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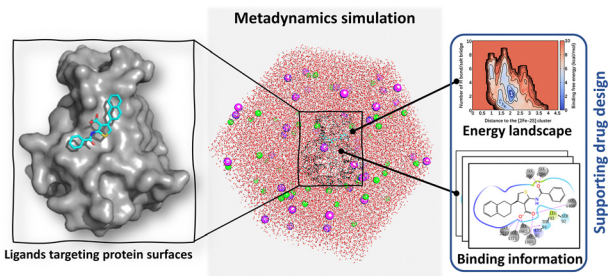
Cover
See Yu Wang and Kazuyuki Takeda, pp. 13838–13845. Image reproduced by permission of Art Action Inc. from *Phys. Chem. Chem. Phys.*, 2023, **25**, 13838.

PERSPECTIVES

13819

Metadynamics simulations of ligands binding to protein surfaces: a novel tool for rational drug design

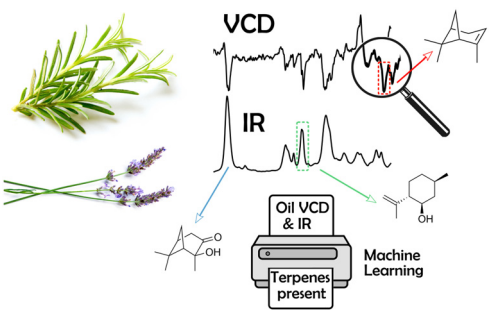
Ke Zuo, Agata Kranjc, Riccardo Capelli, Giulia Rossetti, Rachel Nechushtai and Paolo Carloni*



13825

Pushing the boundaries of VCD spectroscopy in natural product chemistry

Tom Vermeyen, Andrea N. L. Batista, Alessandra L. Valverde, Wouter Herrebout* and João M. Batista Jr.*



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COMMUNICATION

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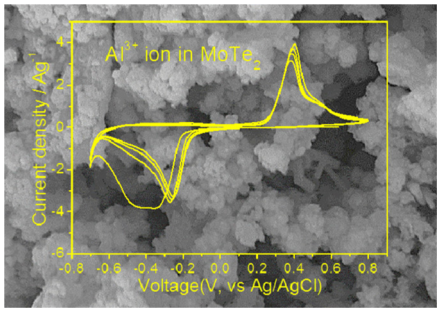
Investigation of reversible metal ion (Li^+, Na^+, Mg^{2+}, Al^{3+}) insertion in $MoTe_2$ for rechargeable aqueous batteries

Sunny Nandi, Yichen Yan, Xintong Yuan, Chongzhen Wang, Ximin He, Yuzhang Li* and Shyamal K. Das*



RESEARCH PAPERS

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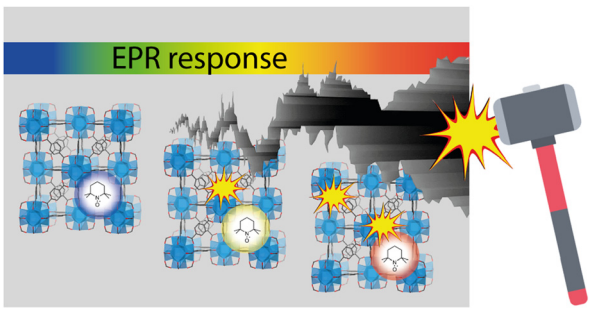
Double nutation cross-polarization between heteronuclear spins in solids

Yu Wang and Kazuyuki Takeda*

13846

UiO-66 framework with an encapsulated spin probe: synthesis and exceptional sensitivity to mechanical pressure

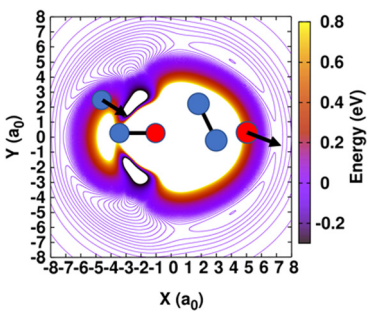
Artem S. Poryvaev,* Kirill P. Larionov, Yana N. Albrekht, Alexander A. Efremov, Alexey S. Kiryutin, Kristina A. Smirnova, Vasiliy Y. Evtushok and Matvey V. Fedin*



