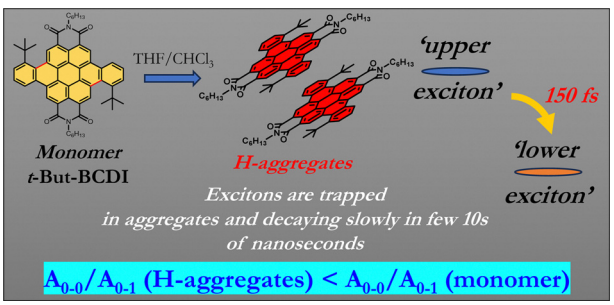

Unveiling emissive H-aggregates of benzocoronenediimide, their photophysics and ultrafast exciton dynamics

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

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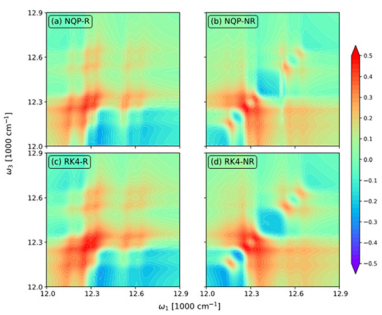

A non-Markovian neural quantum propagator and its application in the simulation of ultrafast nonlinear spectra

Jiaji Zhang* and Lipeng Chen*

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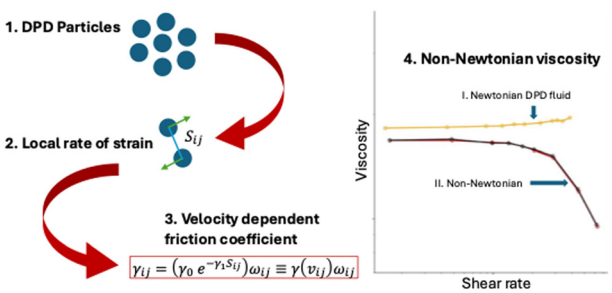

Non-Newtonian dynamics modelled with non-linear transport coefficients at the mesoscale by using dissipative particle dynamics

Ali Naseri, Clara Salueña Perez and Josep Bonet Avalos*

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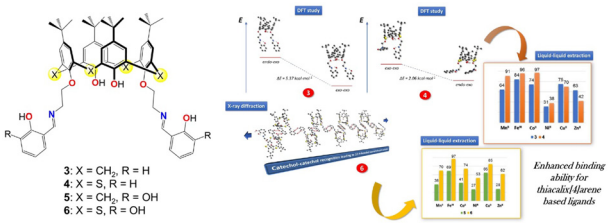
Interplay between conformational flexibility, intermolecular H-bonding and 3d-metal cation extraction ability in a series of thiacalix[4]arene lower rim disubstituted Schiff base derivatives

Iuliia V. Strelnikova, Alexander S. Ovsyannikov,* Aidar T. Gubaidullin, Artem S. Agarkov, Sophiya R. Kleshnina, A. A. Iova, Victor L. Furer, Alexander E. Vandyukov, Svetlana E. Solovieva and Igor S. Antipin



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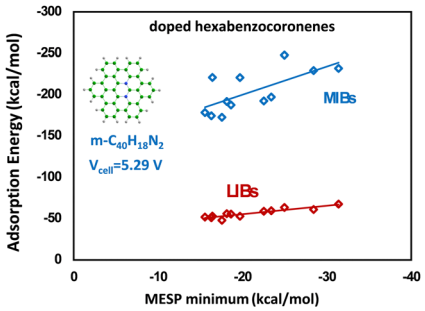
Doped hexa-*peri*-hexabenzocoronene as anode materials for lithium- and magnesium-ion batteries

Remya Geetha Sadasivan Nair,* Arun Kumar Narayanan Nair,* Bicheng Yan* and Shuyu Sun*



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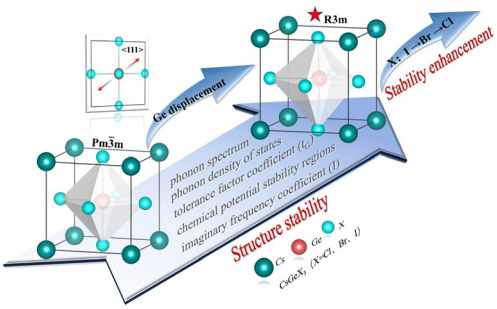
The stability of $CsGeX_3$ (X = I, Br, Cl) selectively tuned by the crystal structures and halide ions as inferred from the calculated phonon spectrum

