

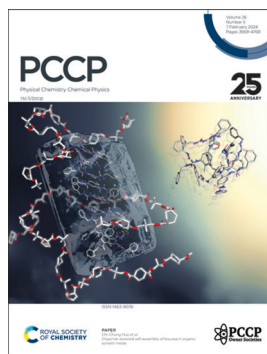
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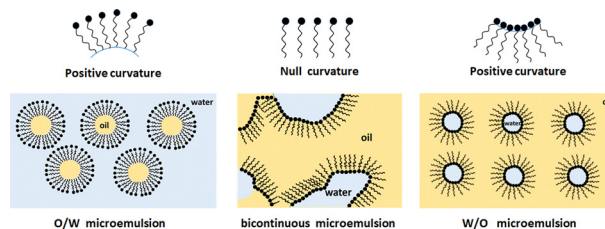
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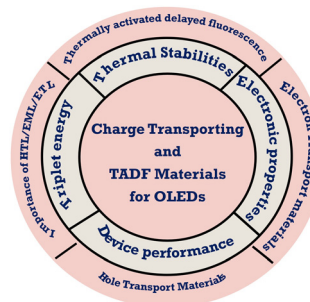
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Charge transporting and thermally activated delayed fluorescence materials for OLED applications

Krishan Kumar



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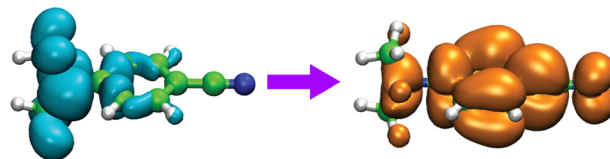


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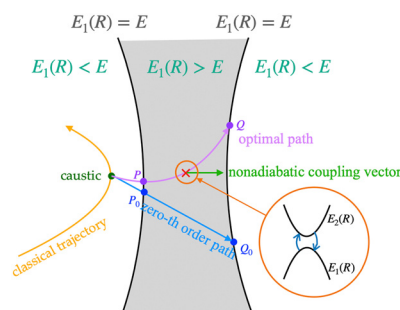


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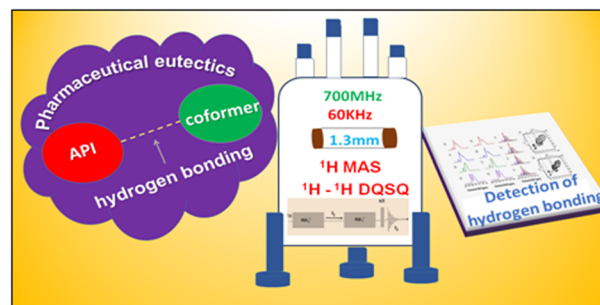
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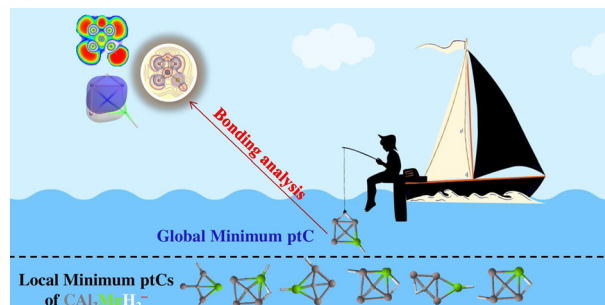
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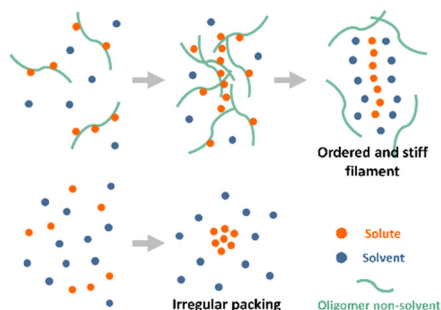
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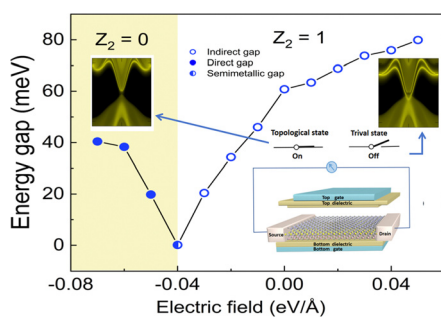
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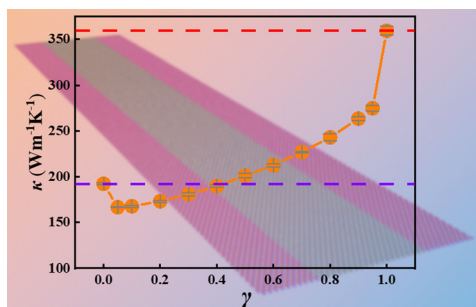
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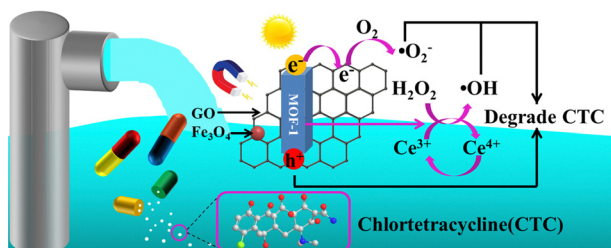
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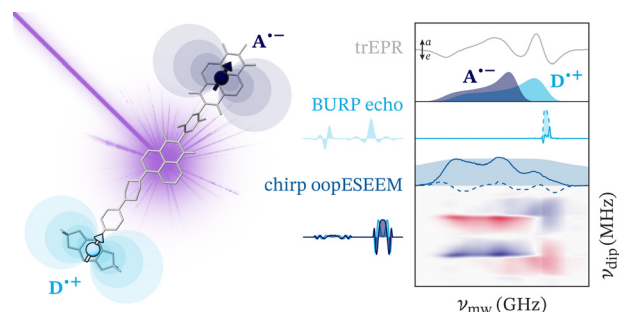


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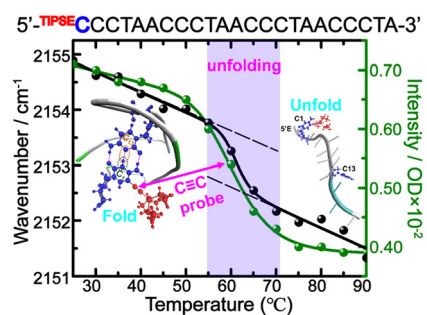
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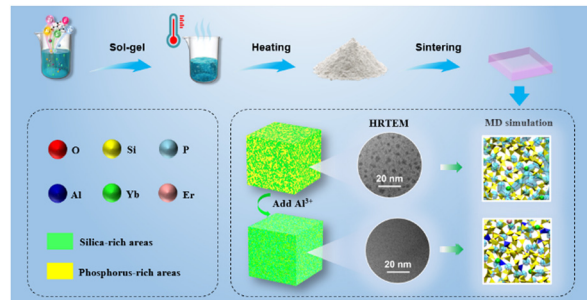
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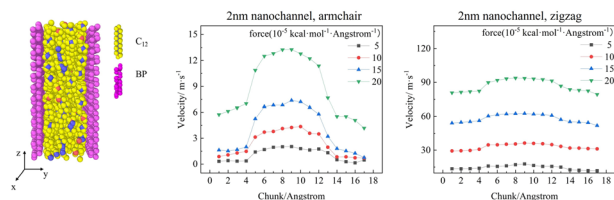
Te-doped-WSe₂/W as a stable monolith catalyst for ampere-level current density hydrogen evolution reaction

Xingchen Zhang, Dongfang Zhang, Xinya Chen, Dingyi Zhou, Jinying Zhang and Zhiyong Wang*



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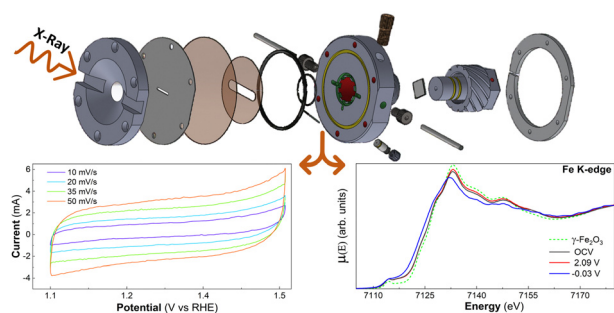
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Anisotropic fluid flows in black phosphorus nanochannels

