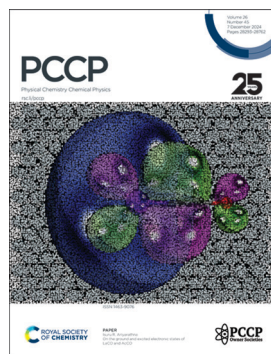


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See Katarzyna M. Krupka and María Pilar de Lara-Castells, pp. 28349–28360. Image reproduced by permission of Katarzyna M. Krupka and María Pilar de Lara-Castells from *Phys. Chem. Chem. Phys.*, 2024, 26, 28349.

REVIEW

28307

Synthesis and modification of boron nitride nanomaterials for gas sensors: from theory to application

Yan Zhang, Yan Wang,* Cong Qin and Jianliang Cao*

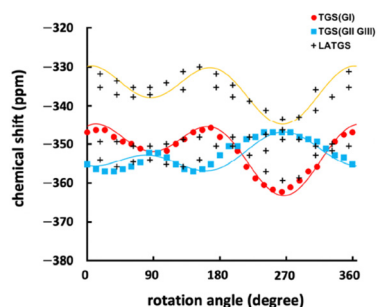


COMMUNICATION

28332

Direct capture of the alanine ghost in alanine-doped triglycine sulfate crystals

Yukana Terasawa,* Toshimichi Shibue and Toru Asahi



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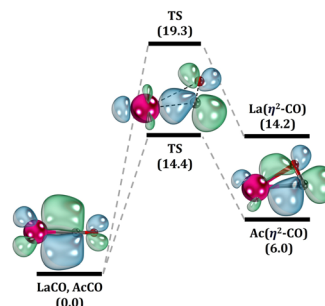
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28337

On the ground and excited electronic states of LaCO and AcCO

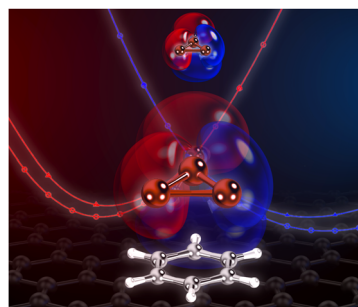
Isuru R. Ariyaratna



28349

Support effects on conical intersections of Jahn–Teller fluxional metal clusters on the sub-nanoscale

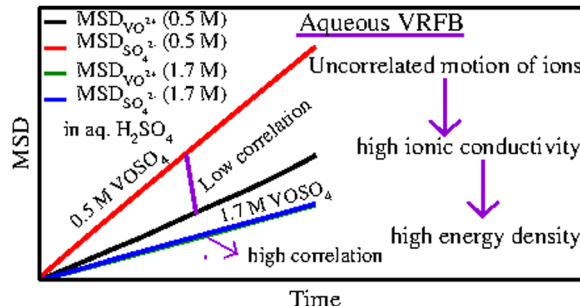
Katarzyna M. Krupka and María Pilar de Lara-Castells*



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Structure and dynamics of aqueous VOSO₄ solutions in conventional flow through cell design: a molecular dynamics simulation study

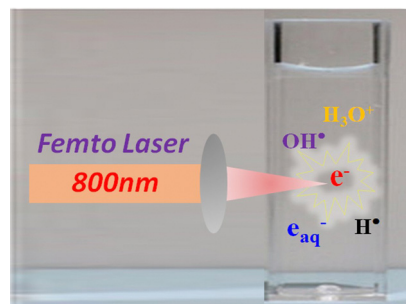
Anwesa Karmakar



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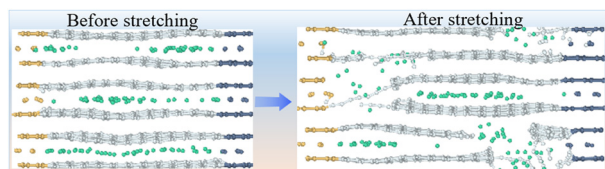
In situ generation and reaction of a sub-picosecond electron pulse: ultrafast broadband spectroscopy