13854

Low-temperature kinetics for the N + NO reaction: experiment guides the way

Kevin M. Hickson,* Juan Carlos San Vicente Veliz, Debasish Koner and Markus Meuwly*



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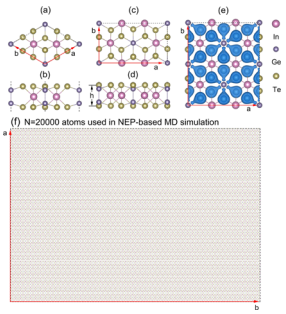
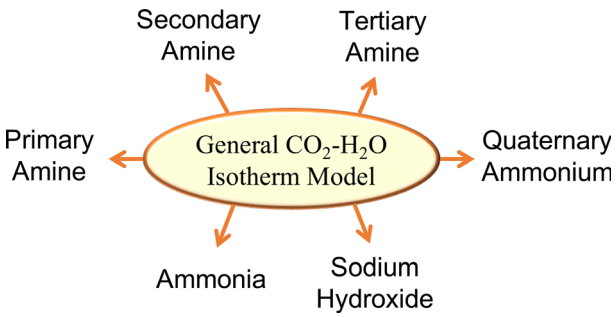


Investigation of the mechanical and transport properties of $InGeX_3$ (X = S, Se and Te) monolayers using density functional theory and machine learning

Yong-Bo Shi, Yuan-Yuan Chen, Hao Wang, Shuo Cao, Yuan-Xu Zhu, Meng-Fan Chu, Zhu-Feng Shao, Hai-Kuan Dong* and Ping Qian*

13877



A general binary isotherm model for amines interacting with CO_2 and H_2O

Yuta Kaneko* and Klaus S. Lackner*

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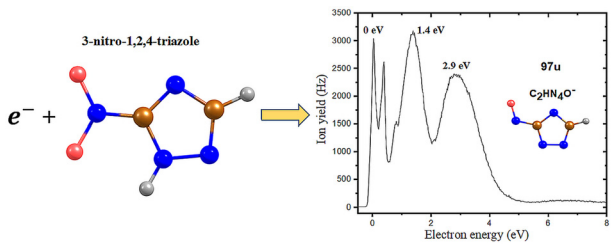

Decomposition of triazole and 3-nitrotriazole upon low-energy electron attachment

Muhammad Saqib, Farhad Izadi, Leon U. Isierhienrhien, Milan Ončák* and Stephan Denifl*

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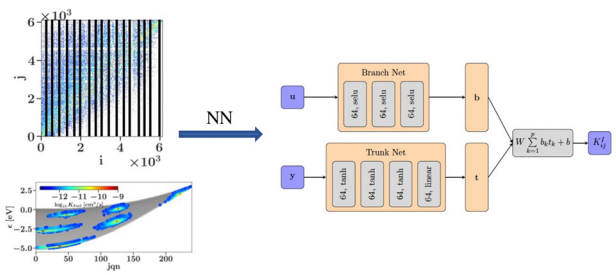

Efficient quasi-classical trajectory calculations by means of neural operator architectures

Maitreyee Sharma Priyadarshini, Simone Venturi, Ivan Zanardi and Marco Panesi*

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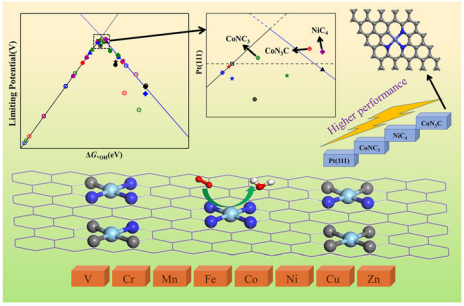
Exploring the catalytic activity of graphene-based TM-N_xC_{4-x} single atom catalysts for the oxygen reduction reaction *via* density functional theory calculation