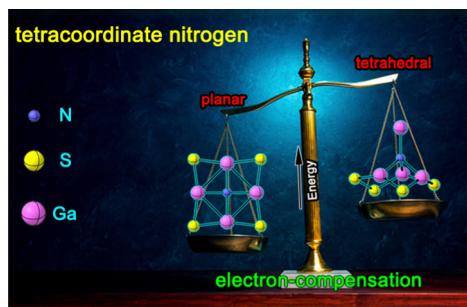
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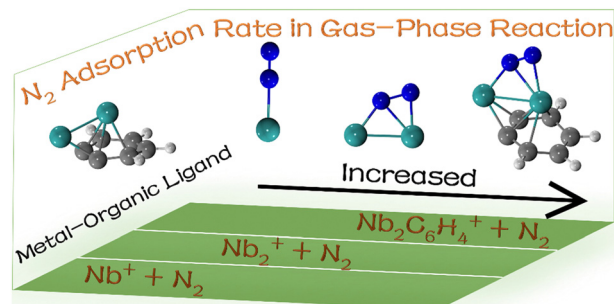
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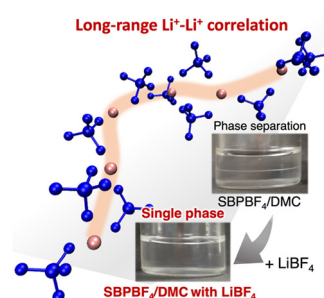


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A structural study on a specific Li-ion ordered complex in dimethyl carbonate-based dual-cation electrolytes

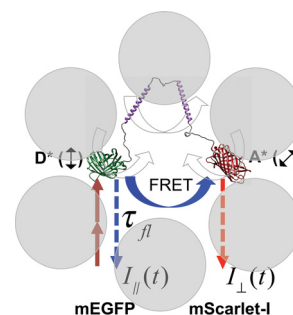
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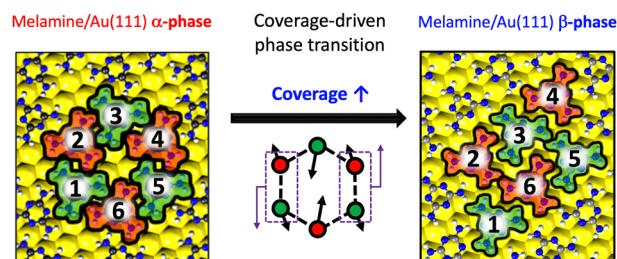
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Transition mechanism of the coverage-dependent polymorphism of self-assembled melamine nanostructures on Au(111)

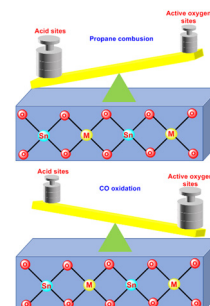
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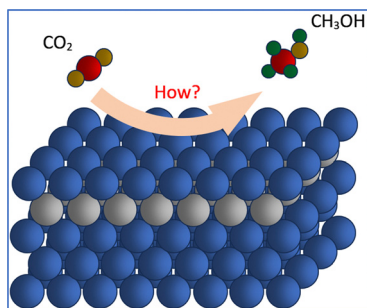
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Haiming Yan, Teng Liu, Yu Lv, Xianglan Xu, Junwei Xu, Xiuzhong Fang and Xiang Wang*



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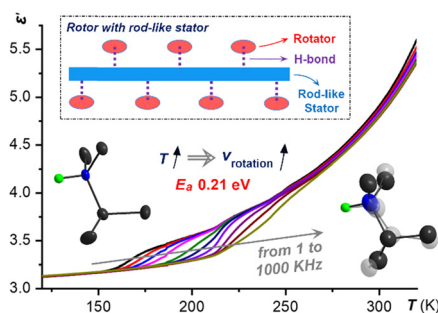
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Carbon dioxide conversion to methanol on a PdCo bimetallic catalyst

Huynh Tat Thanh, Ong Kim Le, Viorel Chihaiia and Do Ngoc Son*

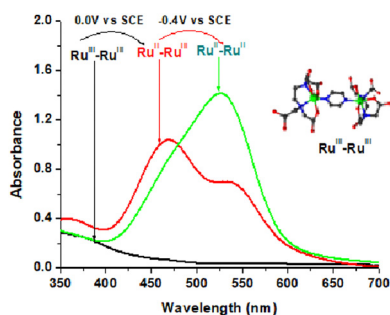
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Molecular rotators anchored on a rod-like anionic coordination polymer adhered by charge-assisted hydrogen bonds

Hui Xiao, Wei-Yu Hu, Qing Wang, Cheng-Hui Zeng, Hao-Hong Li, Haiming Liu, Zi-Yi Du* and Chun-Ting He

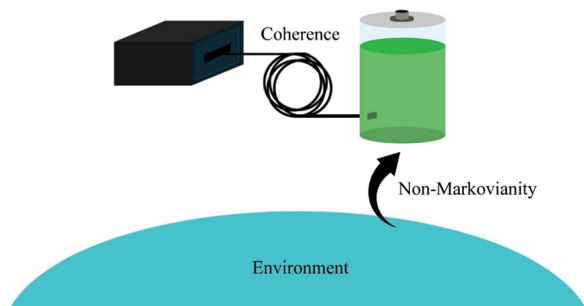
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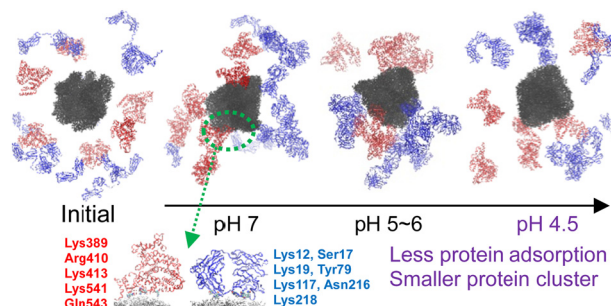


Quantum non-Markovianity, quantum coherence and extractable work in a general quantum process

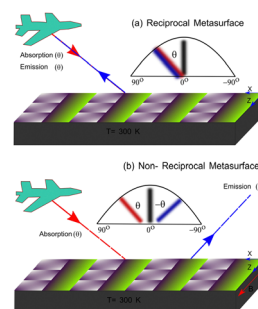
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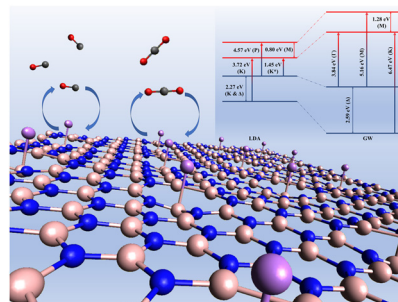
Hwankyu Lee



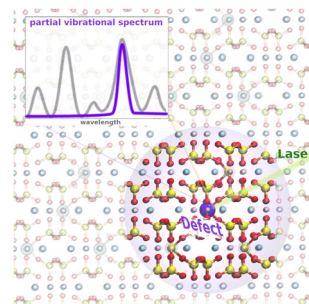
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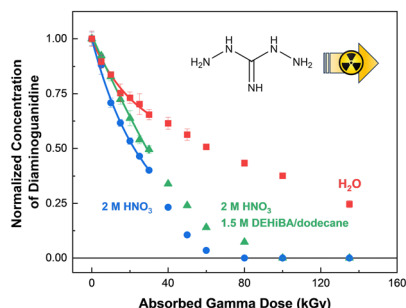


Luca Bellucci,* Michele Cassetta, Henrik Skogby and
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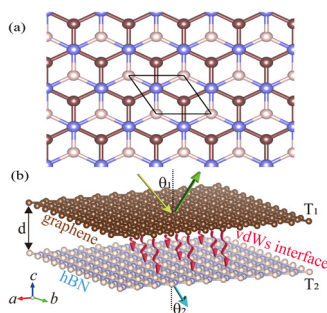
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Radiolytic evaluation of a new technetium redox control reagent for advanced used nuclear fuel separations

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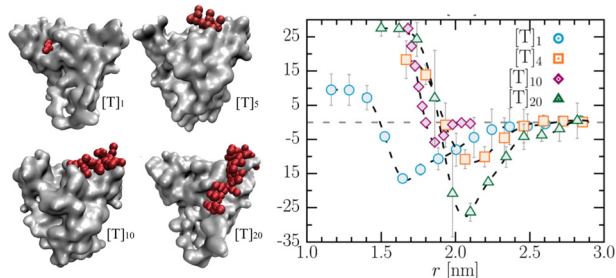
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Interface thermal conductivities induced by van der Waals interactions