Amitabha Nandi, Rajib Ghosh, Aruna K. Mora and Sukhendu Nath*



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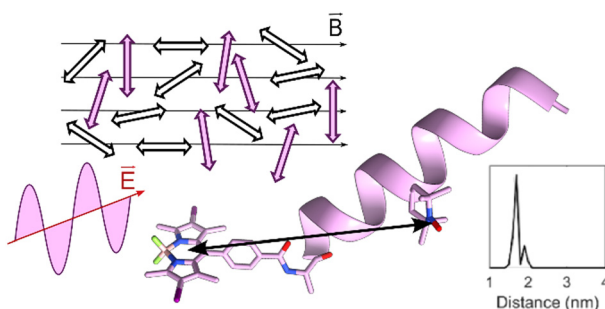
28386



Exploring lithium ion interactions in graphite electrodes through non-equilibrium molecular dynamics and density functional theory

Ding Shen,* ZhaoQi Ren, Shuang Wei, YanZhen Ji, YongHui Ma, YouZhi Yang, Wei Dong and ShuWei Tang

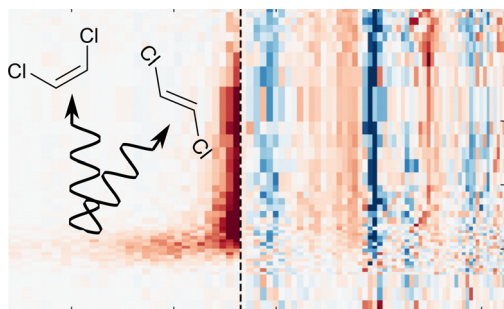
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I₂BODIPY as a new photoswitchable spin label for light-induced pulsed EPR dipolar spectroscopy exploiting magnetophotoselection

Arnau Bertran, Susanna Ciuti, Daniele Panariti, Ciarán J. Rogers, Haiqing Wang, Jianzhang Zhao, Christiane R. Timmel, Marina Gobbo, Antonio Barbon,* Marilena Di Valentin* and Alice M. Bowen*

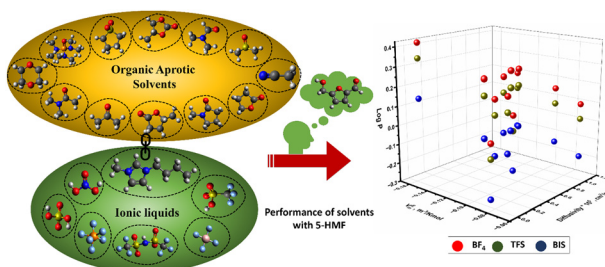
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Ultrafast photochemical processes in 1,2-dichloroethene measured with a universal XUV probe

Henry G. McGhee, Henry J. Thompson, James Thompson, Yu Zhang, Adam S. Wyatt, Emma Springate, Richard T. Chapman, Daniel A. Horke, Russell S. Minns, Rebecca A. Ingle and Michael A. Parkes*

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Structure, dynamic, and free energy analyses of 5-hydroxymethylfurfural in aprotic solvents and imidazolium ionic liquids using all-atom molecular dynamics simulations

Sweta Jha and Praveenkumar Sappidi*

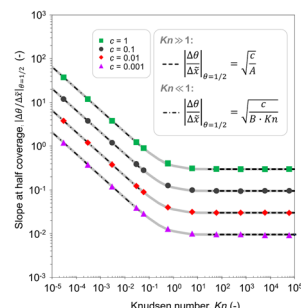


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Simulated conformality of atomic layer deposition in lateral channels: the impact of the Knudsen number on the saturation profile characteristics

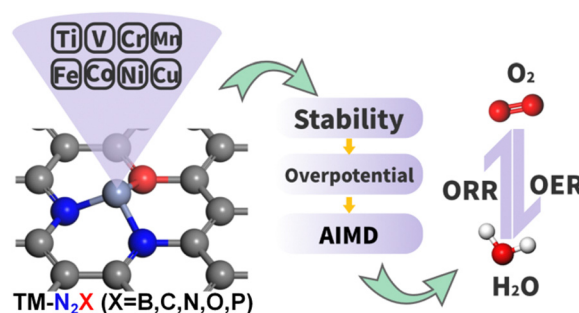
Christine Gonsalves,* Jorge A. Velasco, Jihong Yim, Jānis Jārvilehto, Ville Vuorinen and Riikka L. Puurunen*



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A theoretical investigation on the OER and ORR activity of graphene-based TM-N₃ and TM-N₂X (X = B, C, O, P) single atom catalysts by density functional theory calculations