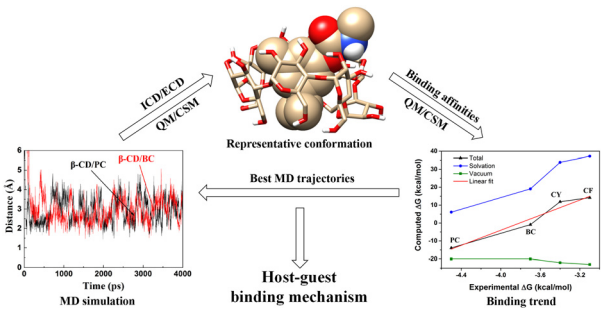
Zhengwei Du, Kaiming Deng, Erjun Kan and Cheng Zhan*



13923

How are *N*-methylcarbamates encapsulated by β-cyclodextrin: insight into the binding mechanism

Xiaofang Bao, Xiao Liu, Ran Dou, Sen Xu, Dabin Liu, Jun Luo, Xuedong Gong, Chung F. Wong and Baojing Zhou*



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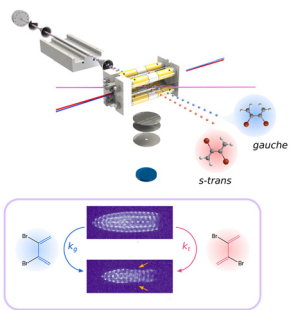
Conformational and state-specific effects in reactions of 2,3-dibromobutadiene with Coulomb-crystallized calcium ions

Ardita Kilaj, Silvan Käser, Jia Wang, Patrik Straňák, Max Schwilk, Lei Xu, O. Anatole von Lilienfeld, Jochen Küpper,* Markus Meuwly* and Stefan Willitsch*



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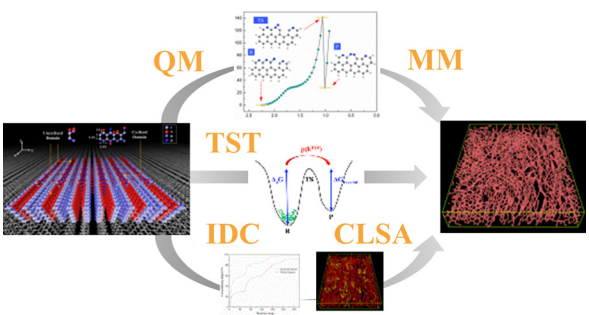
Insights into the carbonization mechanism of PAN-derived carbon precursor fibers and establishment of a kinetics-driven accelerated reaction template for atomistic simulation

Pengcheng Shi, Yingdan Zhu,* Haibing Xu, Chun Yan, Dong Liu, Lingyu Yue and Gang Chen



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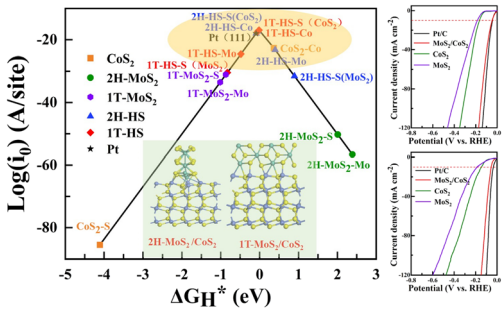

Interface prompted highly efficient hydrogen evolution of MoS_2/CoS_2 heterostructures in a wide pH range

Tian Wang, Pu Chang, Zhipeng Sun, Xiaohu Wang, Junguang Tao* and Lixiu Guan*

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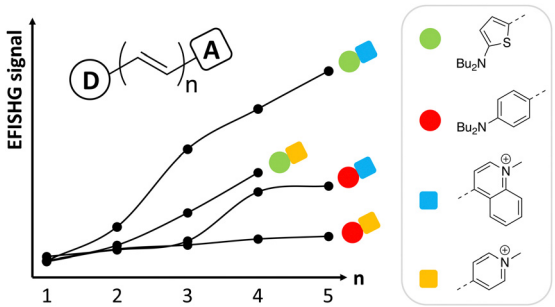
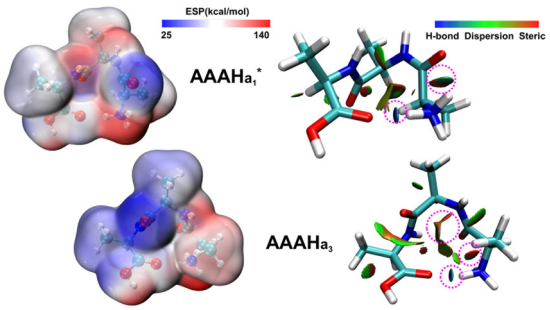