Tengcheng Huang, Zheyu Zhang, Baoyun Liang, Ang Li, Xin Xu, Yujia Gao, Zhuxia Wu, Haiyan Li, Fei Yuan, Pengyi Liu, Tingting Shi* and Weiguang Xie*



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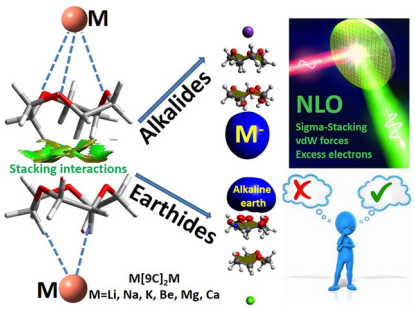
Stacking interactions in stabilizing supramolecular assembly of $M[9C]_2M$ complexes: dynamic stability with remarkable nonlinear optical features

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



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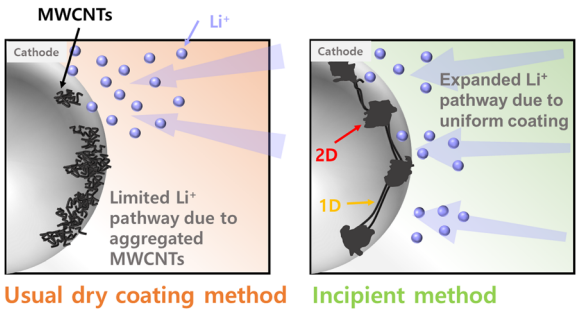

Superior conductive 1D and 2D network structured carbon-coated Ni-rich $Li_{1.05}Ni_{0.88}Co_{0.08}Mn_{0.04}O_2$ as high-ion-diffusion cathodes for lithium-ion batteries

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

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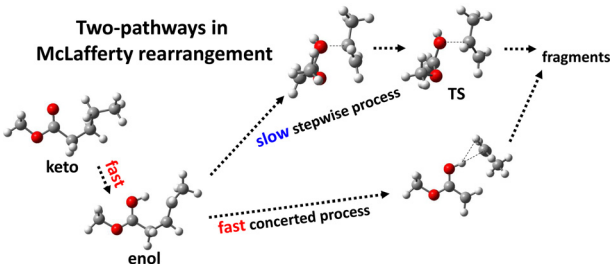

Comprehensive quantum chemical and mass spectrometric analysis of the McLafferty rearrangement of methyl valerate

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

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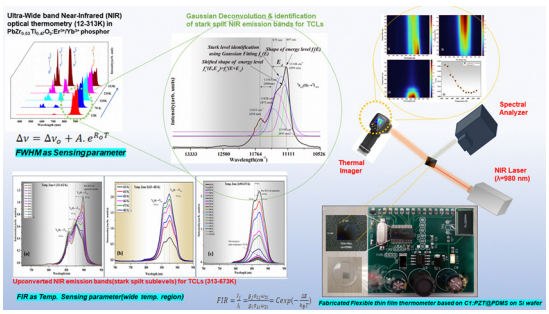

Ultra-wide band near-infrared (NIR) optical thermometry (12–673 K) performance enhanced by Stark sublevel splitting in Er^{3+} ions near the first biological window in the $PbZr_{0.53}Ti_{0.47}O_3$:Er^{3+}/Yb^{3+} phosphor

Prasenjit Prasad Sukul,* Yadvendra Singh and Hendrik Swart

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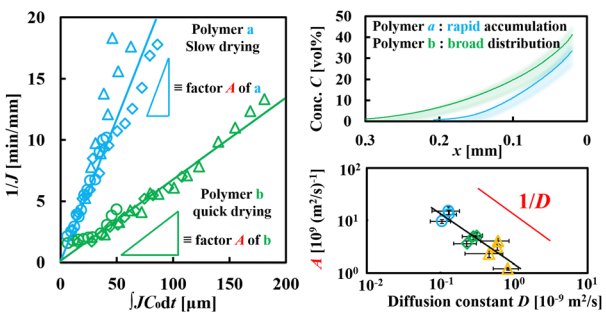

How does the polymer type affect the rate of water evaporation from polymer solutions?