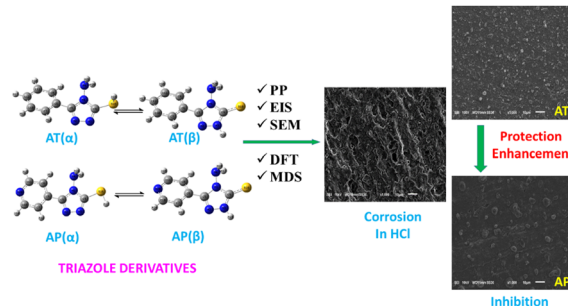
Jiaxiang Wu, Erjun Kan and Cheng Zhan*



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A combination of experimental and theoretical methods in evaluating triazole derivatives' mild steel corrosion inhibition ability in an acidic solution

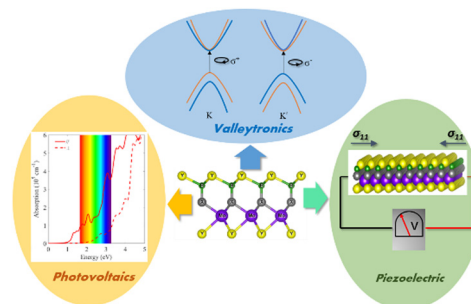
Ngo Hong Cat Van, Nguyen Quang Trung, Pham Dinh Tu Tai, Pham Cam Nam and Dinh Quy Huong*



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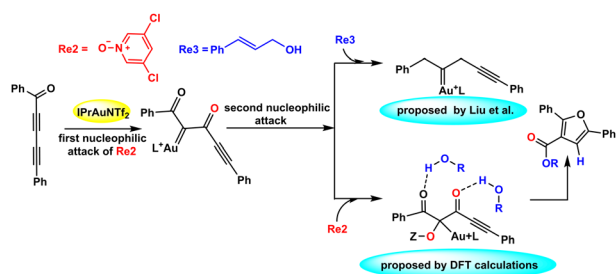
Exploring the valleytronic, optical, and piezoelectric properties of Janus MoBX₂ (X = N, P; Y = S, Se, Te) monolayers for multifunctional applications

Luogang Xie, Lingli Wang, YanDong Ma, Hongyan Lu and Yang Yang*



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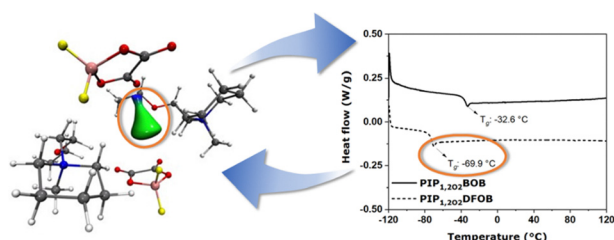
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DFT rationalization of the mechanism and selectivity in a gold-catalyzed oxidative cyclization of diynones with alcohols

Guowei Yan, Ji Ma, Simeng Qi, Alexander M. Kirillov, Lizi Yang* and Ran Fang*

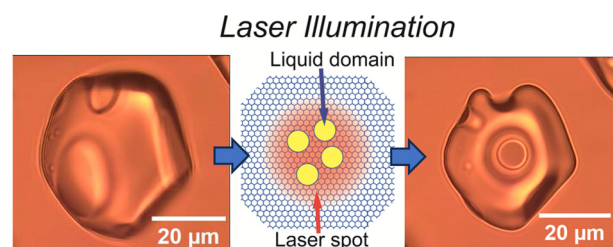
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Insight into physico-chemical properties of oxalatoborate-based ionic liquids through combined experimental-theoretical characterization

Matteo Palluzzi, Giorgia Mannucci, Akiko Tsurumaki, Matteo Busato, Maria Assunta Navarra* and Paola D'Angelo*

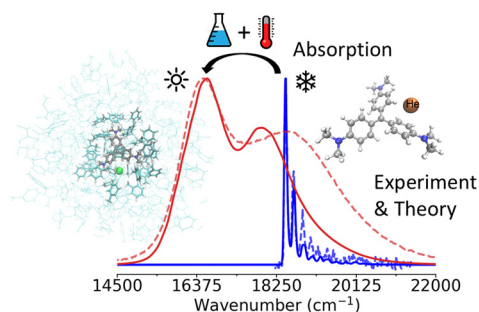
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Laser-induced fabrication of a supercooled liquid droplet embedded in an ice microcrystal