H. M. Dong, H. P. Liang, Z. H. Tao, Y. F. Duan,* M. V. Milošević* and K. Chang*

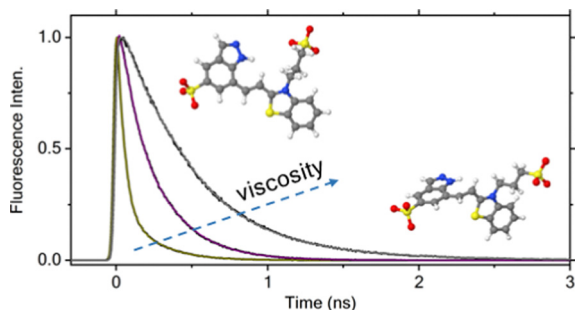
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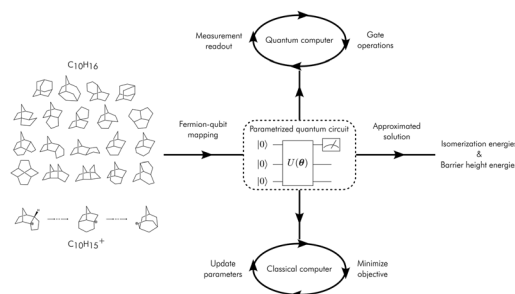


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Applications of noisy quantum computing and quantum error mitigation to “adamantaneland”: a benchmarking study for quantum chemistry

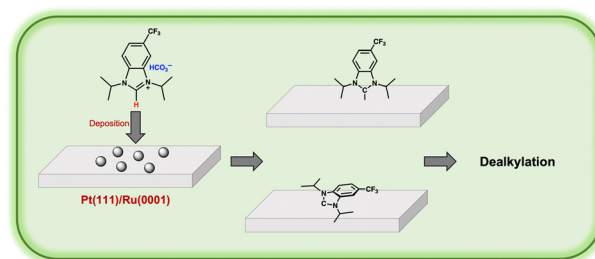
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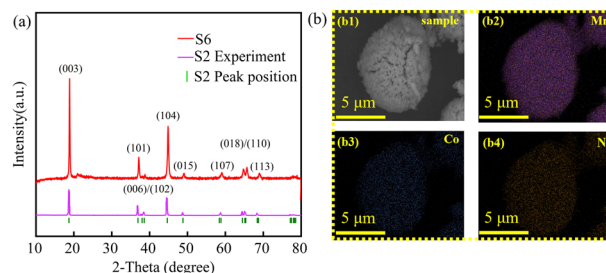
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Design of a new Li-rich Mn-based ternary cathode material based on the Ni, Co, and Mn action mechanism

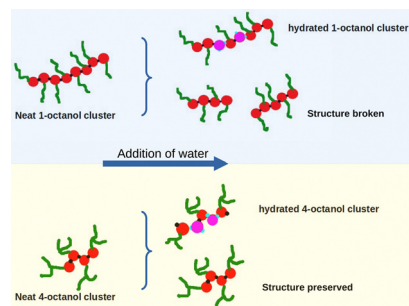
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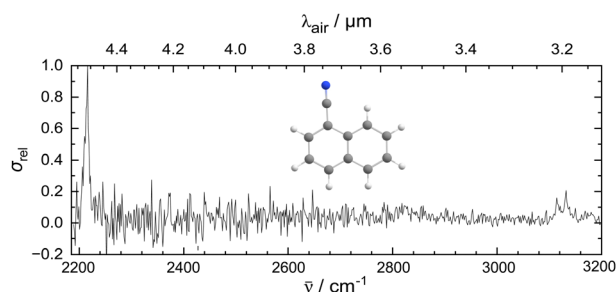
On the dual behaviour of water in octanol-rich aqueous *n*-octanol mixtures: an X-ray scattering and computer simulation study

Martina Požar, Jennifer Bolle, Susanne Dogan-Surmeier, Eric Schneider, Michael Paulus, Christian Sternemann* and Aurélien Perera



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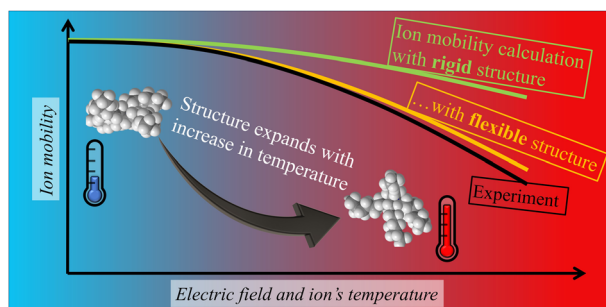
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Mid-infrared spectroscopy of 1-cyanonaphthalene cation for astrochemical consideration

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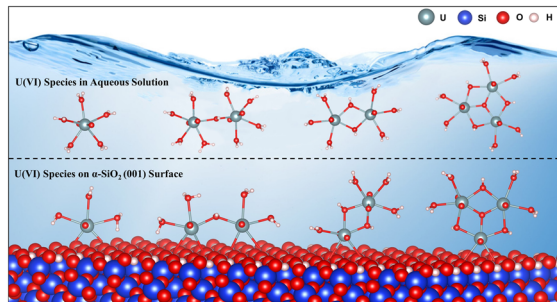
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Ion mobility calculations of flexible all-atom systems at arbitrary fields using two-temperature theory

Farah Mubas-Sirah, Viraj D. Gandhi, Mohsen Latif,
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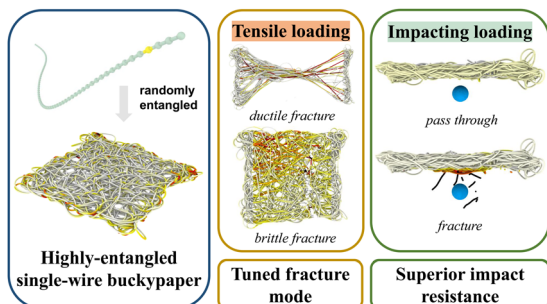
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Structures of multinuclear U(VI) species on the hydroxylated α -SiO₂(001) surface: insights from DFT calculations

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A single carbon nanotube-entangled high-performance buckypaper with tunable fracture mode

Yuna Sang, Chongxiao Cui, Yushun Zhao,*
Xiuping Zhang, Zhuochao Zhang, Fei Wang,
Rong Liu, Chao Sui,* Xiaodong He and Chao Wang*

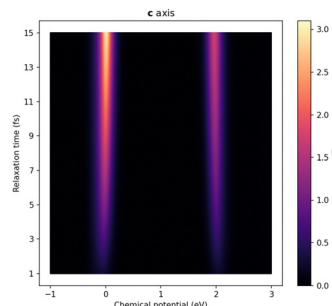


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Computational prediction of high thermoelectric performance in As_2Se_3 by engineering out-of-equilibrium defects

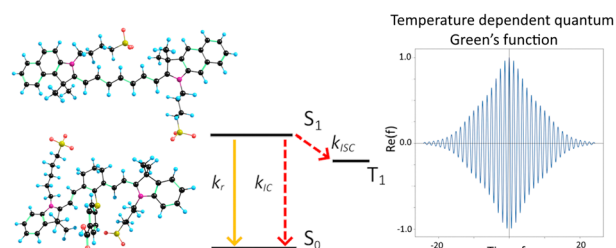
Anderson Silva Chaves, Murilo Aguiar Silva and Alex Antonelli*



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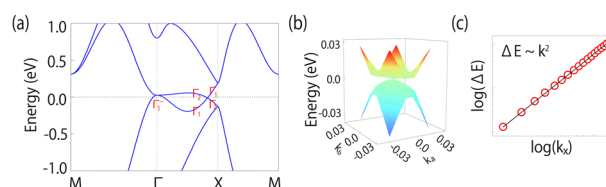
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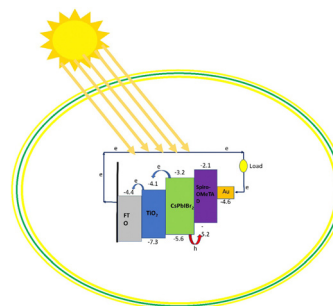
Jin-Yang Li, Xin-Yue Kang, Ying Zhang, Si Li* and Yugui Yao



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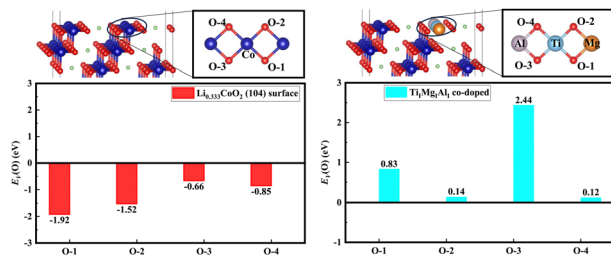
Impact of Ce doping on the optoelectronic and structural properties of a CsPbIBr_2 perovskite solar cell