Masahiko Tanaka and Susumu Inasawa*

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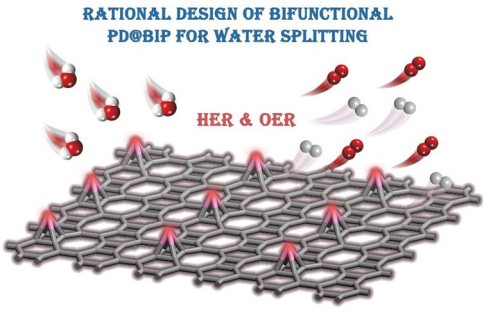
Single-atom Pd directly anchored on biphenylene: a promising bifunctional electrocatalyst for overall water splitting

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



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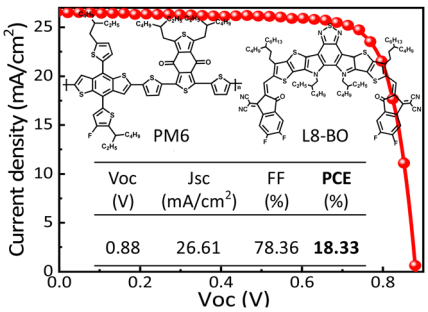
Optimization of active layers for efficient binary organic solar cells

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



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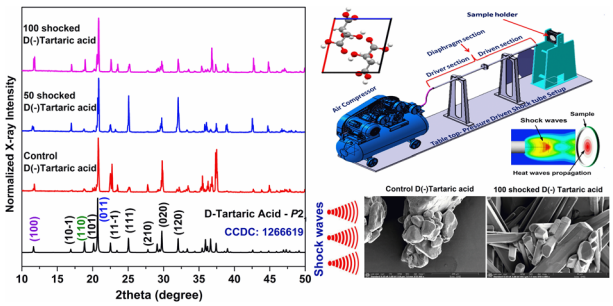
Acoustic shock wave-induced superheating-assisted dynamic recrystallization – a case study of D-tartaric acid

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



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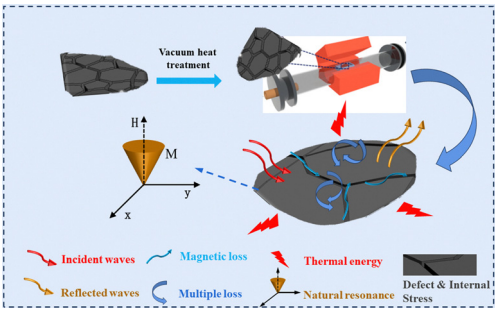
Grain size modulation to optimize the wave-absorbing properties of FeSiCr alloy micropowder

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



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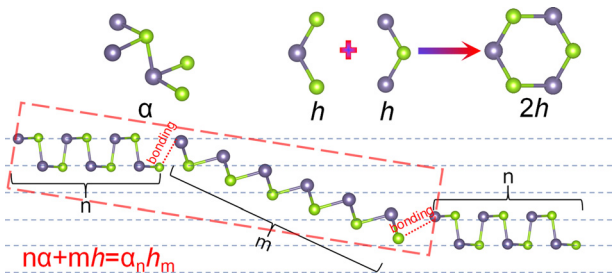

$\alpha_n h_m$-GeSe: a multifunctional semiconductor combining auxeticity and piezoelectricity

Jiajun Zhu, Heyun Zhao and Wanbiao Hu*

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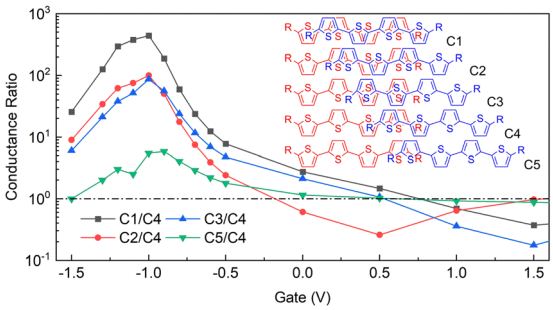

A multi-state supramolecular switch realized *via* a [π···π] dimer

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

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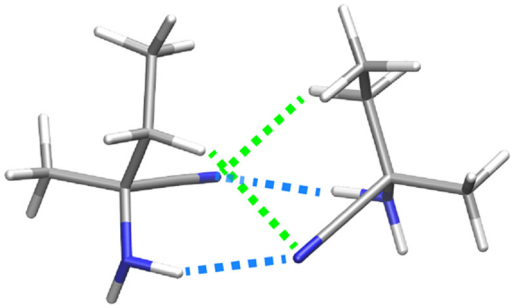