Shuichi Hashimoto* and Takayuki Uwada

28514



Influence of symmetry breaking on the absorption spectrum of crystal violet: from isolated cations at 5 K to room temperature solutions

Alexander Schäfer, Samuele Giannini, Dmitry Strelnikov, Theresa Mohr, Fabrizio Santoro, Javier Cerezo* and Manfred M. Kappes*

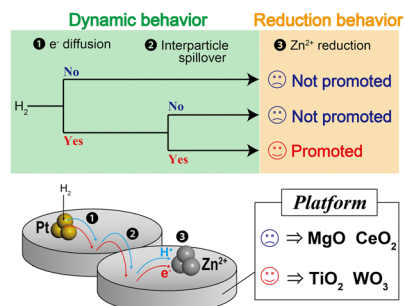


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Effects of oxide platforms on the dynamics and reduction characteristics of hydrogen spillover

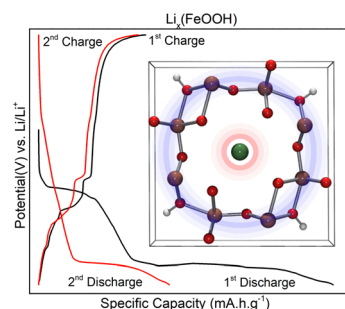
Kazuki Shun, Akihito Fujimoto, Kohsuke Mori* and Hiromi Yamashita



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Exploring the electrochemical properties and lithium insertion mechanisms in akaganeite (β -FeOOH) – a combined DFT/experimental study

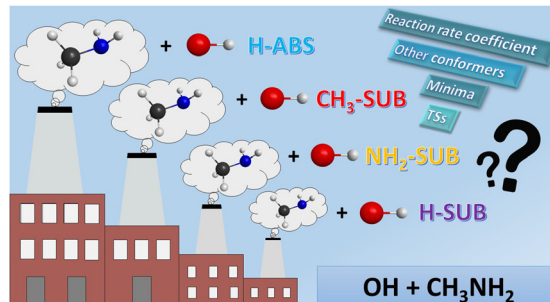
Paulo Roberto Garcês Gonçalves Jr, Heitor Avelino De Abreu, Luciano Andrey Montoro, Gabriela Cordeiro Silva, Angela de Mello Ferreira and Hélio Anderson Duarte*



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High-level *ab initio* characterization of the OH + CH₃NH₂ reaction

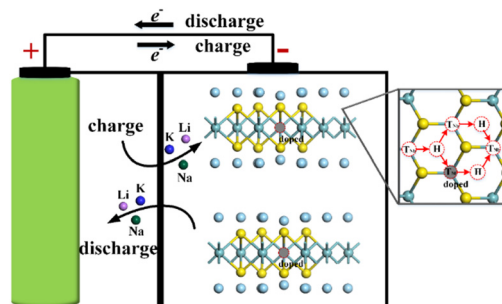
Balázs Gruber and Gábor Czakó*



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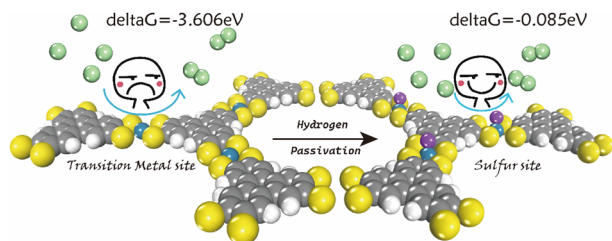
Insight into the potential of M–NbS₂ (M = Pd, Ti and V) monolayers as anode materials for alkali ion (Li/Na/K) batteries

Meixia Xiao,* Shuling Xu, Haiyang Song, Zhifei Sun, Jiaying Bi and Beibei Xiao



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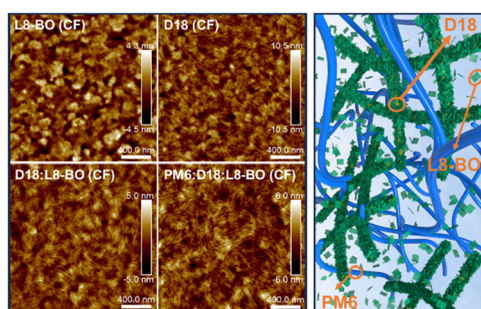
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A hydrogen passivation strategy for the electrocatalytic chlorine evolution reaction on metal–organic frameworks: a theoretical insight