M. I. Khan,* Ali Mujtaba, Mahvish Fatima, Riadh Marzouki, Saddam Hussain and Tauseef Anwar



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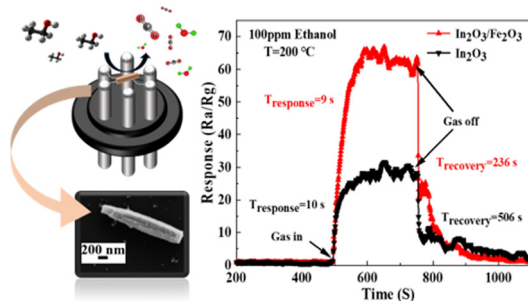
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A synergetic promotion of surface stability for high-voltage LiCoO_2 by multi-element surface doping: a first-principles study

Hongbin Lin, Xiumei Kang, Guigui Xu,* Yue Chen, Kehua Zhong, Jian-Min Zhang and Zhigao Huang*

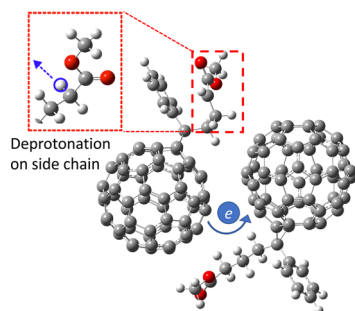
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In-MIL-68 derived $\text{In}_2\text{O}_3/\text{Fe}_2\text{O}_3$ shuttle-like structures with n-n heterojunctions to improve ethanol sensing performance

Zhenyue Liu, Zhenkai Zhang, Chen Yue, Yang Mu, Zhiguo Yang, Davoud Dastan, Xi-Tao Yin* and Xiaoguang Ma*

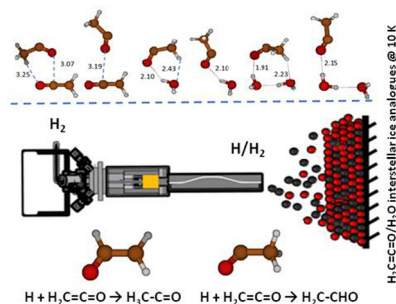
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Charge transfer in superbase n-type doping of PCBM induced by deprotonation

Chuan-Ding Dong,* Fabian Bauch, Yuanyuan Hu and Stefan Schumacher

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The significant role of water in reactions occurring on the surface of interstellar ice grains: Hydrogenation of pure ketene $\text{H}_2\text{C}=\text{C}=\text{O}$ ice versus hydrogenation of mixed $\text{H}_2\text{C}=\text{C}=\text{O}/\text{H}_2\text{O}$ ice at 10 K

Mohamad Ibrahim, Jean-Claude Guillemin, Patrick Chaquin, Alexis Markovits and Lahouari Krim*

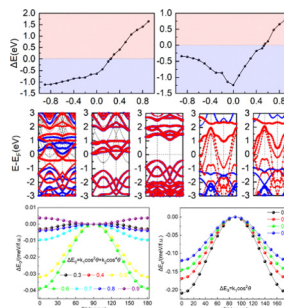


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Carrier doping modulates the magnetoelectronic and magnetic anisotropic properties of two-dimensional MSi_2N_4 ($M = \text{Cr, Mn, Fe, and Co}$) monolayers

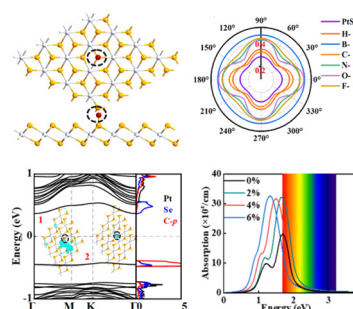
Ziyuan An, Linhui Lv, Ya Su,* Yanyan Jiang and Zhaoyong Guan*



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Single-layer PtSe_2 adsorbed with non-metallic atoms: geometrical, mechanical, electronic and optical properties and strain effects

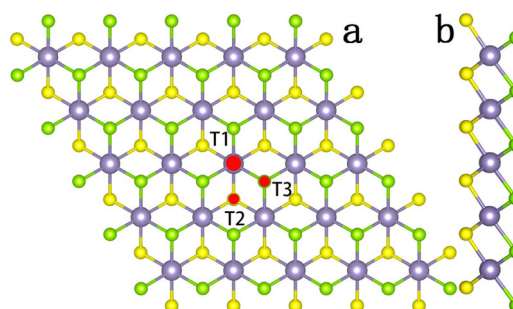
Xinyan Li, Zhanhai Li,* Jianing Han, Shengguo Cao and Zhenhua Zhang*



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First-principles study of magnetic properties and electronic structure of 3d transition-metal atom-adsorbed SnSSe monolayers

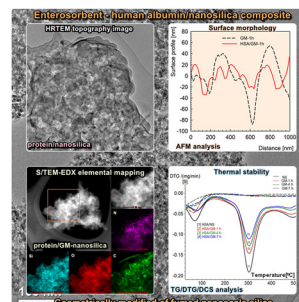
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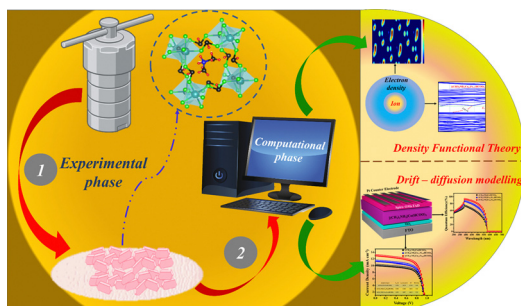
Nanostructure and thermal characteristics of silica/human serum albumin systems based on a modified nanosilica entero-vulnerosorbent

Agnieszka Chrzanowska,* Liudmyla V. Nosach and Anna Derylo-Marczewska



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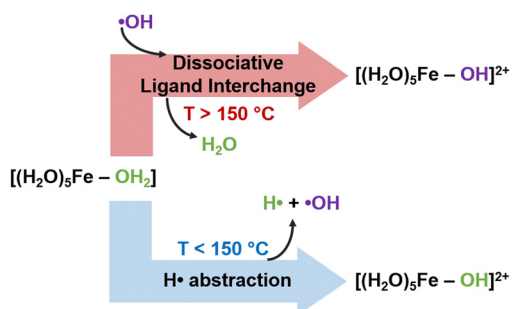
4262



Experimental and computational DFT, drift-diffusion studies of cobalt-based hybrid perovskite crystals as absorbers in perovskite solar cells

Sathish Marimuthu, Saravanan Pandiaraj, Muthumareeswaran Muthuramamoorthy, Khalid E. Alzahrani, Abdullah N. Alodhayb, Sudhagar Pitchaimuthu and Andrews Nirmala Grace*

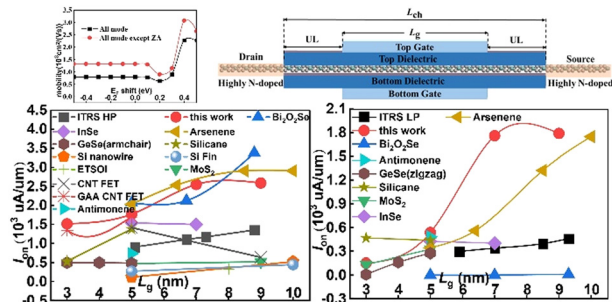
4278



Kinetics of the reaction of ferrous ions with hydroxyl radicals in the temperature range 25–300 °C

Logan Barr,* Jacy K. Conrad, Christine McGregor, Randy Perron, Pamela A. Yakabuskie and Craig R. Stuart

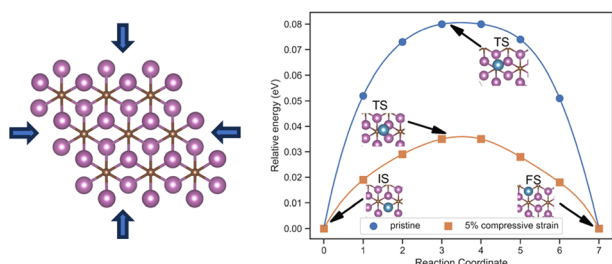
4284



Comprehensive understanding of electron mobility and superior performance in sub-10 nm DG ML tetrahex-GeC₂ n-type MOSFETs

