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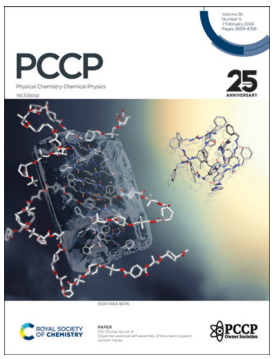

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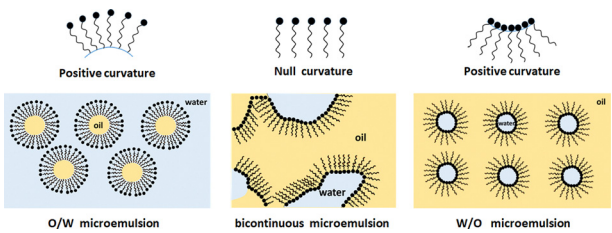
See Chi-Chung Hua *et al.*, pp. 3810–3814. Image reproduced by permission of Ching-Hung Wu and Chi-Chung Hua from *Phys. Chem. Chem. Phys.*, 2024, **26**, 3810.

REVIEWS

3699

Effect of polymer addition on the phase behavior of oil–water–surfactant systems of Winsor III type

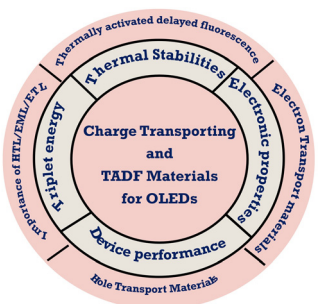
Ming Lu, Björn Lindman* and Krister Holmberg*



3711

Charge transporting and thermally activated delayed fluorescence materials for OLED applications

Krishan Kumar



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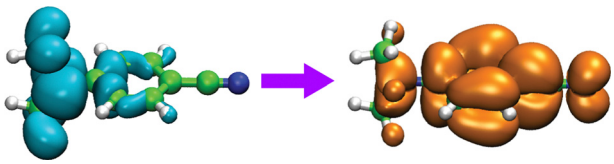
PERSPECTIVE

3755

Visualizing and characterizing excited states from time-dependent density functional theory

John M. Herbert

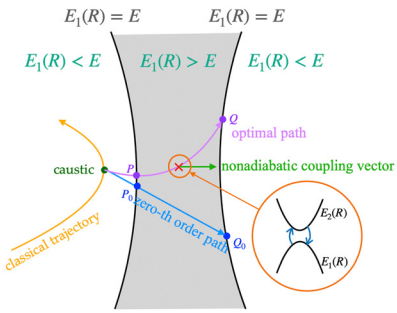


COMMUNICATIONS

3795

Classically forbidden nonadiabatic transitions in multidimensional chemical dynamics

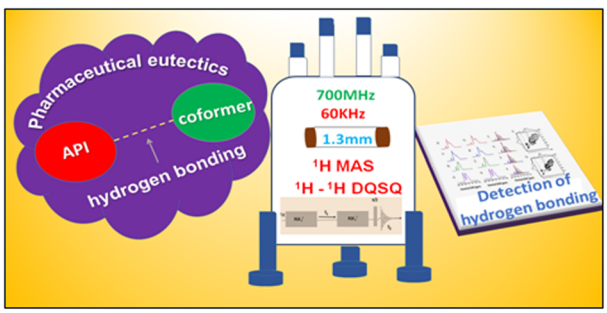
I-Yun Hsiao, Yoshiaki Teranishi* and Hiroki Nakamura



3800

A solid-state NMR method for characterization of pharmaceutical eutectics

Chaithanya Hareendran, Parth S. Shaligram, Rajesh Gonnade and T. G. Ajithkumar*



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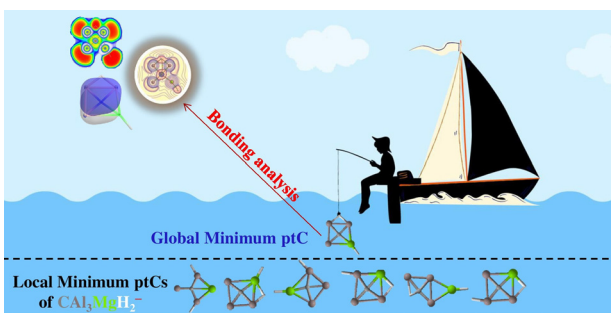
Global minimum and a heap of low-lying isomers with planar tetracoordinate carbon in the $CAl_3MgH_2^-$ system

Abdul Hamid Malhan and Krishnan Thirumoorthy*



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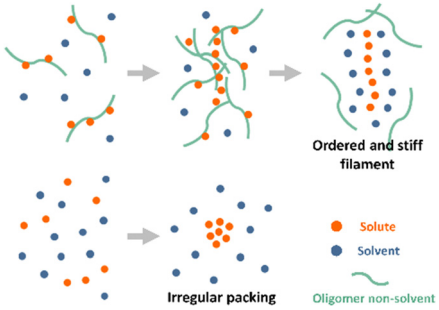

Oligomer-assisted self-assembly of bisurea in organic solvent media

Ching-Hung Wu, Ling-Hua Huang and Chi-Chung Hua*

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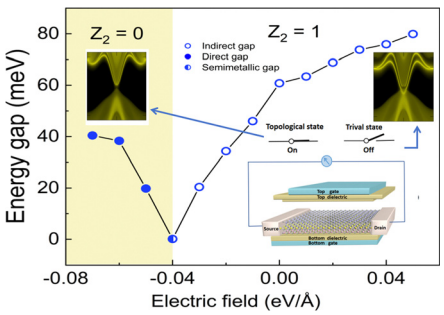
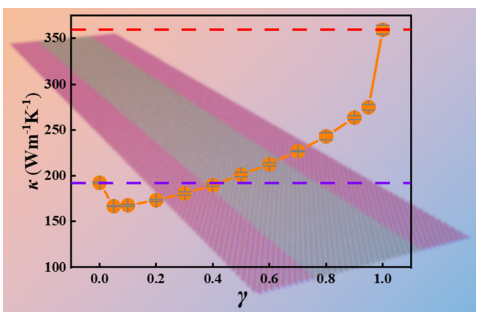


Ideal two-dimensional quantum spin Hall insulators MgA_2Te_4 (A = Ga, In) with Rashba spin splitting and tunable properties

Jiaqi Li, Xinlu Cheng and Hong Zhang*

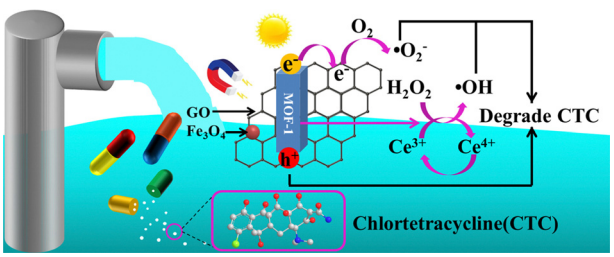
3823



Unexpected reduction in thermal conductivity observed in graphene/h-BN heterostructures

Zhang Wu, Rumeng Liu,* Ning Wei and Lifeng Wang

3832



A magnetically reusable Ce-MOF/GO/Fe_3O_4 composite for effective photocatalytic degradation of chlortetracycline

Yuting Bai, Derek Hao, Sisi Feng,* Liping Lu* and Qi Wang*

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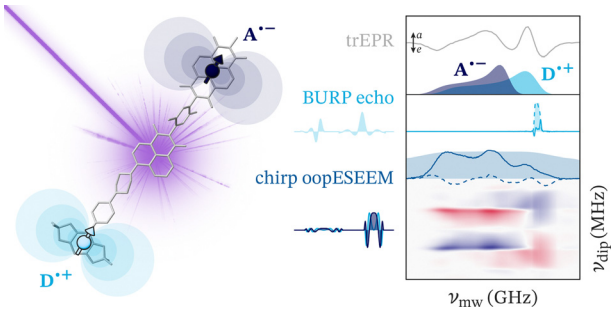
Control of excitation selectivity in pulse EPR on spin-correlated radical pairs with shaped pulses

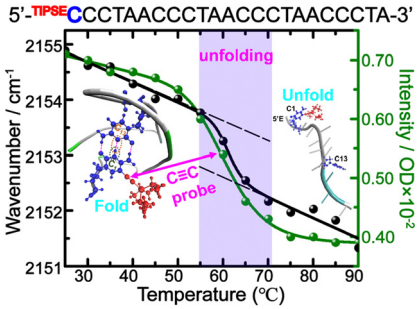
Daniele Panariti, Sarah M. Conron, Jinyuan Zhang, Michael R. Wasielewski, Marilena Di Valentin and Claudia E. Tait*