Jiake Fan, Lei Yang, Hui Li, Zijian Sun, Mengyun Mei and Weihua Zhu*

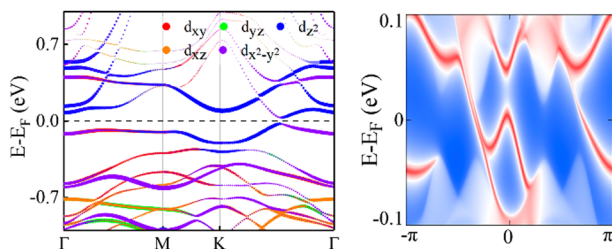
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Morphology optimization *via* pre-aggregation and miscibility matching in PM6:L8-BO ternary organic solar cells

Chuyue Wei, Junwei Zhang, Jing Deng, Xiangyan Yang, Jiahui Luo, Zixiao Xu, Lin Zhang,* Shuaishuai Yuan* and Weihua Zhou*

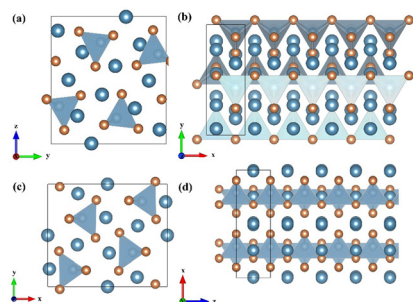
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High Chern number quantum anomalous Hall effect in monolayer $\text{Co}_3\text{X}_3\text{Sse}$ ($\text{X} = \text{Sn}, \text{Pb}$) kagomes

Xiang Yin, Li Deng, Fei Wang, Yanzhao Wu, Junwei Tong and Xianmin Zhang*

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Lattice thermal conductivity reduction in Ca_3AlSb_3 and $\text{Ca}_5\text{Al}_2\text{Sb}_6$ by manipulating the covalent tetrahedral chain

Chi Zhang, Wenya Zhai, Jingyu Li, Jianbo Zhu, Zengfu Ou, Lanwei Li, Peng-Fei Liu, Xiaobing Liu, Yuli Yan* and Yongsheng Zhang*

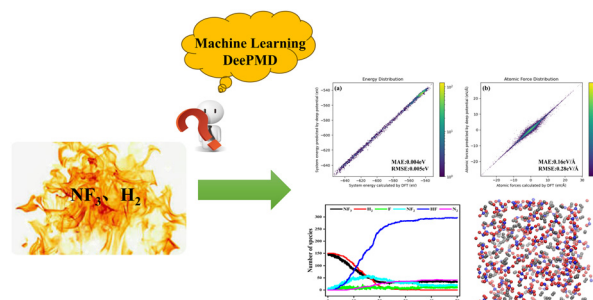


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Investigation on the combustion mechanism for NF_3/H_2 in DF/HF chemical lasers: a new perspective based on deep potential molecular dynamics simulations

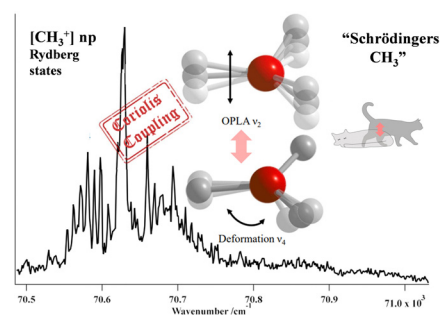
Yinhua Ma, Dongmei Mu, Meiheng Lv, Nan Wang, Huaxin Liu, Fangjian Shang and Jianyong Liu*



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Photofragmentation and fragment analysis; Coriolis interactions in excited states of CH_3

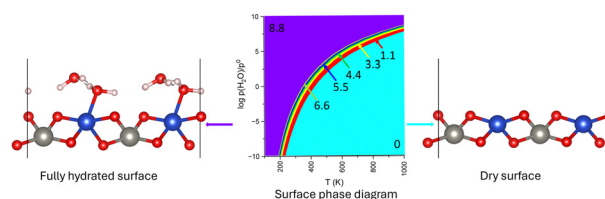
Meng-Xu Jiang and Ágúst Kvaran*



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Water adsorption at the (010) and (101) surfaces of CuWO_4