Yuehua Xu,* Daqing Li, He Sun, Haowen Xu and Pengfei Li

4298



Biaxial compressive strain enhances calcium binding and mobility on two-dimensional Sc₂C: a density functional theory investigation

Darwin B. Putungan,* Christian Loer T. Llemit, Alexandra B. Santos-Putungan, Roland V. Sarmago and Ralph Gebauer

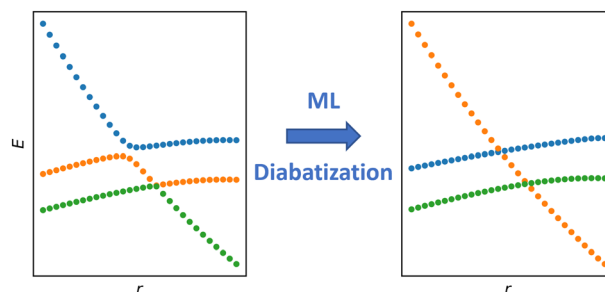


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4306

Fast and accurate excited states predictions: machine learning and diabaticization

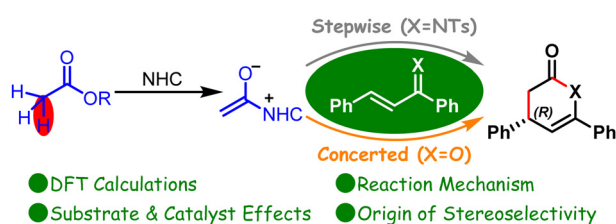
Štěpán Sršeň,* O. Anatole von Lilienfeld and Petr Slaviček*



4320

Elucidating the mechanism and origin of stereoselectivity in the activation/transformation of an acetic ester catalyzed by an N-heterocyclic carbene

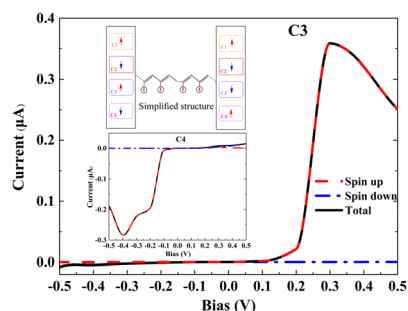
Pingxin Liang, Haoran Yang* and Yang Wang*



4329

Molecular rectification induced by magnetization alignment in organic-ferromagnetic devices

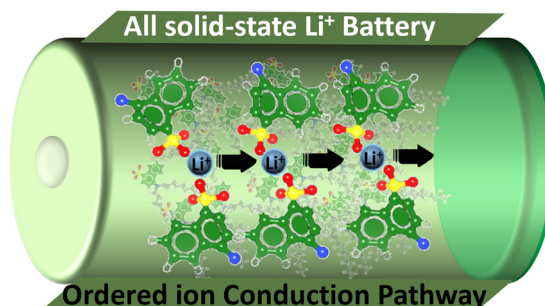
H. Ma, H. X. Li, H. Q. Zhang, Y. Wang, J. T. Li, C. Wang, J. F. Ren and G. C. Hu*



4338

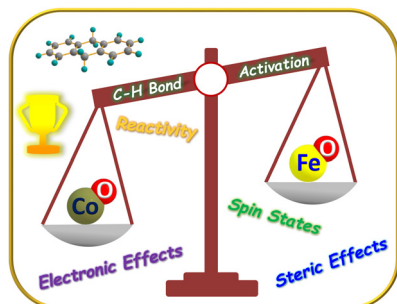
Modelling structure and ionic diffusion in a class of ionic liquid crystal-based solid electrolytes

Md Sharif Khan,* Ambroise Van Roieghem, Stefano Mossa, Flavien Ivol, Laurent Bernard, Lionel Picard and Natalio Mingo*



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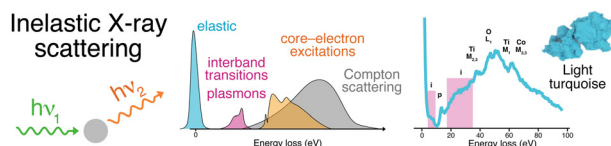
4349



C–H bond activation by high-valent iron/ cobalt–oxo complexes: a quantum chemical modeling approach

Manjeet Kumar, Manoj Kumar Gupta, Mursaleem Ansari* and Azaj Ansari*

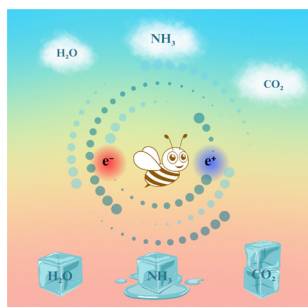
4363



Non-resonant inelastic X-ray scattering for discrimination of pigments

Lauren Dalecky, Francesco Sottile, Linda Hung, Laure Cazals, Agnès Desolneux, Aurélia Chevalier, Jean-Pascal Rueff and Loïc Bertrand*

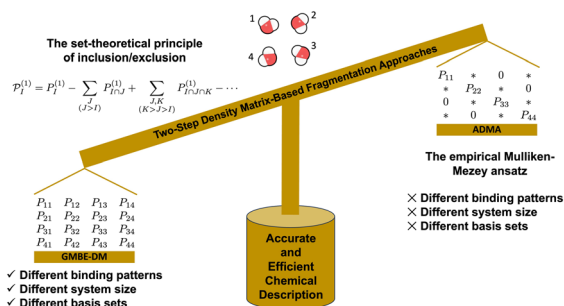
4372



Electron- and positron-driven molecular processes for H₂O, CO₂, and NH₃ in their gas and ice phases

Neha Barad and Chetan Limbachiya*

4386



Analysis of two overlapping fragmentation approaches in density matrix construction: GMBE-DM vs. ADMA

Francisco Ballesteros and Ka Un Lao*

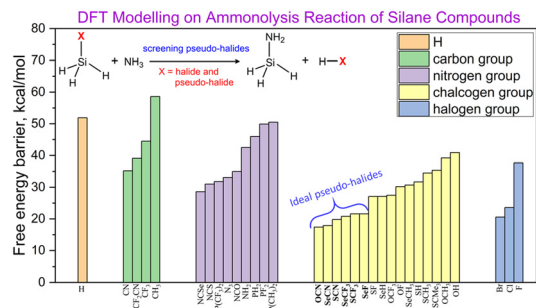


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4395

Enhancing silicon-nitride formation through ammonolysis of silanes with pseudo-halide substituents

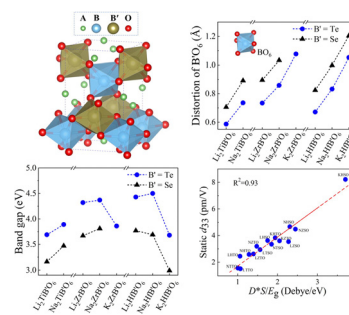
Anil Kumar Tummanapelli, Yingqian Chen and Ming Wah Wong*



4403

Investigation of nonlinear optical properties in α -A₂BB'O₆ (A = Li, Na, K; B = Ti, Zr, Hf; B' = Se, Te) by first-principles calculations

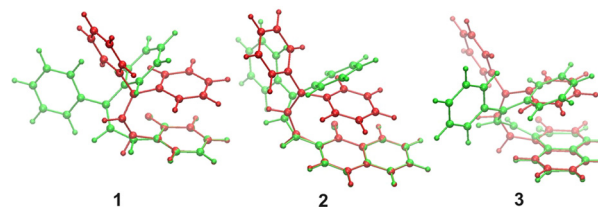
Gaojing Fang, Xiaojun Teng, Luo Yan, Yu Wu, Kui Xue, Xiaofeng Zhang, Yi-min Ding,* Liujiang Zhou* and Qiye Wen*



4412

Intramolecular excimers of open forms of 2H-benzopyran, 2H- and 3H-naphthopyrans in solution: TD-DFT/DFT analysis

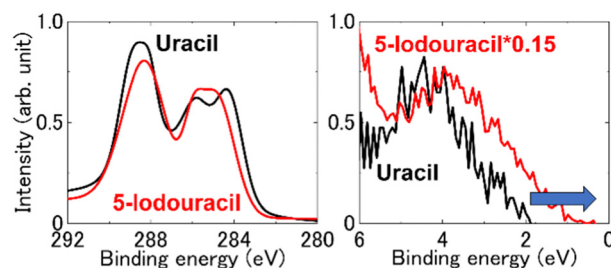
Daiana S. Tabirja and Victor V. Kostjukov*