Enantioselective interactions of aminonitrile dimers

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

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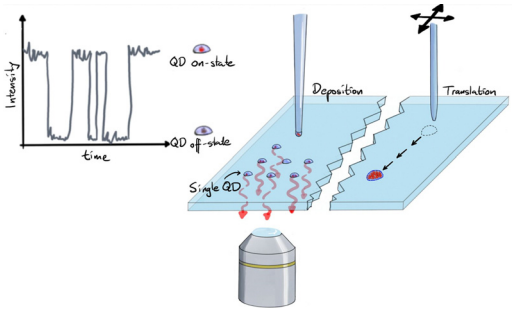

Controlled encapsulation of colloidal semiconductor quantum dots in a microdroplet

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

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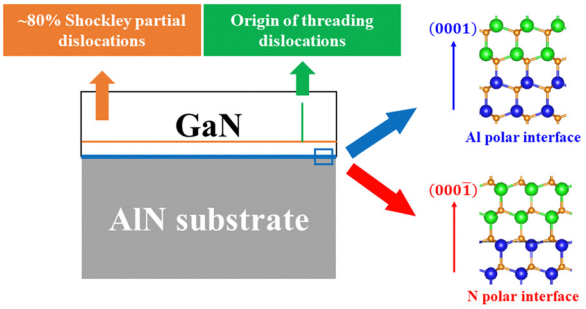
The effect of interface polarity on the basal dislocations at the GaN/AlN interface

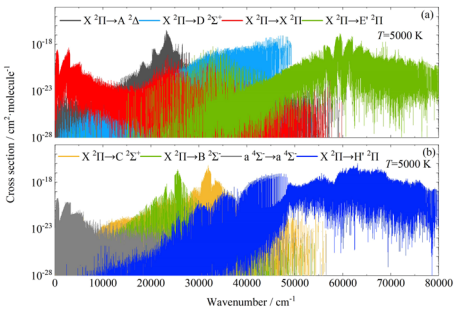
Yuming Yang, Xuemei Zhang, Mi Qin, Jun Liu, Chuanguo Zhang, Zhixin Hui, Yonggang Li, Zhi Zeng and Yongsheng Zhang*



367

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

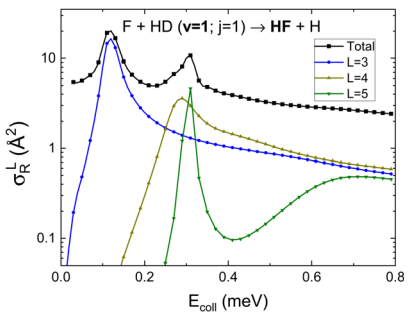
Zhenlu Hou and Linhua Liu*



376

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

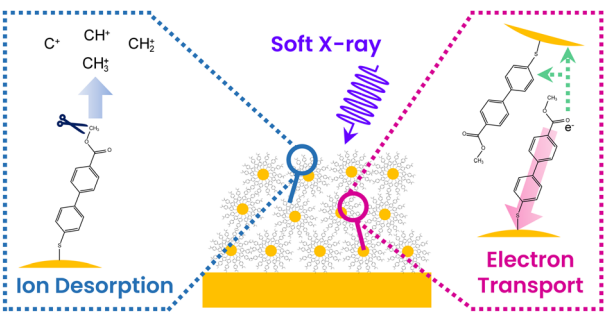
V. Sáez-Rábanos,* G. Sáez-Cano, J. E. Verdasco, F. J. Aoiz and V. J. Herrero



388

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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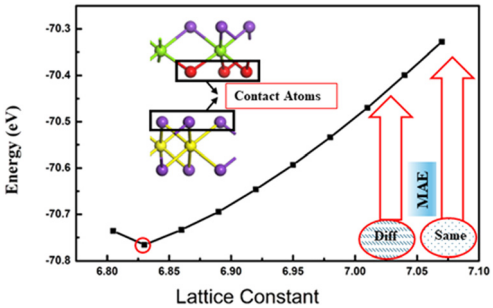