3857

Site specifically probing the unfolding process of human telomere i-motif DNA using vibrationally enhanced alkynyl stretch

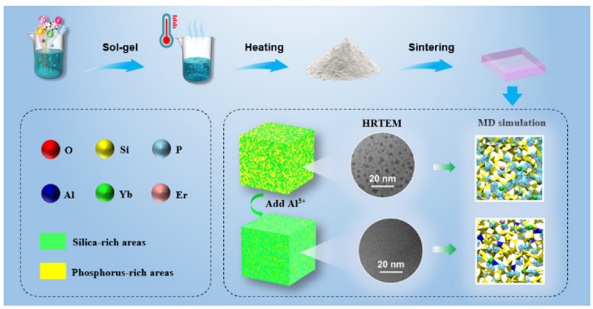
Tiantian Dong, Pengyun Yu, Juan Zhao and Jianping Wang*



3869

Theoretical and experimental investigation of Al^{3+} ion-suppressed phase-separation structures in rare-earth-doped high-phosphorus silica glasses

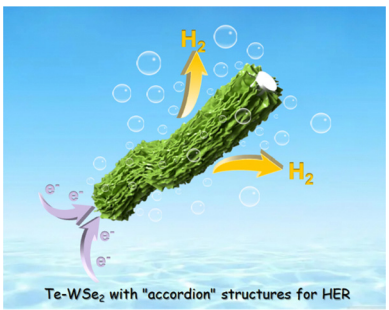
He-He Dong, Jin-Jun Ren, Ying-Gang Chen, Fan Wang, Dan-Ping Chen, Lu Deng, Chong-Yun Shao, Shi-Kai Wang,* Chun-Lei Yu* and Li-Li Hu*



3880

Te-doped-WSe_2/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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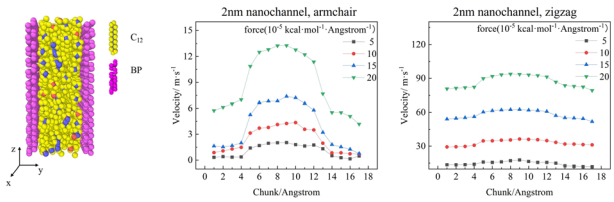

Anisotropic fluid flows in black phosphorus nanochannels

Ruda Jian, Shiwen Wu, Siyu Tian, Amirarsalan Mashhadian, Zhihao Xu, Stefano Leonardi, Tengfei Luo* and Guoping Xiong*

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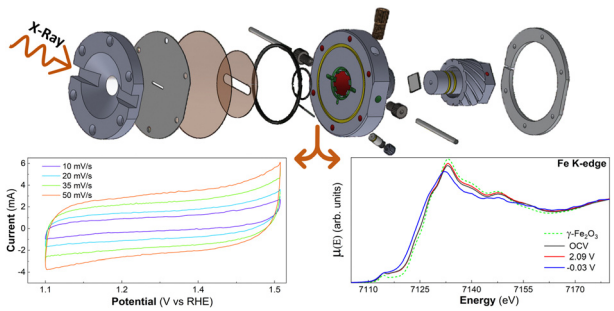
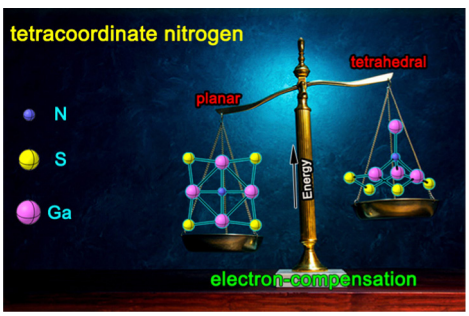


A novel electrochemical flow-cell for *operando* XAS investigations in X-ray opaque supports

Francesco Paparoni,* Guillaume Alizon, Andrea Zitolo, Seyed Javad Rezvani, Andrea Di Cicco, Hélène Magnan and Emiliano Fonda*

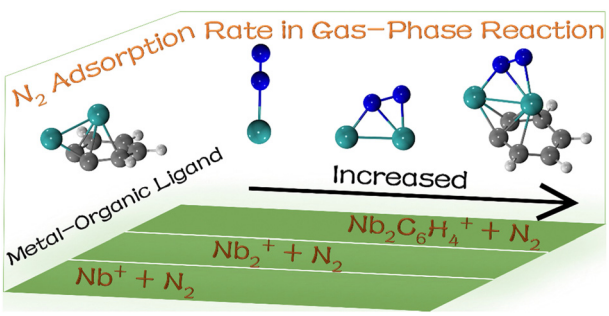
3907



Breaking the Hoff/Le Bel rule by an electron-compensation strategy: the global energy minimum of $NGa_4S_4^+$

Xiu-dong Jia* and Zhi-wei Du

3912



Nitrogen adsorption on $Nb_2C_6H_4^+$ cations: the important role of benzyne (*ortho*-C_6H_4)

Feng-Xiang Zhang, Yi-Heng Zhang, Ming Wang and Jia-Bi Ma*

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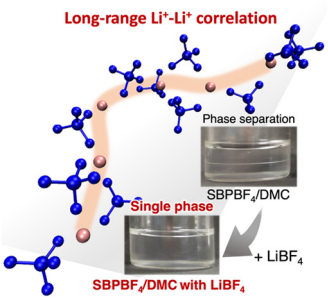
A structural study on a specific Li-ion ordered complex in dimethyl carbonate-based dual-cation electrolytes

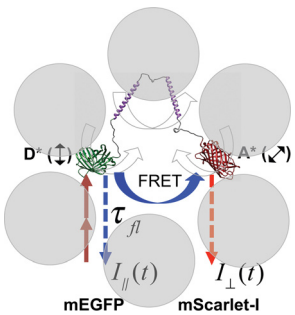
Yu Chikaoka,* Tomoya Tashiro, Saki Sawayama, Ayana Kobayashi, Ayuna Matsumoto, Etsuro Iwama, Katsuhiko Naoi* and Kenta Fujii*



3927

Two-photon excited-state dynamics of mEGFP-linker-mScarlet-I crowding biosensor in controlled environments

Sarah A. Mersch, Sarah Bergman, Erin D. Sheets, Arnold J. Boersma and Ahmed A. Heikal*



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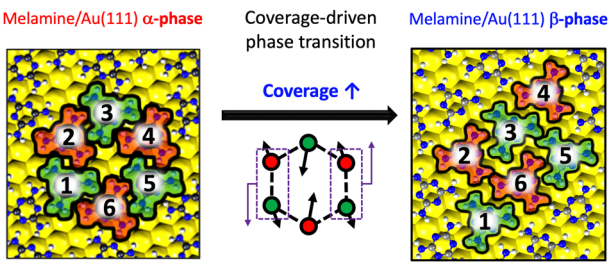
Transition mechanism of the coverage-dependent polymorphism of self-assembled melamine nanostructures on Au(111)

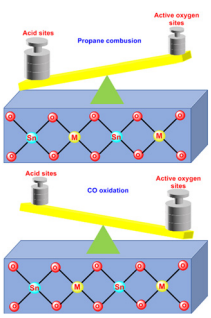
Jorge Manuel Zamalloa-Serrano, José María Gómez-Fernández, Carlos Sánchez-Sánchez, María Francisca López, José Ignacio Martínez,* José Ángel Martín-Gago and Irene Palacio*



3950

Doping SnO_2 with metal ions of varying valence states: discerning the importance of active surface oxygen species *vs.* acid sites for C_3H_8 and CO oxidation

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



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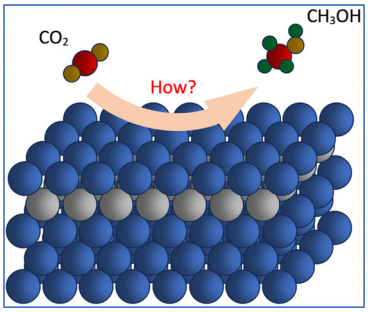
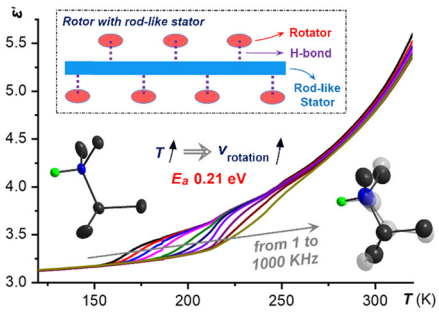