Electric-field induced second harmonic generation responses of push–pull polyenic dyes: experimental and theoretical characterizations

Carmelo Naim, Raphaël Vangheluwe, Isabelle Ledoux-Rak, Benoît Champagne, Claire Tonnelé,* Mireille Blanchard-Desce,* Eduard Matito* and Frédéric Castet*

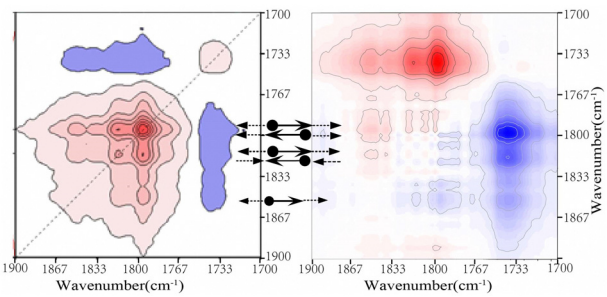
13989



Identifying the protonation site and the scope of non-proline *cis*-peptide bond conformations: a first-principles study on protonated oligopeptides

Rui Xiong, Li Xu, Yong Tang, Mengge Cao and Hongbao Li*

13999



The intermolecular polar bond interaction and coupling induced spectral splitting phenomenon for a binary mixture

Huigang Wang,* Zian Wang, Jiwen Jian, Caiying Jiang* and Lanying Pan*

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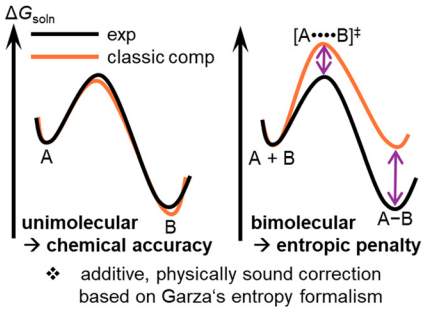
The entropic penalty for associative reactions and their physical treatment during routine computations

Jama Ariai* and Urs Gellrich*



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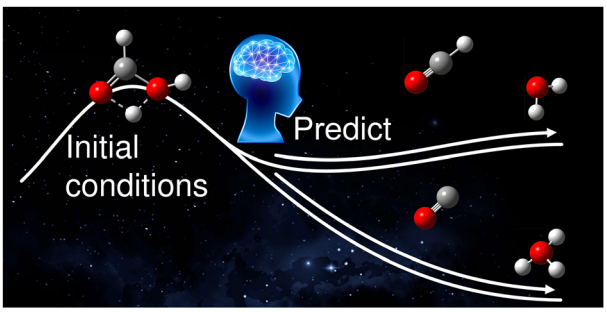
Dynamics study of the post-transition-state-bifurcation process of the $(HCOOH)H^+ \rightarrow CO + H_3O^+/HCO^+ + H_2O$ dissociation: application of machine-learning techniques

Tatsuhiro Murakami,* Shunichi Ibuki, Yu Hashimoto, Yuya Kikuma and Toshiyuki Takayanagi



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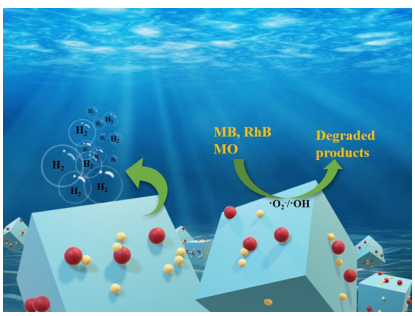
Synthesis and highly efficient photocatalysis applications of CdS QDs and Au NPs Co-modified $KTaO_3$ perovskite cubes