4422

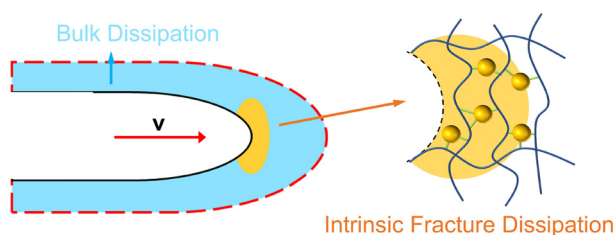
Comparison of core and valence band electronic structures of bulk uracil and 5-halouracils

Yudai Izumi,* Maki Ohara, Yuji Baba and Akinari Yokoya



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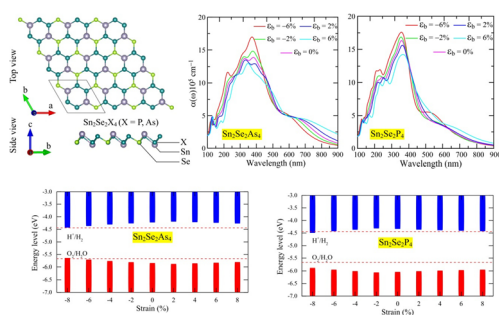
4429



Insight into the fracture energy dissipation mechanism in elastomer composites via sacrificial bonds and fillers

Dongyi He, Xiaxia Cheng, Chunyu Wong, Xiangliang Zeng, Linling Li, Chao Teng,* Guoping Du, Chenxu Zhang,* Linlin Ren, Xiaoliang Zeng* and Rong Sun

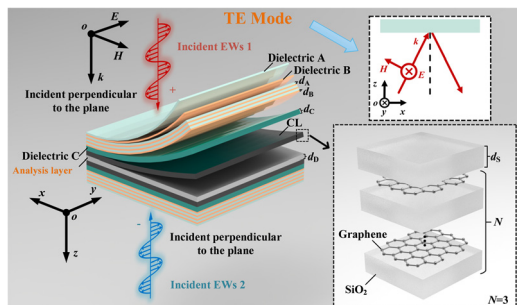
4437



First principles study of strain effects on prospective 2D photocatalysts $\text{Sn}_2\text{Se}_2\text{X}_4$ (X = P, As) with ultra-high charge carrier mobility

Pham D. Trung* and Hien D. Tong*

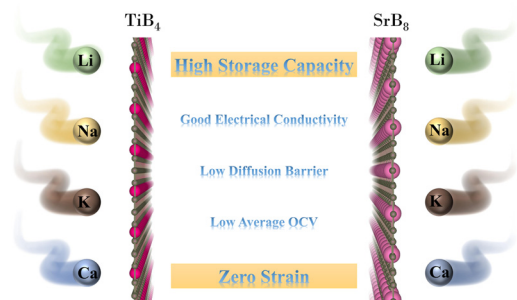
4447



A multiple cancer cell optical biosensing metastructure realized by CPA

Jia-Hao Zou, Jun-Yang Sui, You-Ran Wu and Hai-Feng Zhang*

4455



TiB_4 and SrB_8 monolayers: high capacity and zero strain-like anode materials for Li/Na/K/Ca ion batteries

Yunxin Wang, Sisi Liang, Juncheng Tian, Huixian Duan, Ying Lv, Lijia Wan, Chunlai Huang, Musheng Wu, Chuying Ouyang and Junping Hu*

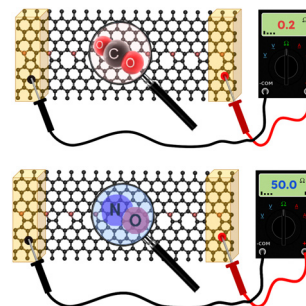


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4466

Boron-doped graphene topological defects: unveiling high sensitivity to NO molecule for gas sensing applications

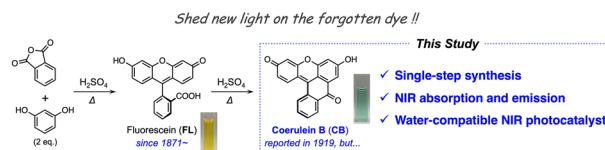
B. Keshav Rao, Tadeu Luiz Gomes Cabral, Debora Carvalho de Melo Rodrigues, Fábio A. L. de Souza, Wanderlã L. Scopel, Rodrigo G. Amorim* and Ravindra Pandey



4474

Coerulein B: a water-soluble and water-compatible near-infrared photoredox catalyst

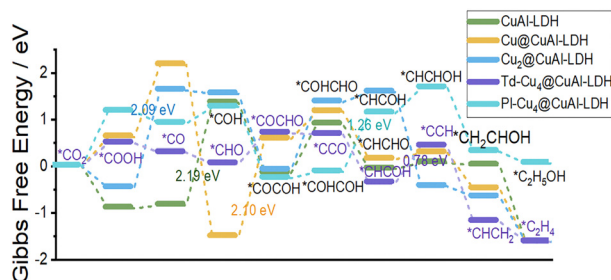
Masaru Tanioka,* Masaya Oyama, Kaito Nakajima, Minori Mori, Mei Harada, Yuji Matsuya* and Shinichiro Kamino*



4480

Theoretical study on electrocatalytic carbon dioxide reduction over copper with copper-based layered double hydroxides

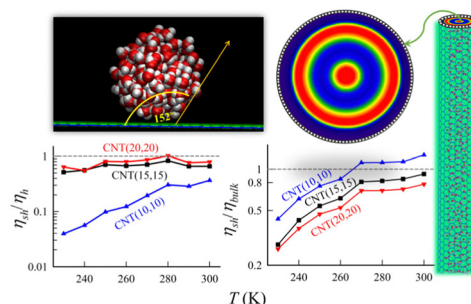
Xin-Yu Xu, Jing-Yi Guo, Wei Zhang, Yao Jie, Hui-Ting Song, Hao Lu, Yi-Fan Zhang, Jia Zhao, Chen-Xu Hu and Hong Yan*



4492

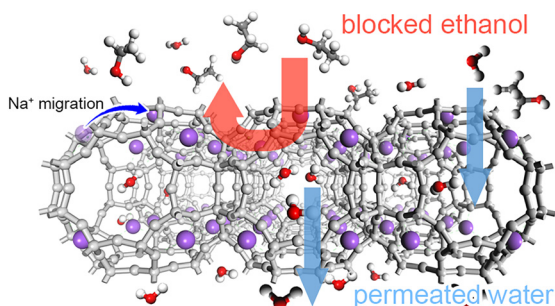
Enhanced fluidity of water in superhydrophobic nanotubes: estimating viscosity using jump-corrected confined Stokes–Einstein approach

Golam Rosul Khan and Snehasis Daschakraborty*



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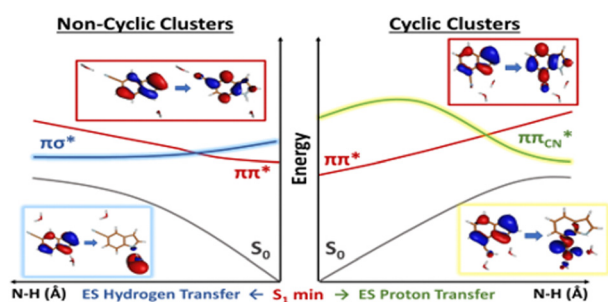
4505



Computational understanding of Na-LTA for ethanol–water separation

Zicheng Wan, Chen Zhou, Yichao Lin,*
Liang Chen and Ziqi Tian*

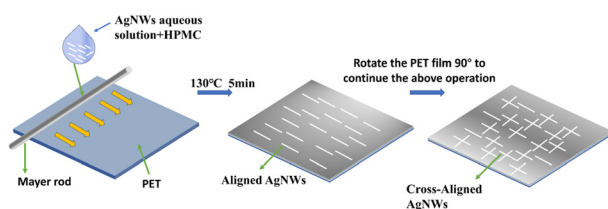
4511



Excited state hydrogen or proton transfer pathways in microsolvated *n*-cyanoindole fluorescent probes

Salsabil Abou-Hatab and Spiridoula Matsika*

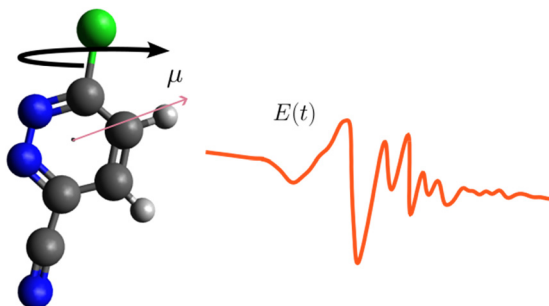
4524



Silver nanowires/cellulose flexible transparent conductive films for electromagnetic interference shielding and electrothermal conversion