Carbon dioxide conversion to methanol on a PdCo bimetallic catalyst

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

3974



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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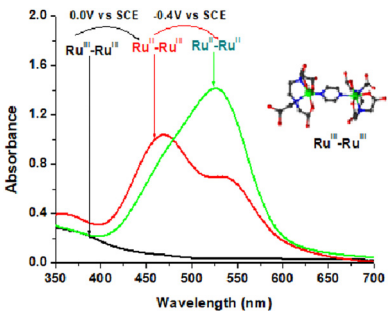
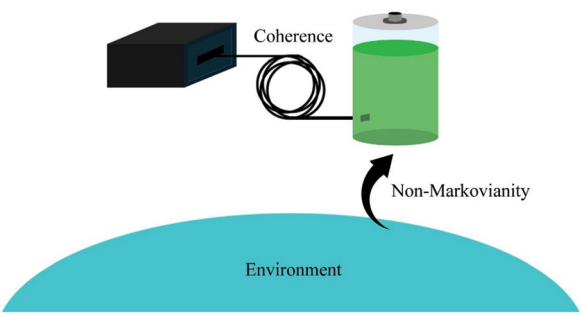


Redox reactions of a pyrazine-bridged Ru^{III}(edta) binuclear complex: spectrochemical, spectroelectrochemical and theoretical studies

Olga Impert,* Maciej Witwicki, Urszula K. Komarnicka, Alina Bieńko, Alessandro Niorettini and Debabrata Chatterjee*

3990



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

Amin Mohammadi and Afshin Shafiee*

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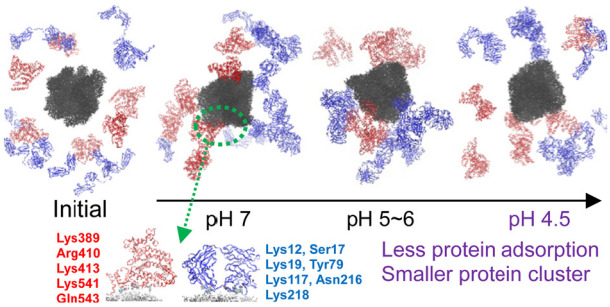
4000

Separation of protein corona from nanoparticles under intracellular acidic conditions: effect of protonation on nanoparticle–protein and protein–protein interactions

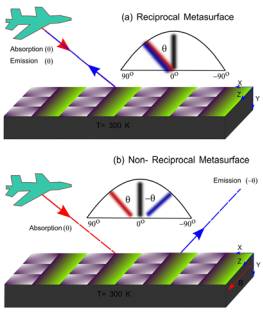
Hwankyu Lee



4011

Wide-angle camouflage detectors by manipulating emissivity using a non-reciprocal metasurface array

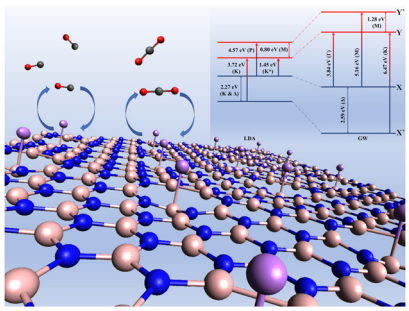
Bowei Zhang, Bin Wang and Sandeep Kumar Chamoli*



4021

Electronic, optical, and adsorption properties of Li-doped hexagonal boron nitride: a GW approach

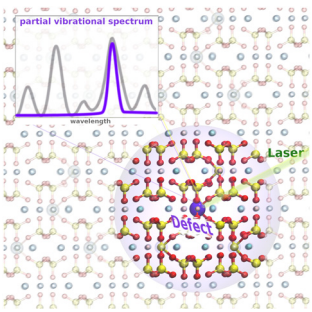
Dhanjit Talukdar,* Shilpi Stuti Bora and Gazi A. Ahmed



4029

Pure and Sc-doped diopside ($CaMgSi_2O_6$) vibrational spectra: modelling and experiments

Luca Bellucci,* Michele Cassetta, Henrik Skogby and Sabrina Nazzareni*



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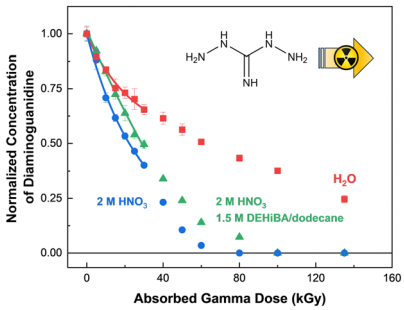
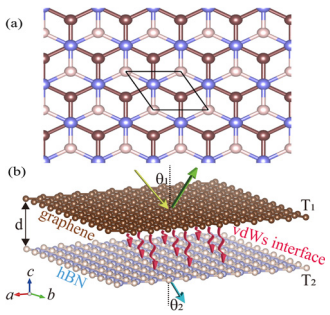


Radiolytic evaluation of a new technetium redox control reagent for advanced used nuclear fuel separations

Anh N. Dang, Maya H. Rogalski, Corey D. Pilgrim, Joseph R. Wilbanks, Dean R. Peterman, Jesse D. Carrie, Peter R. Zalupski, Stephen P. Mezyk* and Gregory P. Horne*

4047



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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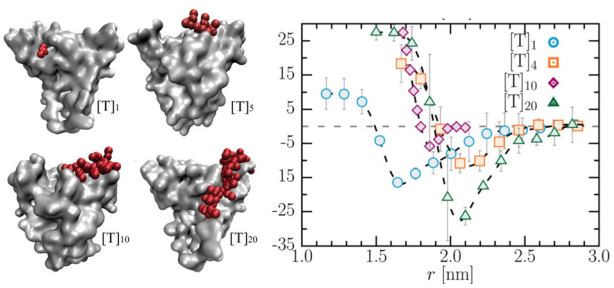
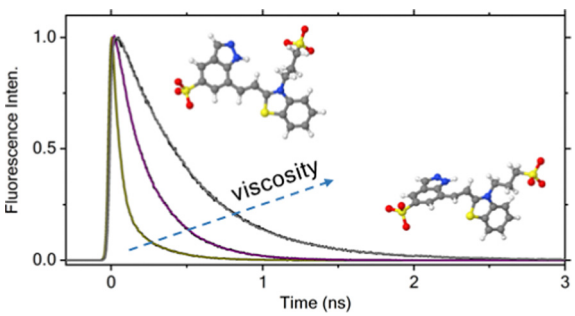


Control of polymer–protein interactions by tuning the composition and length of polymer chains

Menghan Xie, Xu Jia* and Xiao Xu*

4062



Unravelling photoisomerization dynamics in a metastable-state photoacid

Ying-Zhong Ma,* Uvinduni I. Premadasa, Vyacheslav S. Bryantsev, Audrey R. Miles, Ilia N. Ivanov, Adnan Elgattar, Yi Liao and Benjamin Doughty

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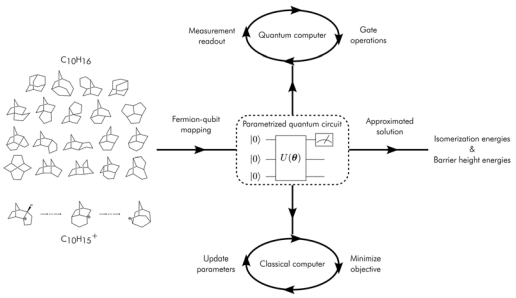
Applications of noisy quantum computing and quantum error mitigation to "adamantaneland": a benchmarking study for quantum chemistry

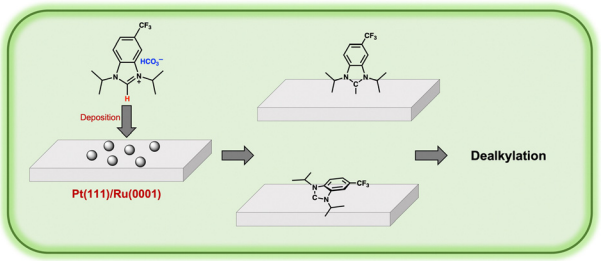
Viki Kumar Prasad, Freeman Cheng, Ulrich Fekl* and Hans-Arno Jacobsen*