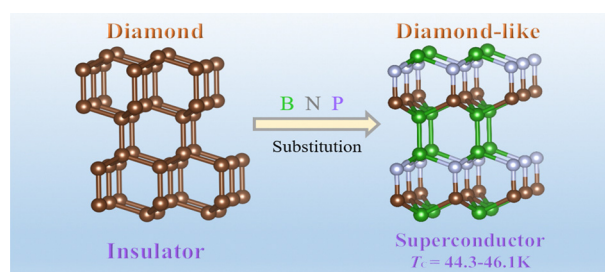
Xuan Chu, David Santos-Carballal* and Nora H. de Leeuw*



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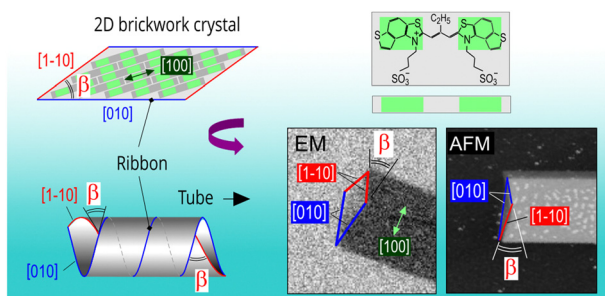
Prediction of high-temperature superconductors at ambient pressure with diamond-like structures: B_2CX (X = N, P)

Yi Wan, Ying-Jie Chen,* Shu-Xiang Qiao, Kai-Yue Jiang, Guo-Hua Liu, Na Jiao, Ping Zhang and Hong-Yan Lu*



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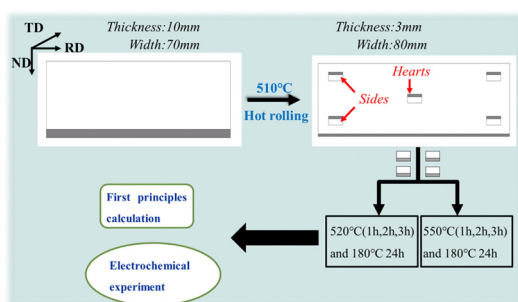
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Crystallographic models of ribbons and ribbon-based J-aggregate nanotubes from the geometry of tube ends

Valery V. Prokhorov,* Kirill A. Prusakov, Sergey I. Pozin, Olga M. Pereyginina, Eugene I. Mal'tsev and Alexander A. Nekrasov

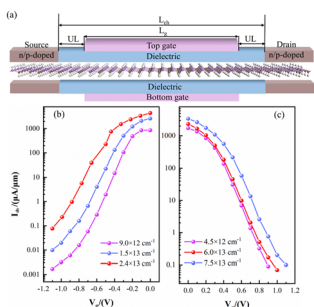
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Multi-scale study on the electrochemical behavior and corrosion mechanism of 5083 aluminum alloy with different microstructures in a NaCl environment

Zhijie Dai, Zhengbing Xiao,* Dahong Zhao, Sunhang Xiao, Yuanchun Huang and Qingsong Dai

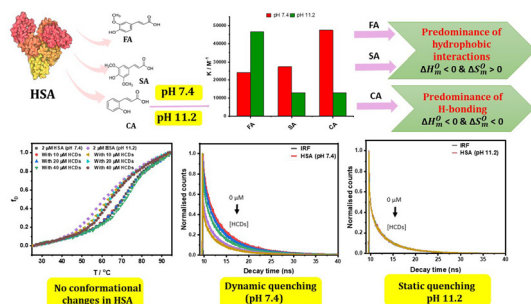
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Ballistic transport in sub-10 nm monolayer InAs transistors for high-performance applications

Tianruo Xie and Yuliang Mao*

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Deciphering the spectroscopic and thermodynamic aspects of binding of biologically important antioxidants with the alkali induced state of human serum albumin