Zhijiang Guo, Xiaoli Li, Ning Li, Xuanji Liu, Longhui Hao,
Yuxuan Wang, Wei Deng, Haoxuan Bai, Jianguo Liang*
and Zhanchun Chen*

4533



Full control of the orientation of non-symmetric molecules using weak and moderate electric fields

Rosario González-Férez and Juan J. Omiste*

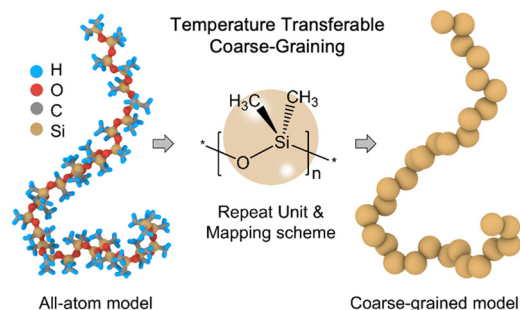


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4541

Energy renormalization for temperature transferable coarse-graining of silicone polymer

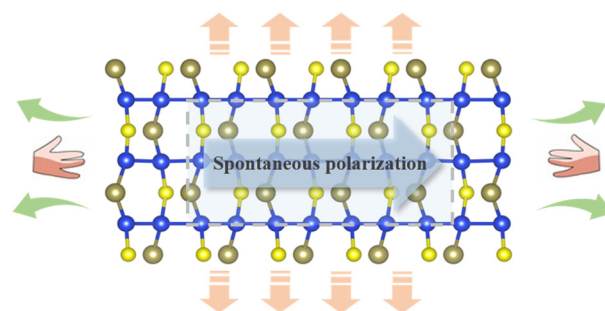
Dawei Zhang, Yang Wang, Maryam Safaripour, Daniel A. Bellido-Aguilar, Kurt R. Van Donselaar, Dean C. Webster, Andrew B. Croll and Wenjie Xia*



4555

First-principles prediction of ferroelectric Janus Si_2XY ($\text{X/Y} = \text{S/Se/Te}$, $\text{X} \neq \text{Y}$) monolayers with negative Poisson's ratios

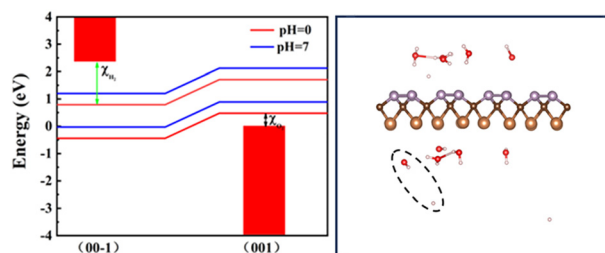
Yunlai Zhu, Zihan Qu, Jishun Zhang, Xiaoteng Wang, Shuo Jiang, Zuyu Xu, Fei Yang, Zuheng Wu* and Yuehua Dai*



4564

Janus monolayer PXC ($\text{X} = \text{As/Sb}$) for photocatalytic water splitting with a negative Poisson's ratio

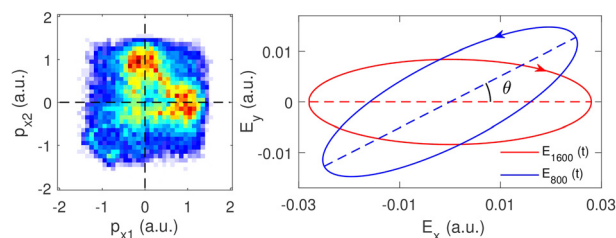
Yunlai Zhu, Shuo Jiang, Jishun Zhang, Zihan Qu, Zuheng Wu, Zuyu Xu, Wei Hu, Yuehua Dai and Fei Yang*



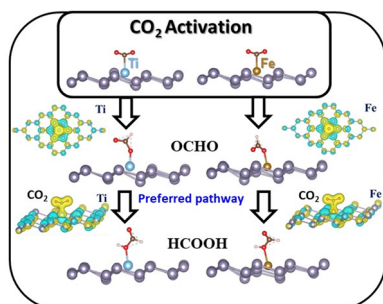
4572

The Coulomb effect in nonsequential double ionization by counter-rotating two-color elliptical polarization fields

Zichao Liu, Cheng Huang,* Tongtong He, Jianying Liao, Yingbin Li and Benhai Yu



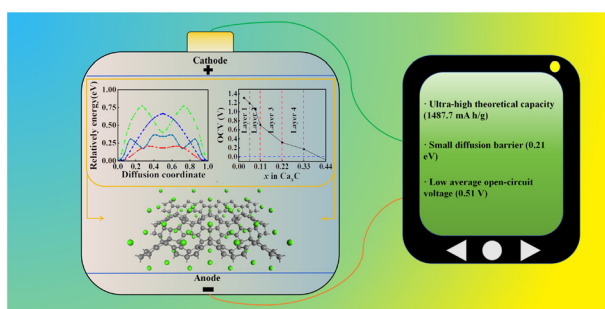
4579



A first-principles study of electro-catalytic reduction of CO₂ on transition metal-doped stanene

Sudatta Giri, Satyesh K. Yadav and Debolina Misra*

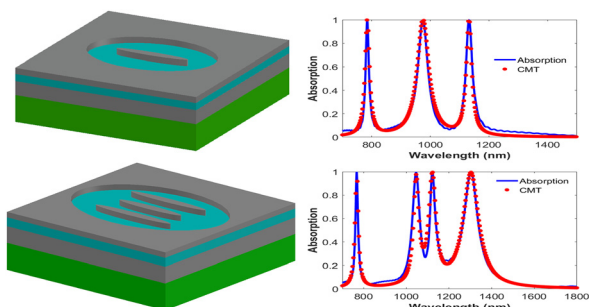
4589



Two-dimensional graphene+ as an anode material for calcium-ion batteries with ultra-high capacity: a first-principles study

Tao Yang, Tian-Ci Ma, Xiao-Juan Ye,* Xiao-Hong Zheng, Ran Jia, Xiao-Hong Yan and Chun-Sheng Liu*

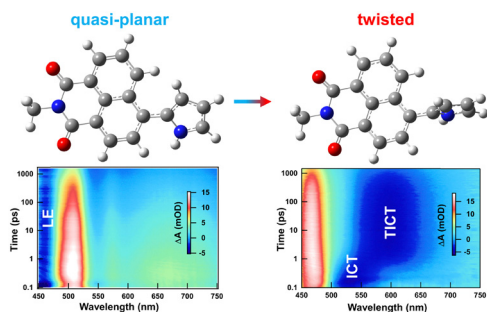
4597



Multi-band perfect absorber based on an elliptical cavity coupled with an elliptical metal nanorod

Yizhao Pan, Yuchang Li, Fang Chen,* Shubo Cheng, Wenxing Yang, Boyun Wang and Zao Yi

4607



Deciphering the photophysical properties of naphthalimide derivatives using ultrafast spectroscopy

Wei Zhang, Yalei Ma, Hongwei Song, Rong Miao,* Jie Kong* and Meng Zhou*

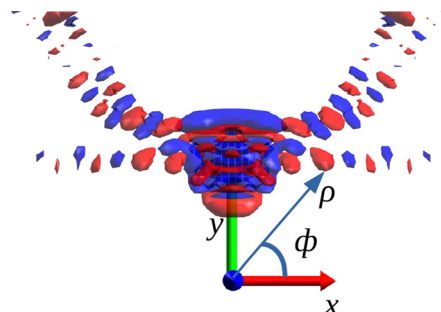


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4614

Lifetimes and decay mechanisms of isotopically substituted ozone above the dissociation threshold: matching quantum and classical dynamics

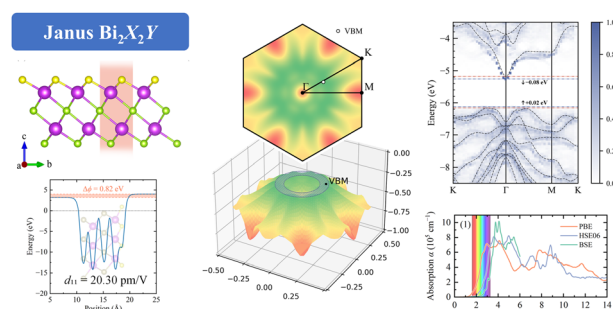
Viatcheslav Kokooouline,* Alexander Alijah and Vladimir Tyuterev