4083

N-heterocyclic carbene adsorption states on Pt(111) and Ru(0001)

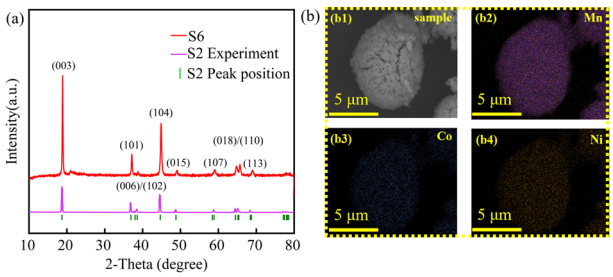
Tianchi Zhang, Sonali B. Khomane, Ishwar Singh, Cathleen M. Crudden* and Peter H. McBreen*



4091

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

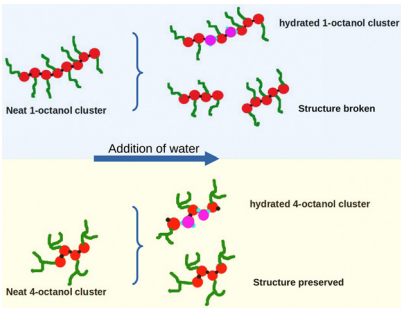
Chengbin Yin, Keyang Wu, Chengzhou Liu, Beibei Ma, Ju Rong* and Yuan Wang*



4099

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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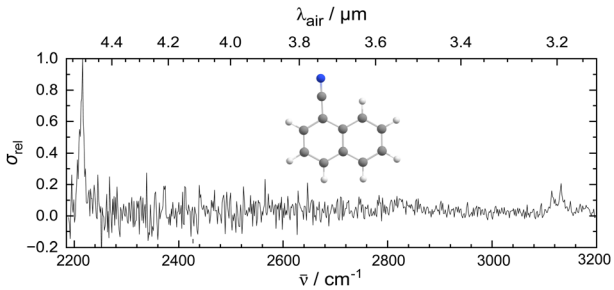
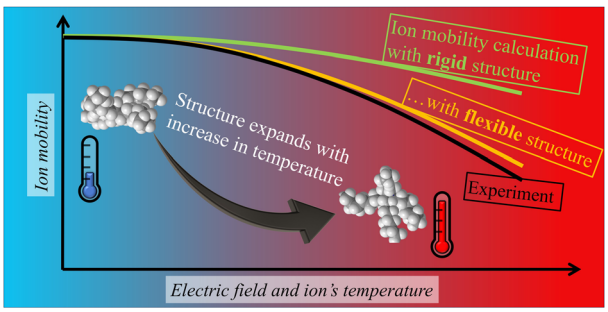
4111



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

Julianna Palotás, Francis C. Daly, Thomas E. Douglas-Walker and Ewen K. Campbell*

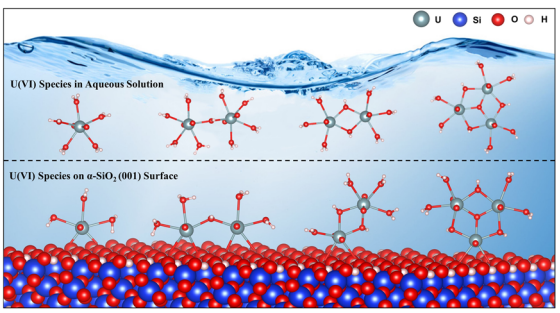
4118



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

Farah Mubas-Sirah, Viraj D. Gandhi, Mohsen Latif, Leyan Hua, Amirreza Tootchi and Carlos Larriba-Andaluz*

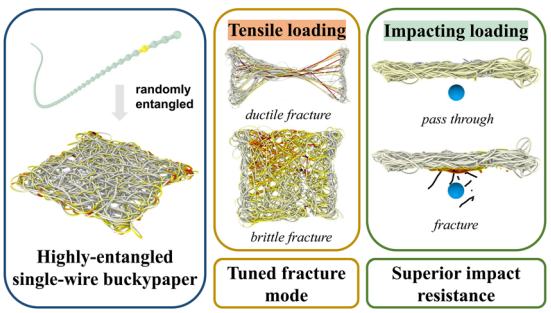
4125



Structures of multinuclear U(VI) species on the hydroxylated α-SiO_2(001) surface: insights from DFT calculations

Pengyuan Gao, Qiang Jin, Zongyuan Chen, Dongqi Wang, Christophe Tournassat and Zhijun Guo*

4135



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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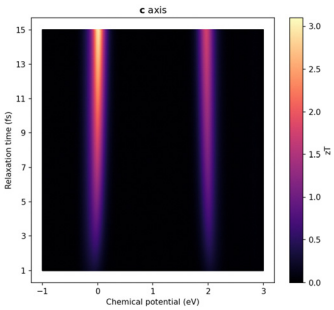
4144

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

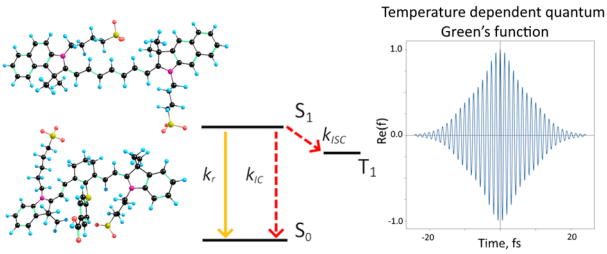
Anderson Silva Chaves, Murilo Aguiar Silva and Alex Antonelli*



4151

Intramolecular rate-constant calculations based on the correlation function using temperature dependent quantum Green's functions

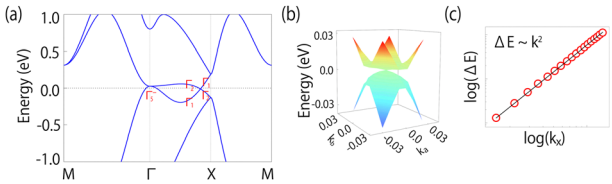
R. R. Valiev,* B. S. Merzlikin, R. T. Nasibullin, V. N. Cherepanov, D. Sundholm and T. Kurtén



4159

Two-dimensional quadratic Weyl points, nodal loops, and spin–orbit Dirac points in PtS, PtSe, and PtTe monolayers

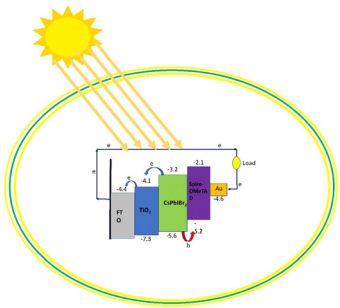
Jin-Yang Li, Xin-Yue Kang, Ying Zhang, Si Li* and Yugui Yao



4166

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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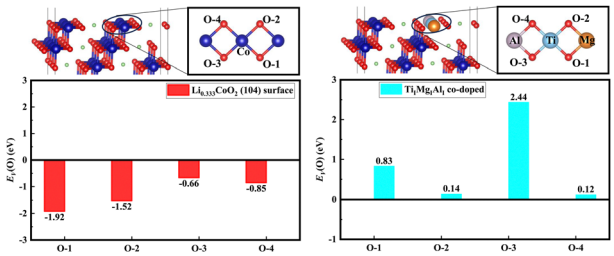
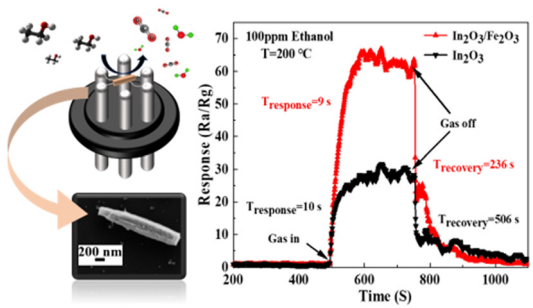
4174



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*

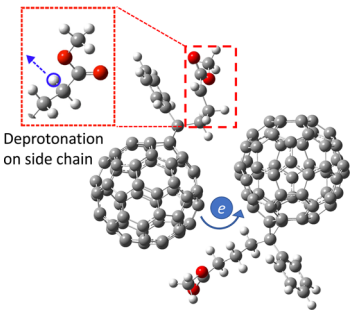
4184



In-MIL-68 derived In_2O_3/Fe_2O_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*