Pressure-driven magnetic phase change in the $CrI_3/Br_3Cr_2I_3$ heterostructure

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

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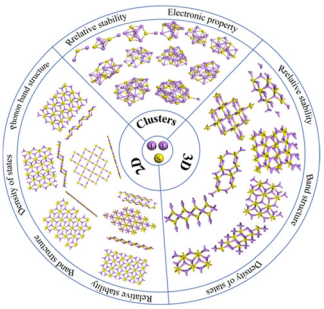
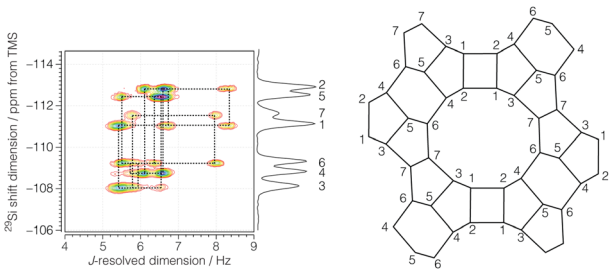


Structure and property exploration of two-dimensional, bulk, and cluster lithium sulfide using the IM^{2}ODE method

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

419



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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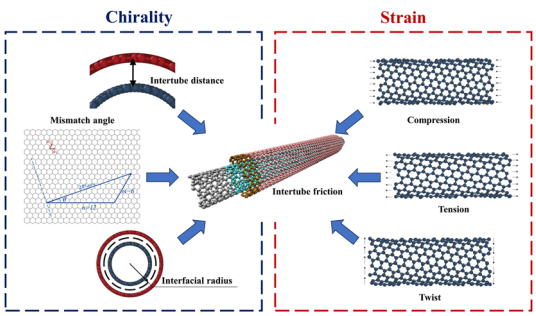

Mechanisms of interlayer friction in low-dimensional homogeneous thin-wall shell structures and its strain effect

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

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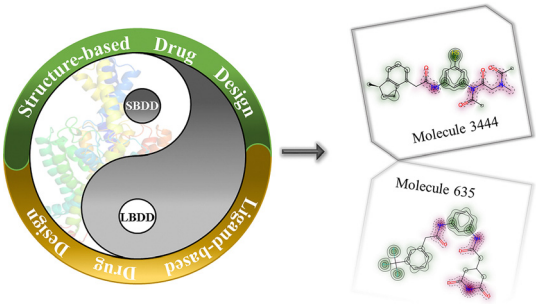
Design of bisamide inhibitors of the TASK-1 potassium channel *in silico*

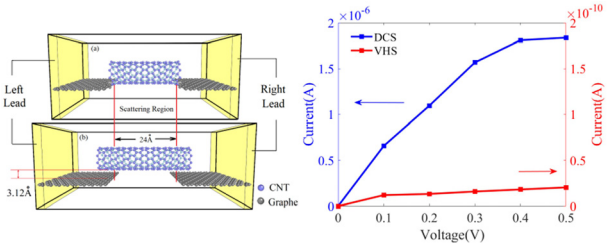
Lu Liu, Jixiang Liu, Liang Chen, Risong Na, Lianjuan Yang, Xiaoping Liu and Xi Zhao*



463

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

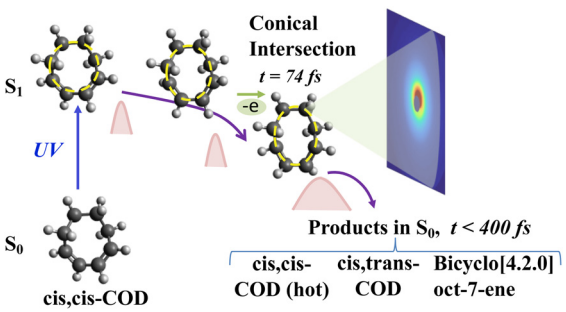
Bo Zhang, Xiaojie Liu,* Huan Wang,* Lifeng Feng* and Haitao Yin*