4629

The coexistence of high piezoelectricity and superior optical absorption in Janus $\text{Bi}_2\text{X}_2\text{Y}$ ($\text{X} = \text{Te, Se}$; $\text{Y} = \text{Te, Se, S}$) monolayers

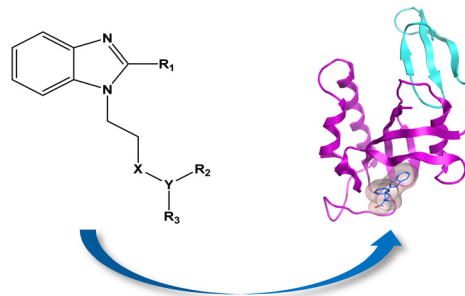
Shu-Hao Cao, Tian Zhang,* Hua-Yun Geng and Xiang-Rong Chen*



4643

Molecular docking, 3D-QASR and molecular dynamics simulations of benzimidazole Pin1 inhibitors

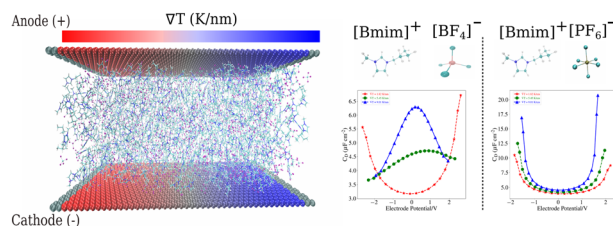
Min Liu, Bingli Wang, Huan Liu, Haolun Xia and Lina Ding*



4657

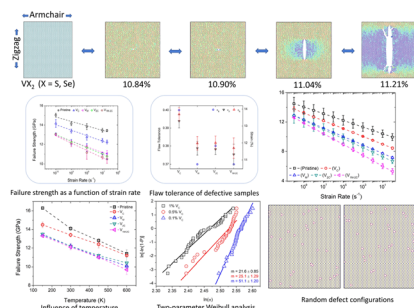
Temperature-dependent differential capacitance of an ionic liquid-graphene-based supercapacitor

Kiran Prakash and Sarith P. Sathian*



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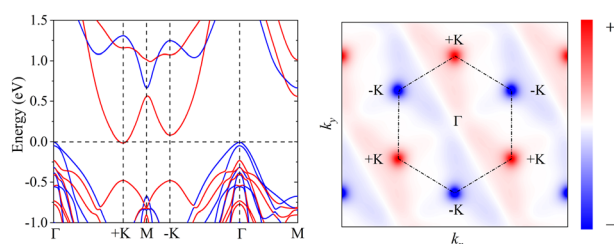
4668



Vacancy-mediated inelasticity in two-dimensional vanadium-based dichalcogenides

Akash Baski, Zimmi Singh and Sankha Mukherjee*

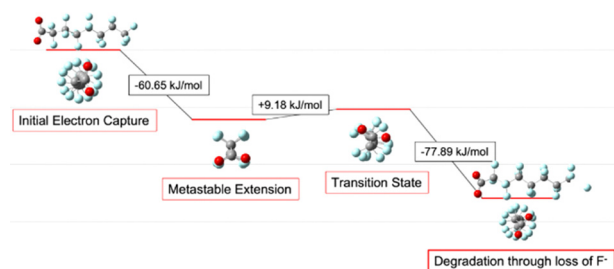
4683



Novel valley character and tunable quasi-half-valley metal state in Janus monolayer VSIGeP₄

Kang Jia, Xiao-Jing Dong, Sheng-Shi Li, Wei-Xiao Ji and Chang-Wen Zhang*

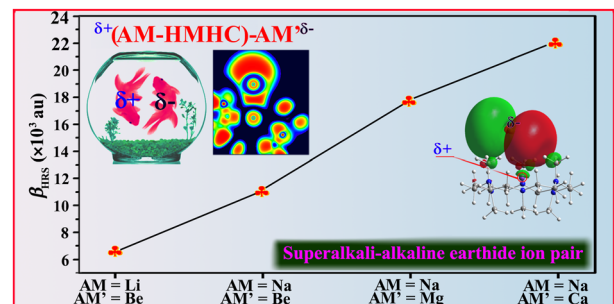
4692



The role of helicity in PFAS resistance to degradation: DFT simulation of electron capture and defluorination

Matt McTaggart and Cécile Malardier-Jugroot*

4702



Supercalculable alkaline earth ion pairs of δ^+ (AM-HMHC)- $\text{AM}'^{\delta-}$ (AM = Li, Na and K; AM' = Be, Mg and Ca) possessing large NLO responses and excellent electronic stabilities and alkali characteristics: a DFT study

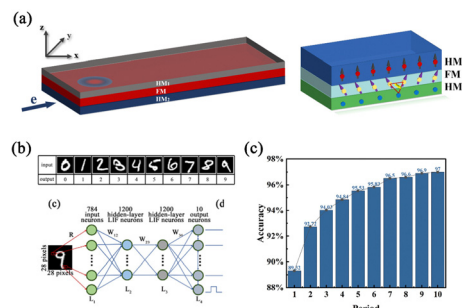
Jianguan Huang, Yin-Feng Wang,* Kai Yang, Wen Zhang, Zhi-Jun Wang, Xuexia Liu* and Zhi-Ru Li*



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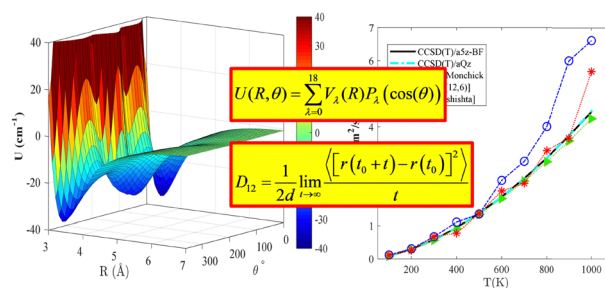
Optimizing skyrmionium movement and stability via stray magnetic fields in trilayer nanowire constructs

Bin Gong, Luowen Wang, Sunan Wang, Ziyang Yu,*
Lun Xiong, Rui Xiong, Qingbo Liu* and Yue Zhang

4724

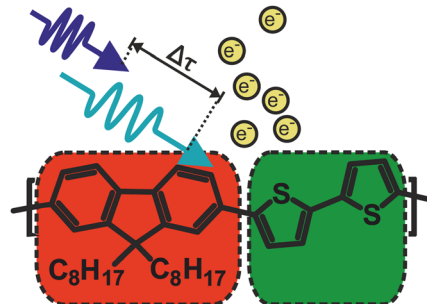
PES and transport properties of the He...HBr complex from kinetic theory and molecular dynamics simulations

Fatemeh Aghababaei and Ebrahim Nemati-Kande*



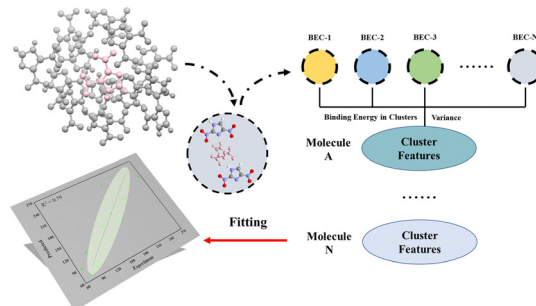
4736

Ultrafast electron dynamics in excited states of conjugated thiophene–fluorene organic polymer (pF8T2) thin films

T. Reiker,* Z. Liu, C. Winter, M. V. Cappellari,
D. Gonzalez Abradelo, C. A. Strassert, D. Zhang and
H. Zacharias

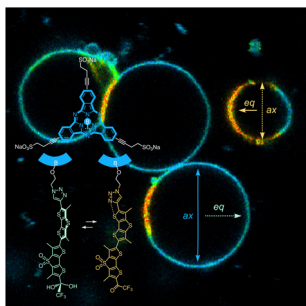
4752

Insight into melting point differences of dinitroimidazoles and dinitropyrazoles from the perspective of intermolecular interactions

Junnan Wu, Siwei Song, Xiujuan Qi,* Haijun Yang* and
Yi Wang*

RESEARCH PAPERS

4759



Subphthalocyanine-flipper dyads for selective membrane staining

José García-Calvo,* Xiao-Xiao Chen, Naomi Sakai, Stefan Matile and Tomás Torres*

CORRECTION

4766

Correction: Optical bands of dodecanuclear compounds $\text{H}_4\text{PVMo}_{11}\text{O}_{40} \cdot y\text{H}_2\text{O}$ with Keggin structure. Semiclassical vibronic model

S. Klokishner,* J. Melsheimer, F. C. Jentoft and R. Schlögl