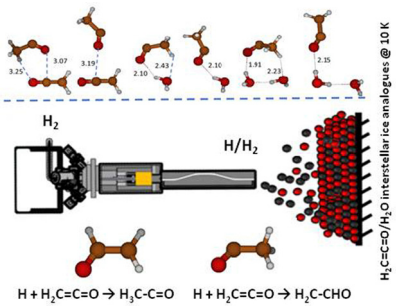
4194



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

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

4200



The significant role of water in reactions occurring on the surface of interstellar ice grains: Hydrogenation of pure ketene $H_2C{=}C{=}O$ ice *versus* hydrogenation of mixed $H_2C{=}C{=}O/H_2O$ ice at 10 K

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

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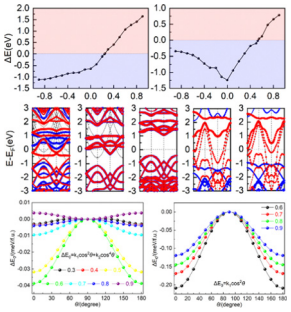
4208

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

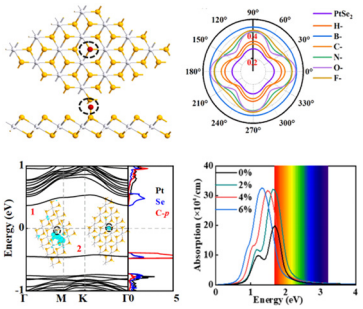
Ziyuan An, Linhui Lv, Ya Su,* Yanyan Jiang and Zhaoyong Guan*



4218

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

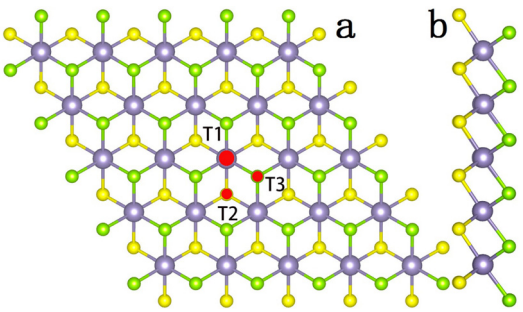
Xinyan Li, Zhanhai Li,* Jianing Han, Shengguo Cao and Zhenhua Zhang*



4231

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

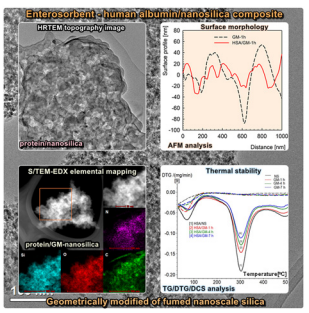
Bin Xu,* Cheng Qian, Zheng Wang, Jing Zhang, Shanshan Ma, Yusheng Wang and Lin Yi



4240

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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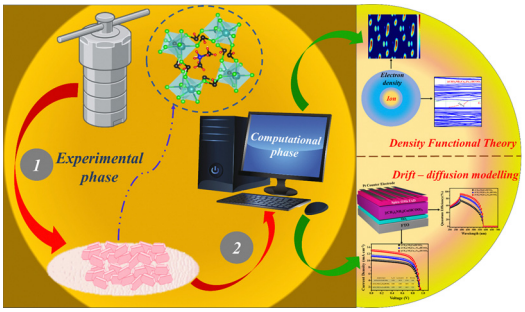
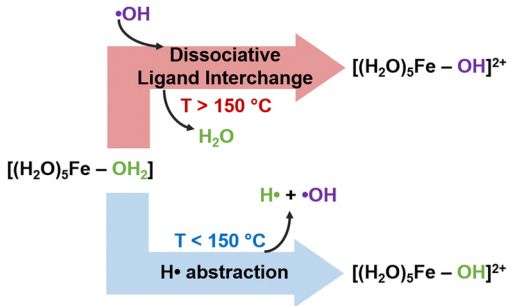
4262



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*

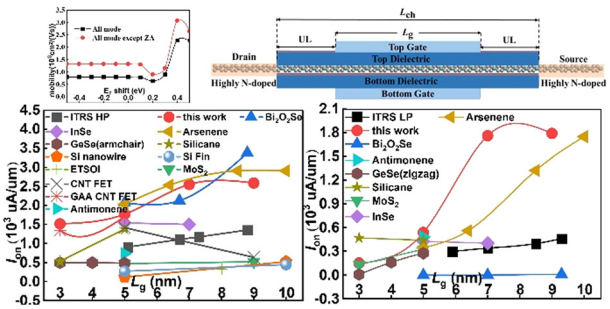
4278



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

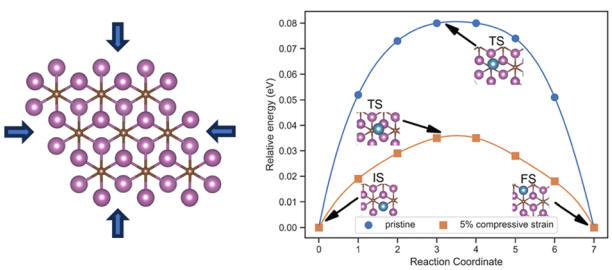
4284



Comprehensive understanding of electron mobility and superior performance in sub-10 nm DG ML tetrahex-GeC_2 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 Sc_2C: 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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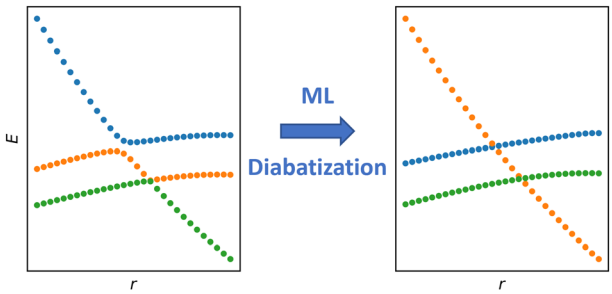
4306

Fast and accurate excited states predictions: machine learning and diabatization

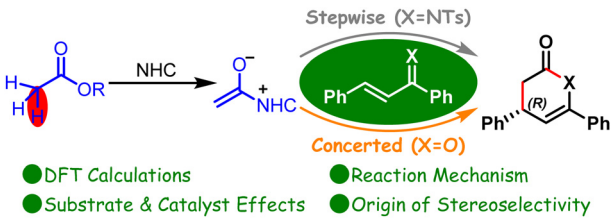
Štěpán Sršeň,* O. Anatole von Lilienfeld and Petr Slavíček*



4320

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

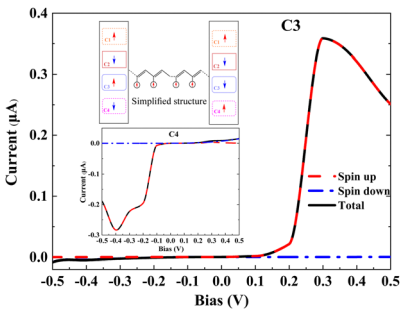
Pingxin Liang, Haoran Yang* and Yang Wang*



4329

Molecular rectification induced by magnetization alignment in organic-ferromagnetic devices

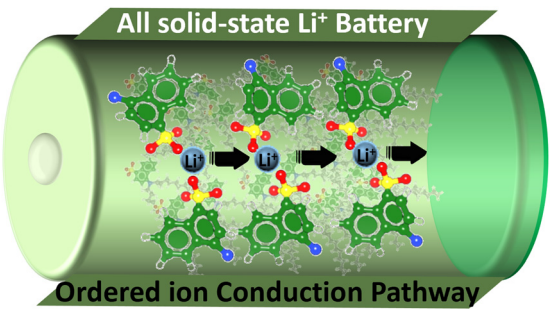
H. Ma, H. X. Li, H. Q. Zhang, Y. Wang, J. T. Li, C. Wang, J. F. Ren and G. C. Hu*



4338

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

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



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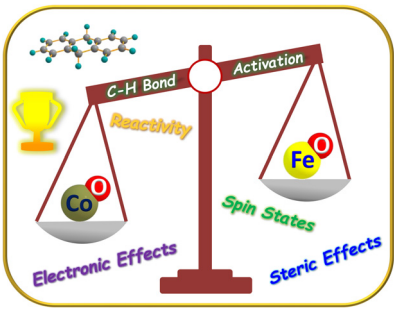
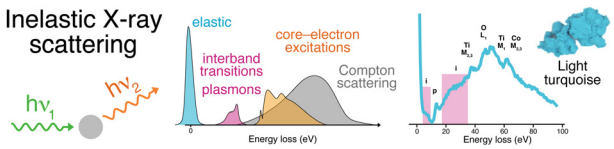