471

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

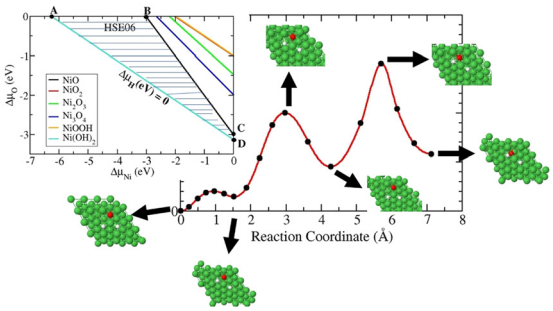
S. B. Muvva,* Y. Liu, P. Chakraborty, J. P. F. Nunes, A. R. Attar, S. Bhattacharyya, K. Borne, E. G. Champenois, N. Goff, K. Hegazy, M. C. Hoffmann, F. Ji, M.-F. Lin, D. Luo, L. Ma, A. Odate, S. Pathak, D. Rolles, A. Rudenko, S. K. Saha, X. Shen, X. Wang, M. R. Ware, S. Weathersby, P. M. Weber, K. J.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



481

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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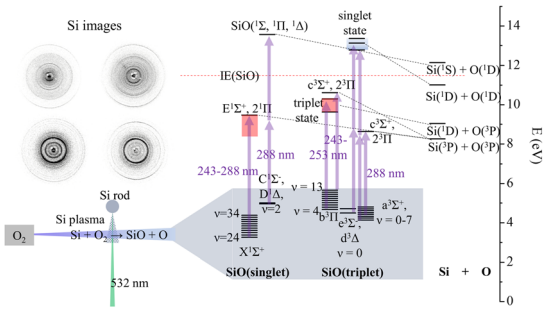

Unveiling ultraviolet photodissociation dynamics of SiO from a laser-ablated supersonic beam with time-sliced ion velocity imaging

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

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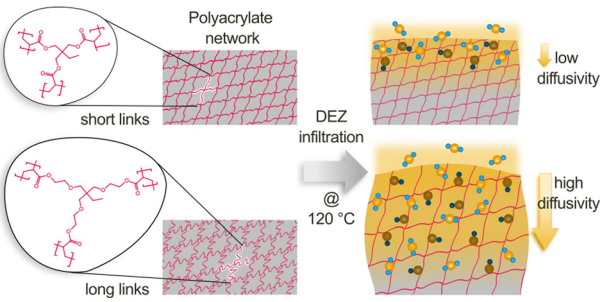

Effects of polymer network flexibility on the kinetics of DEZ vapor phase infiltration into photo-polymerized polyacrylates

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

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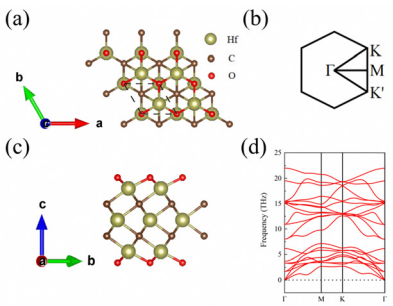

Valley splitting of monolayer $Hf_3C_2O_2$ by the spin–orbit coupling effect: first principles calculations using the HSE06 methods

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

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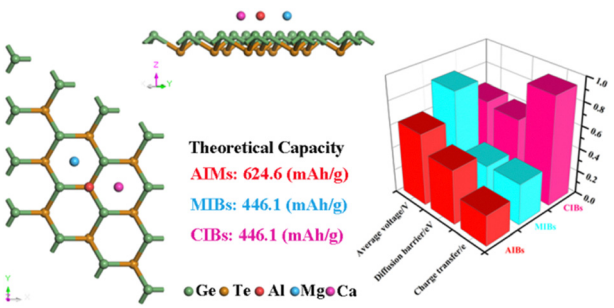

First principles study on monolayer GeTe as an anode material for multivalent ion batteries

Junjie Chen,* Zhiyu Zhou and Ruidan Zhang*

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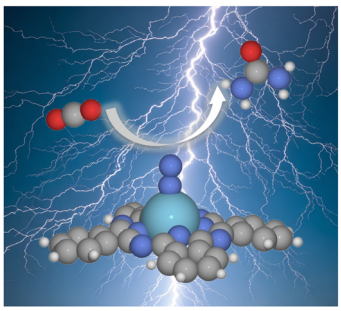
Are transition metal phthalocyanines active for urea synthesis *via* electrocatalytic coupling of CO_2 and N_2?