Niuniu Zhang, Xia Wu, Kangjia Lv, Yujie Chu, Guan Wang* and Dongdi Zhang*



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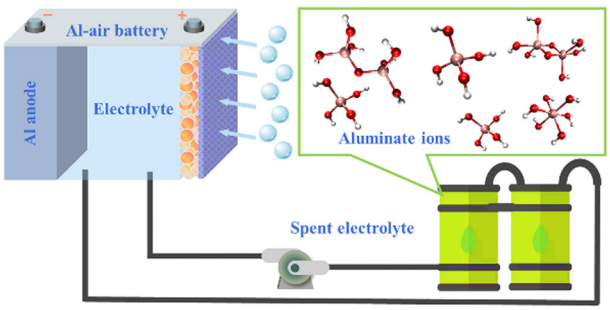
Properties and composition of the spent electrolyte for premium circulation mediated by Al–air batteries

Hao Cheng, Zhifan Hua, Yuan Zhu, Tao Wang, Zheng Li, Yao Lu, Zhongliang Tian* and Wenyi Lu*



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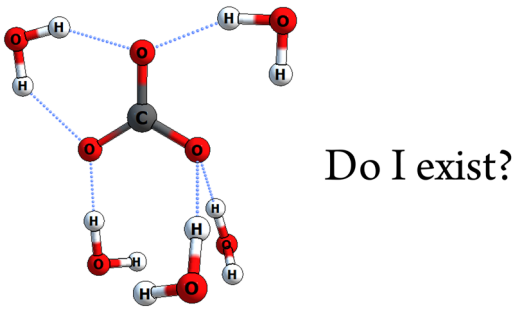
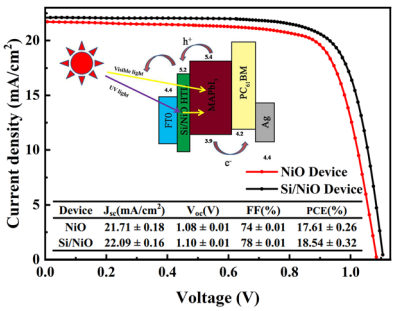


On the existence of CO_3^{2-} microsolvated clusters: a theoretical study

Pavel Rublev, Nikolay V. Tkachenko, Pavel A. Dub and Alexander I. Boldyrev*

14056



Silicon/nickel oxide core/shell nanospheres as a hole transport layer for high efficiency and light-stable perovskite solar cells

Jifeng Zhai, Xin Yin, Jie Xiong,* Pingfan Du, Wei-Hsiang Chen and Lixin Song*

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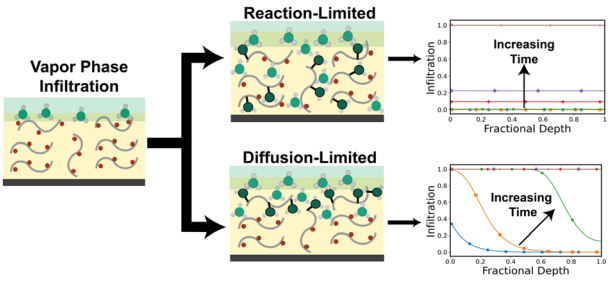
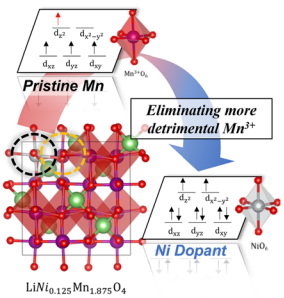


Interpreting inorganic compositional depth profiles to understand the rate-limiting step in vapor phase infiltration processes

Shuaib A. Balogun, Yi Ren, Ryan P. Lively and Mark D. Losego*

14074



Dopant-induced electronic design of redox-active elements in $LiMn_2O_4$ spinel structures

Jae Seung Seol, Seungho Yu and Ki Chul Kim*

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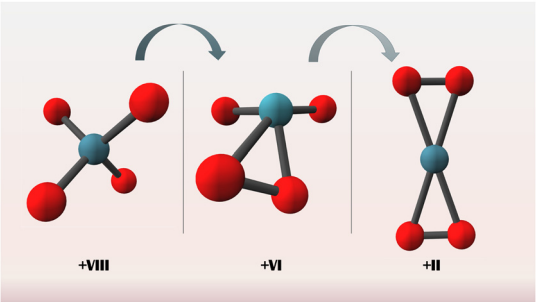
14084