C–H bond activation by high-valent iron/cobalt–oxo complexes: a quantum chemical modeling approach

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

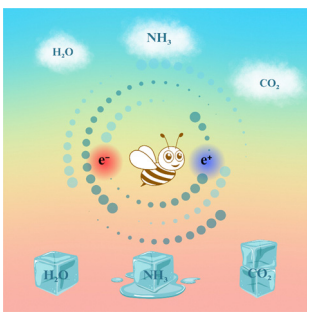
4363



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*

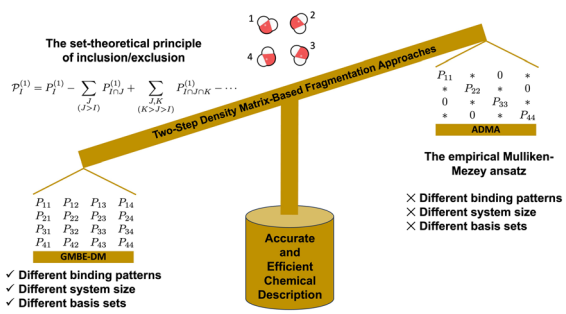
4372



Electron- and positron-driven molecular processes for H_2O, CO_2, and NH_3 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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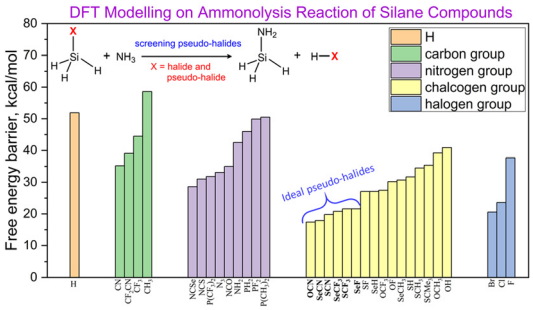
4395

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

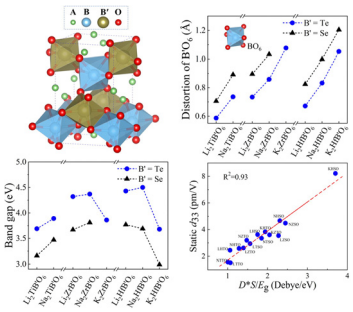
Anil Kumar Tummanapelli, Yingqian Chen and Ming Wah Wong*



4403

Investigation of nonlinear optical properties in α-$A_2BB'O_6$ (A = Li, Na, K; B = Ti, Zr, Hf; B′ = Se, Te) by first-principles calculations

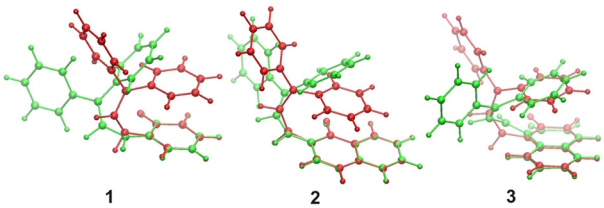
Gaojing Fang, Xiaojun Teng, Luo Yan, Yu Wu, Kui Xue, Xiaofeng Zhang, Yi-min Ding,* Liujiang Zhou* and Qiye Wen*



4412

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

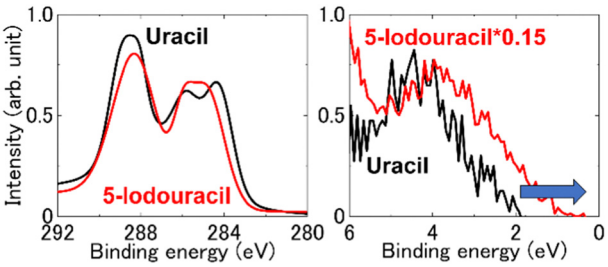
Daiana S. Tabirja and Victor V. Kostjukov*



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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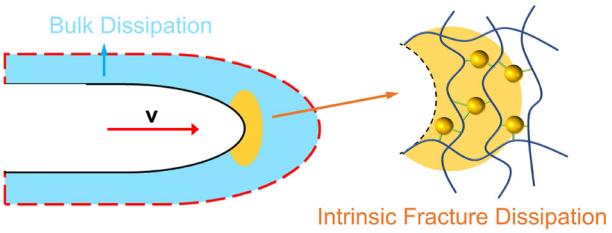
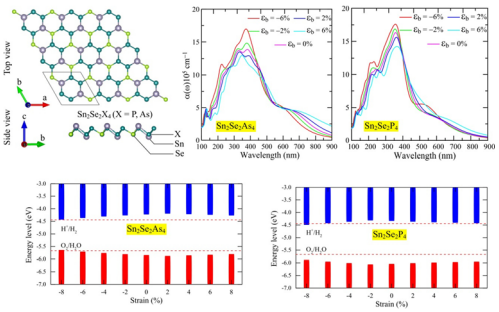


Insight into the fracture energy dissipation mechanism in elastomer composites *via* sacrificial bonds and fillers

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

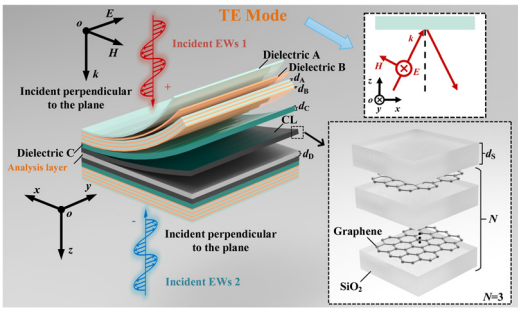
4437



First principles study of strain effects on prospective 2D photocatalysts $Sn_2Se_2X_4$ (X = P, As) with ultra-high charge carrier mobility

Pham D. Trung* and Hien D. Tong*

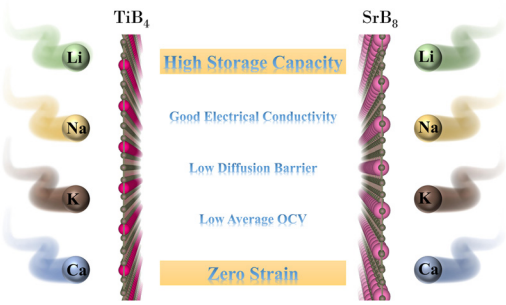
4447



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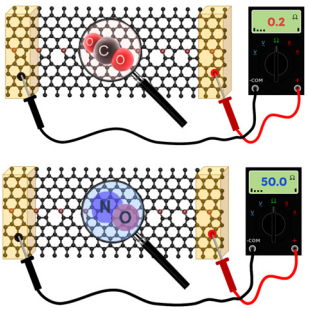
Boron-doped graphene topological defects: unveiling high sensitivity to NO molecule for gas sensing applications

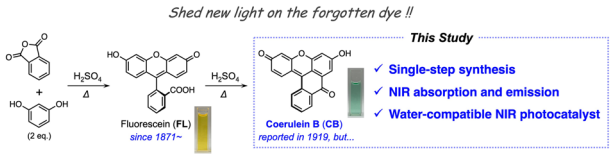
B. Keshav Rao, Tadeu Luiz Gomes Cabral, Debora Carvalho de Melo Rodrigues, Fábio A. L. de Souza, Wanderlã L. Scopel, Rodrigo G. Amorim* and Ravindra Pandey



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*



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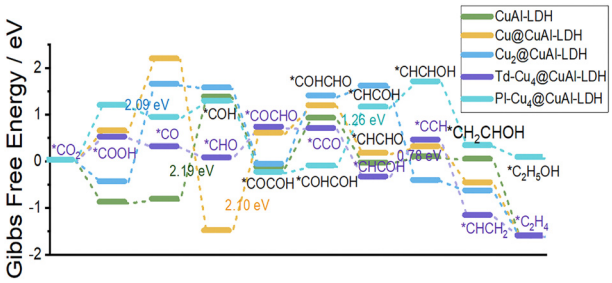
Theoretical study on electrocatalytic carbon dioxide reduction over copper with copper-based layered double hydroxides

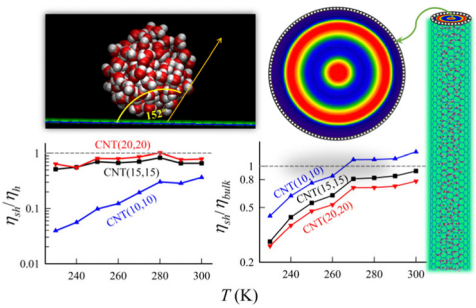
Xin-Yu Xu, Jing-Yi Guo, Wei Zhang, Yao Jie, Hui-Ting Song, Hao Lu, Yi-Fan Zhang, Jia Zhao, Chen-Xu Hu and Hong Yan*