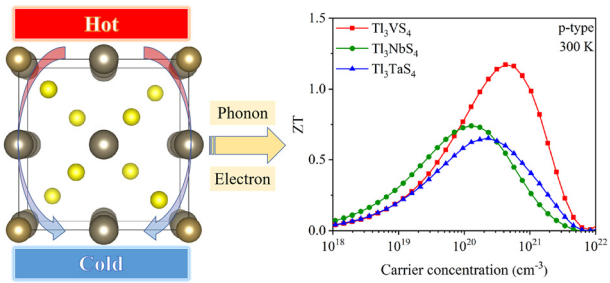
Yungan Huang, Ting Fan and Yongfei Ji*



539

Potential thermoelectric material Tl_3XS_4 (X = V, Nb, Ta) with ultralow lattice thermal conductivity

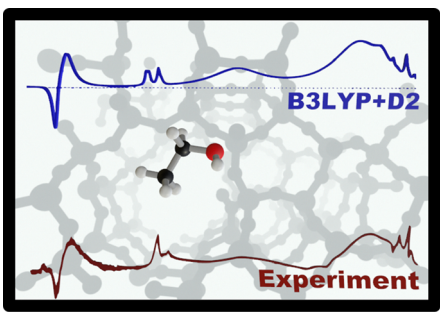
Xiefei Song,* Guangzhao Wang, Wenzhong Li, Siyu Gan, Yan Cai, Dianxu Ma, Yuhui Luo, Yao He* and Ning Wang*



550

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

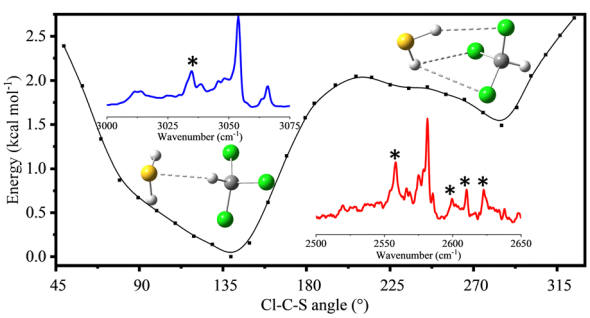
Dipanshu Kumar, Joachim Sauer, Alessia Airi,* Silvia Bordiga and Daria Ruth Galimberti*



564

Competition between C–H···S and S–H···Cl H-bonds in a $CHCl_3$–H_2S complex: a combined matrix isolation IR spectroscopic and quantum chemical investigation

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



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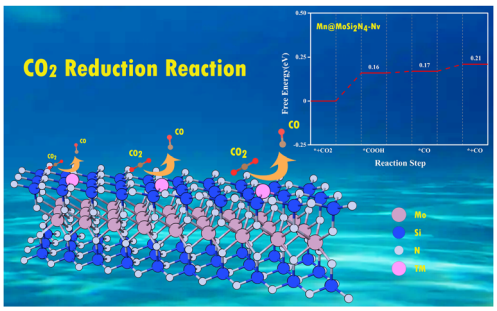

Theoretical investigations of transition metal atom-doped $MoSi_2N_4$ monolayers as catalysts for electrochemical CO_2 reduction reactions

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

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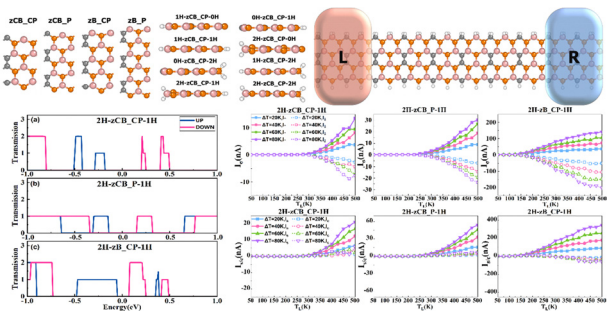

Pure spin currents induced by asymmetric H-passivation in $B_3C_2P_3$ nanoribbons

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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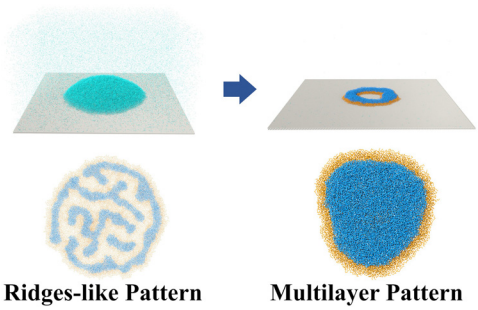

Influence of polymer chain length and concentration on the deposition patterns of linear diblock copolymer solution nanodroplets

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

EXPRESSION OF CONCERN

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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*

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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*

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