Anjali Maheshwari and Nand Kishore*

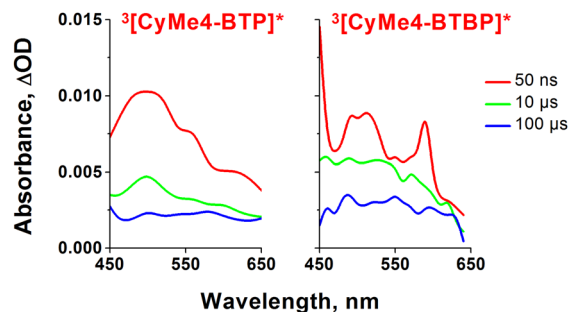


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Radiolytic degradation of selective actinide extractants from the bis-1,2,4-triazine family in cyclohexanone solutions

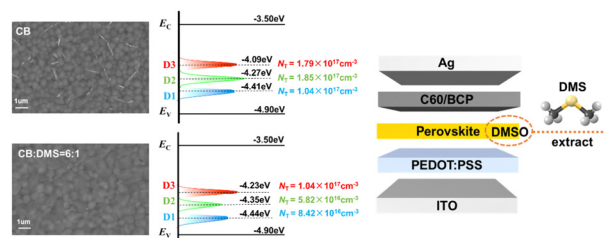
Adrian Sulich,* Jan Grodkowski and Krzysztof Bobrowski



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Improved perovskite crystallization by antisolvent engineering in tin-perovskite photovoltaics

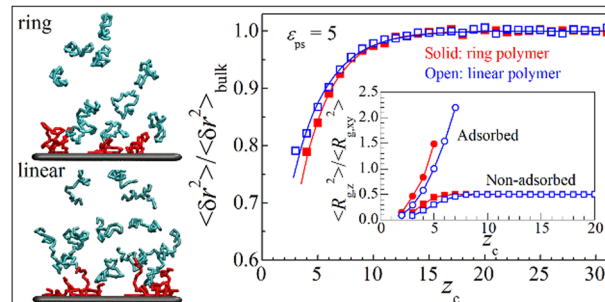
Xin Zhang, Yu Liu, Xinyao Chen, Chunqian Zhang, Jigang Wang, Jin Cheng and Junming Li*



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Simulation study of the conformation and dynamics of substrate-supported ring and linear polymer films

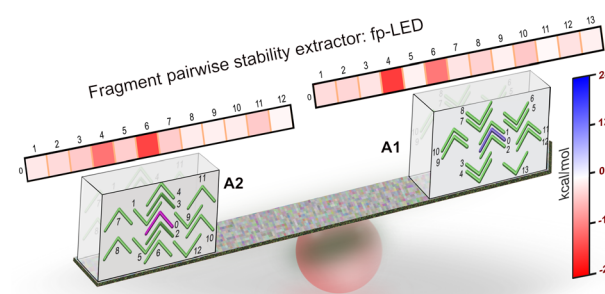
Jianhua Huang,* Hongzhu Ji, Jin Zhang and Zhunpeng Wang



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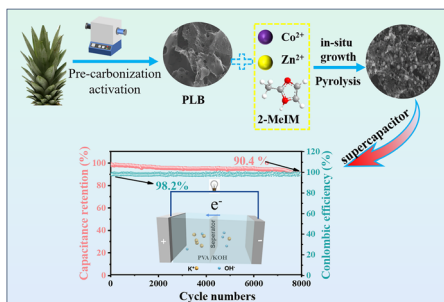
Rationalizing polymorphism with local correlation-based methods: a case study of pnictogen molecular crystals

Ahmet Altun, Eduardo Schiavo, Michael Mehring, Stephan Schulz, Giovanni Bistoni* and Alexander A. Auer*



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A composite of pineapple leaf-derived porous carbon integrated with ZnCo-MOF for high-performance supercapacitors

Xiaoxiao Ma, Yunfan Bai, Shuangli Chen, Zhixian He, Pingping Wu, Yabing Qi and Sijing Zhang*

CORRECTIONS

28757

Correction: Spin-dependent Seebeck effect in zigzag-edge antimonene nanoribbons

Liyan Lin, Yue Jiang,* Xinyi Gao, Yandong Guo,* Hongli Zeng and Xiaohong Yan*

28758

Correction: Impact of lanthanide ion complexation and temperature on the chemical reactivity of *N,N,N',N'*-tetraoctyl diglycolamide (TODGA) with the dodecane radical cation

Gregory P. Horne,* Cristian Celis-Barros, Jacy K. Conrad, Travis S. Grimes, Jeffrey R. McLachlan, Brian M. Rotermund, Andrew R. Cook and Stephen P. Mezyk*