The inert pair effect on heavy noble gases: insights from radon tetroxide

Nuno A. G. Bandeira* and Joaquim Marçalo



14089

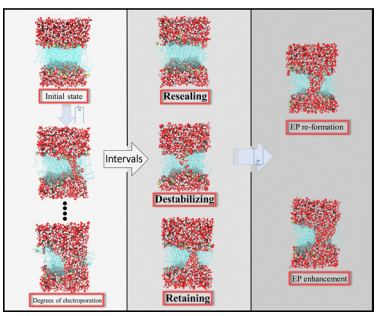
Locally spontaneous dynamic oxygen migration on biphenylene: a DFT study

Boyi Situ, Zihan Yan, Rubin Huo, Kongbo Wang, Liang Chen, Zhe Zhang, Liang Zhao* and Yusong Tu*

14096

A molecular dynamics study of phospholipid membrane electroporation induced by bipolar pulses with different intervals

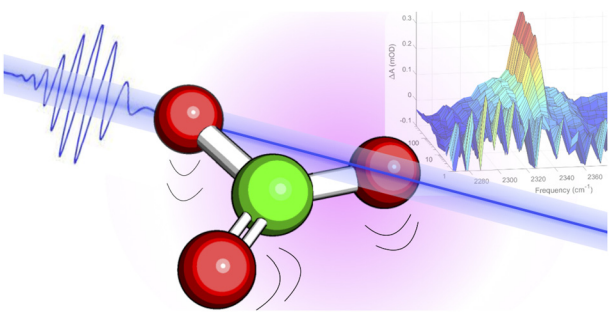
Fei Guo,* Jiong Zhou, Ji Wang, Kun Qian and Hongchun Qu



14104

The primary photolysis of aqueous carbonate di-anions

Jan Thøgersen, Tobias Weidner and Frank Jensen*



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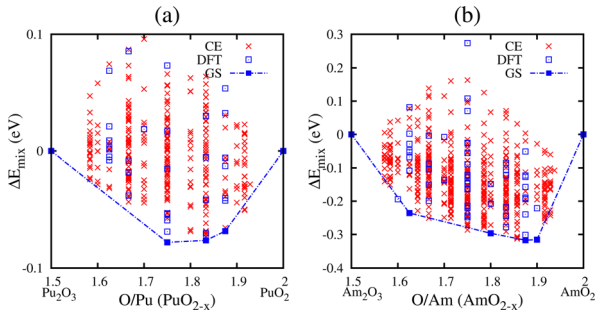
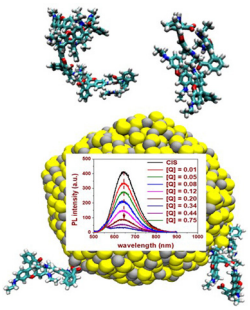
14117



Evidence of vacancy ordered structures in PuO_{2-x} and AmO_{2-x} from first-principles calculations

P. S. Ghosh* and A. Arya

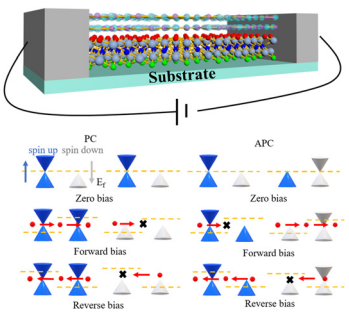
14126



Dye-induced photoluminescence quenching of quantum dots: role of excited state lifetime and confinement of charge carriers

Saleem Al-Maskari, Abey Issac,* Srinivasa Rao Varanasi, Richard Hildner, R. G. Sumesh Sofin, A. Ramadan Ibrahim and Osama K. Abou-Zied

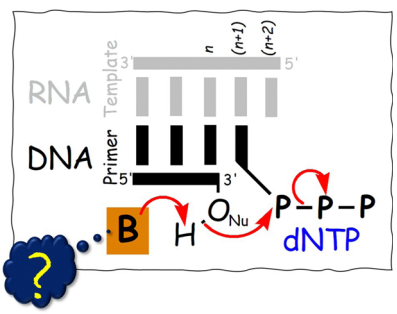
14138



Spin-gapless van der Waals heterostructure for spin gating through magnetic injection devices