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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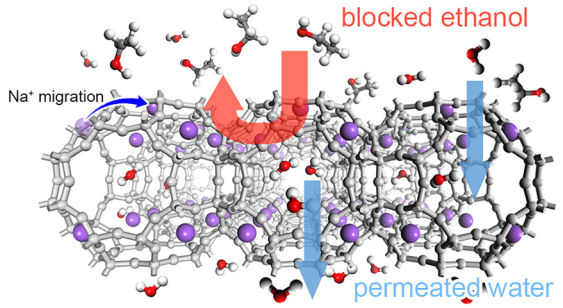
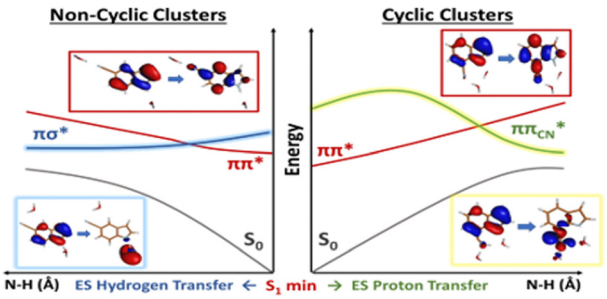


Computational understanding of Na-LTA for ethanol–water separation

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

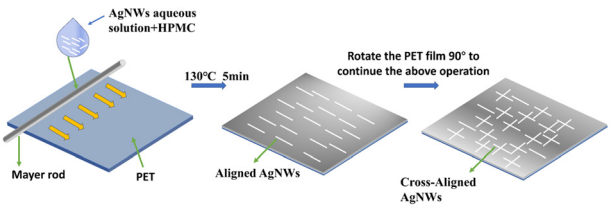
4511



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

Salsabil Abou-Hatab and Spiridoula Matsika*

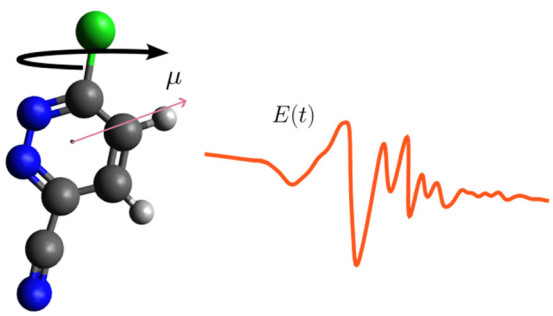
4524



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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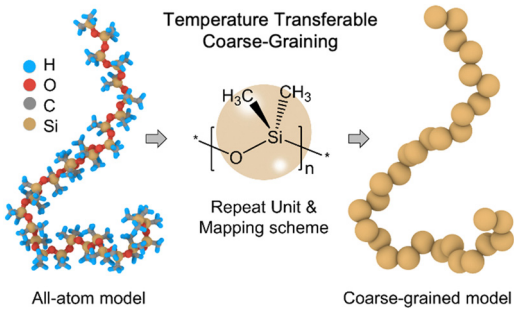
4541

Energy renormalization for temperature transferable coarse-graining of silicone polymer

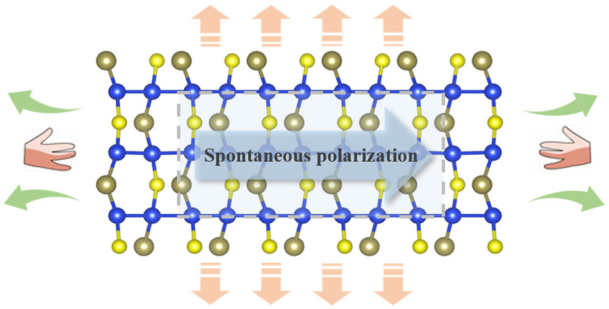
Dawei Zhang, Yang Wang, Maryam Safaripour, Daniel A. Bellido-Aguilar, Kurt R. Van Donselaar, Dean C. Webster, Andrew B. Croll and Wenjie Xia*



4555

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

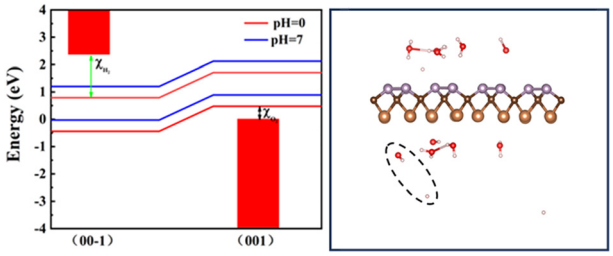
Yunlai Zhu, Zihan Qu, Jishun Zhang, Xiaoteng Wang, Shuo Jiang, Zuyu Xu, Fei Yang, Zuheng Wu* and Yuehua Dai*



4564

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

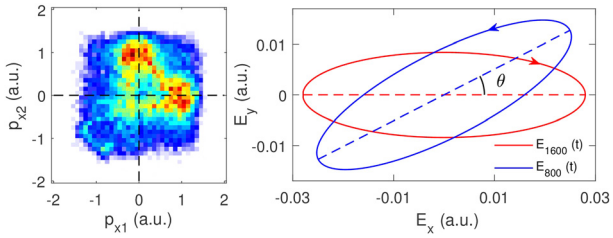
Yunlai Zhu, Shuo Jiang, Jishun Zhang, Zihan Qu, Zuheng Wu, Zuyu Xu, Wei Hu, Yuehua Dai and Fei Yang*



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



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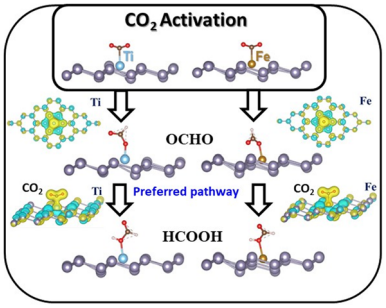
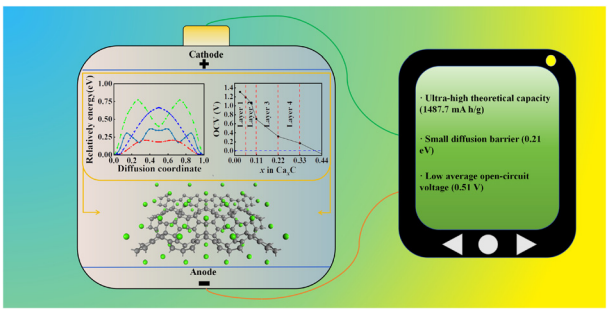


A first-principles study of electro-catalytic reduction of CO_2 on transition metal-doped stanene

Sudatta Giri, Satyesh K. Yadav and Debolina Misra*

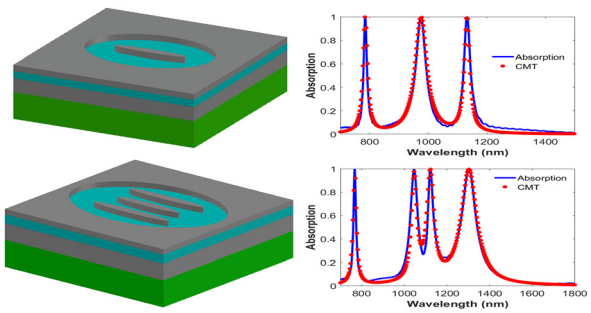
4589



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*

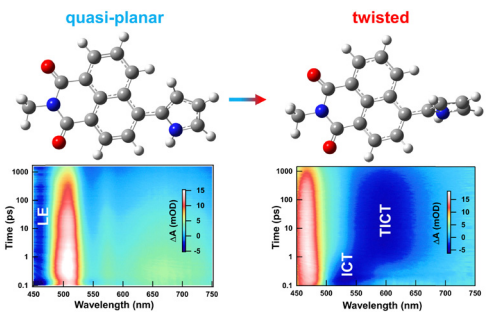
4597



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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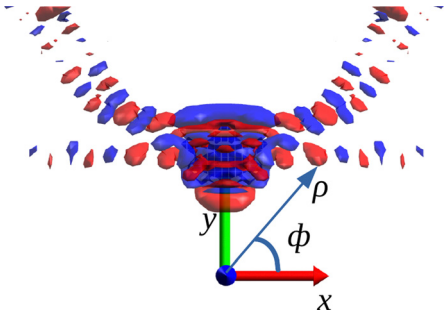
4614

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

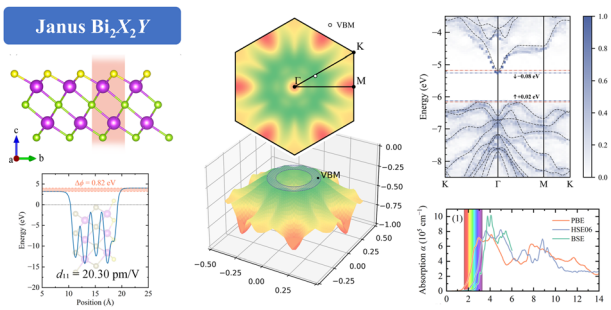
Viatcheslav Kokoouline,* Alexander Alijah and Vladimir Tyuterev



4629

The coexistence of high piezoelectricity and superior optical absorption in Janus Bi_2X_2Y (X = Te, Se; Y = Te, Se, S) monolayers

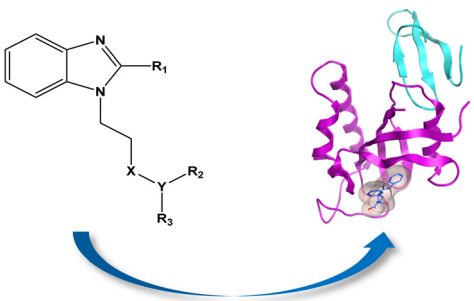
Shu-Hao Cao, Tian Zhang,* Hua-Yun Geng and Xiang-Rong Chen*



4643

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

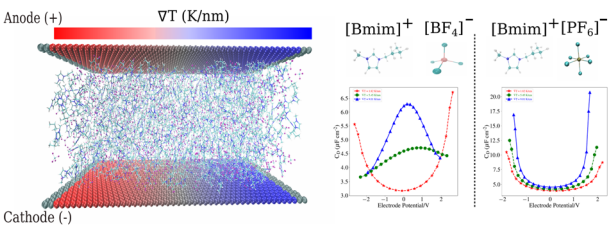
Min Liu, Bingli Wang, Huan Liu, Haolun Xia and Lina Ding*



4657

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

Kiran Prakash and Sarith P. Sathian*



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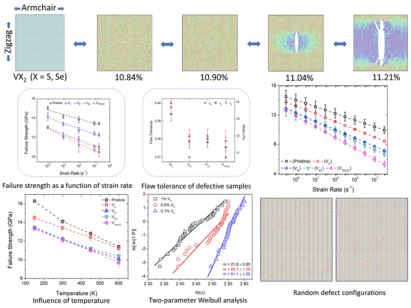
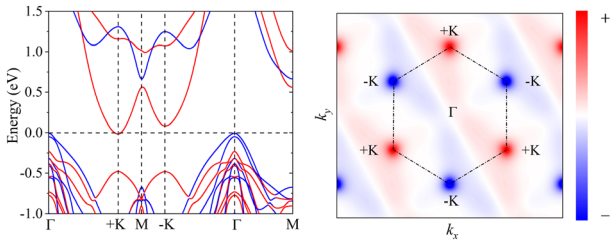


Vacancy-mediated inelasticity in two-dimensional vanadium-based dichalcogenides

Akash Baski, Zimmi Singh and Sankha Mukherjee*

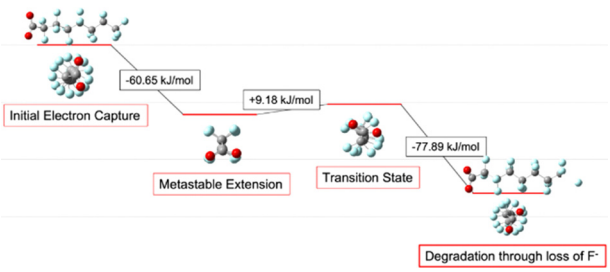
4683



Novel valley character and tunable quasi-half-valley metal state in Janus monolayer $VSiGeP_4$

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

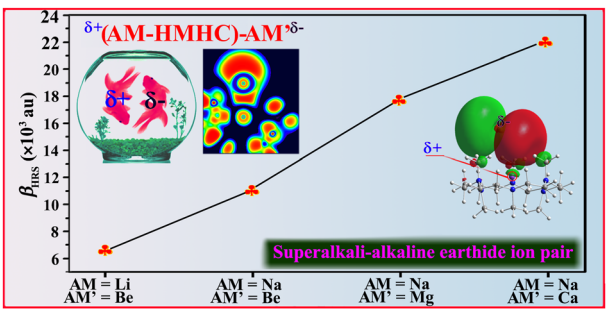
4692



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

Matt McTaggart and Cécile Malardier-Jugroot*

4702



Superalkali-alkaline earthide ion pairs of $^{\delta+}$(AM-HMHC)-AM′$^{\delta-}$ (AM = Li, Na and K; AM′ = Be, Mg and Ca) possessing large NLO responses and excellent electronic stabilities and alkalide characteristics: a DFT study

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

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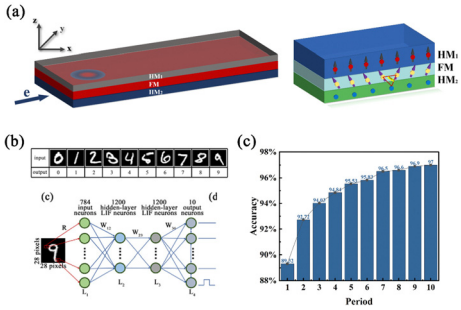
4716

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

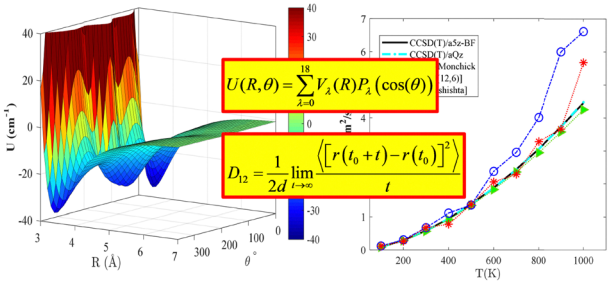
Bin Gong, Luowen Wang, Sunan Wang, Ziyang Yu,* Lun Xiong, Rui Xiong, Qingbo Liu* and Yue Zhang



4724

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

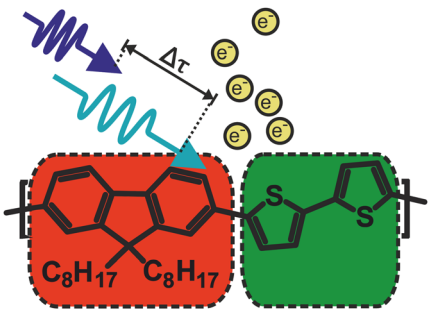
Fatemeh Aghababaei and Ebrahim Nemati-Kande*



4736

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

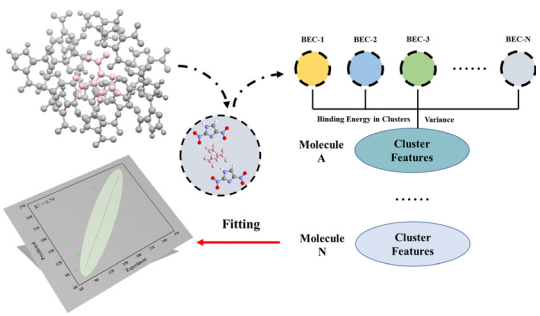
T. Reiker,* Z. Liu, C. Winter, M. V. Cappellari, D. Gonzalez Abradelo, C. A. Strassert, D. Zhang and H. Zacharias



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*



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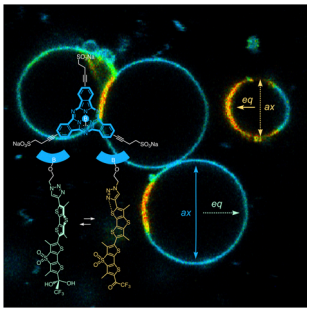

Subphthalocyanine-flipper dyads for selective membrane staining

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

CORRECTION

4766

Correction: Optical bands of dodecanuclear compounds $H_4PVMo_{11}O_{40}\cdot yH_2O$ with Keggin structure. Semiclassical vibronic model

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

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