Xiaolin Zhang, Pengwei Gong, Fangqi Liu and Sicong Zhu*

14147



Probing the general base for DNA polymerization in telomerase: a molecular dynamics investigation

Chandan Kumar Das, Abhinav Gupta and Nisanth N. Nair*

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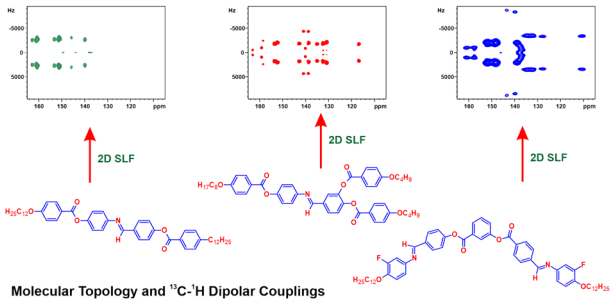
14158

Direct method to grasp molecular topology of mesogens through $^{13}C–^{1}H$ dipolar couplings

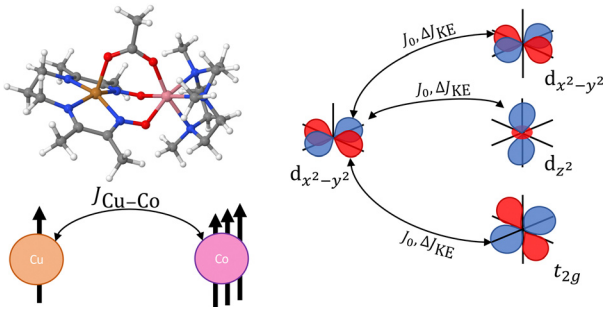
M. Kesava Reddy, P. Jaya Shalini, Nitin P. Lobo, Arun Roy and T. Narasimhaswamy*



14170

Revisiting magnetic exchange couplings in heterodinuclear complexes through the decomposition method in KS-DFT

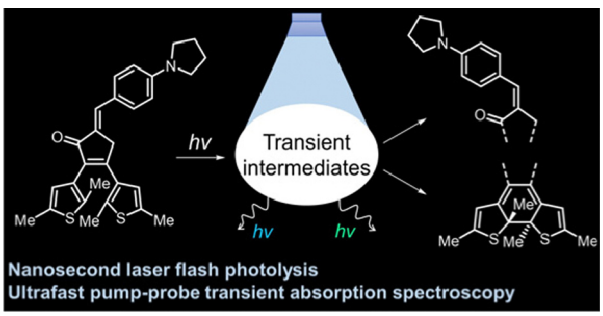
Gwenhaël Duplaix-Rata, Boris Le Guennic and Grégoire David*



14179

Multifunctional fluorescent diarylethene: time-resolved study of photochemistry

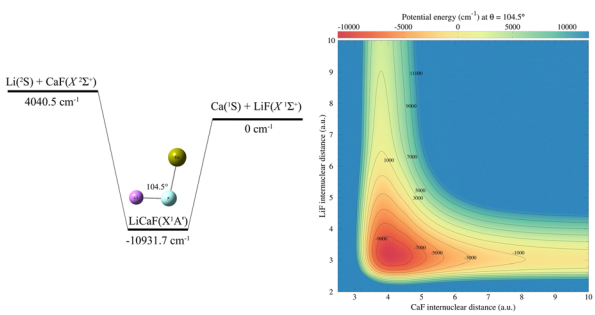
Veronica V. Semionova, Ivan P. Pozdnyakov, Vjacheslav P. Grivin, Victor F. Plyusnin, Yuri P. Tsentalovich, Valerii Z. Shirinian, Alexei A. Melnikov, Sergei V. Chekalin, Andrey G. Lvov* and Evgeni M. Glebov*



14193

The Li + CaF → Ca + LiF chemical reaction under cold conditions

Humberto da Silva Jr, Qian Yao, Masato Morita, Brian K. Kendrick, Hua Guo* and Naduvalath Balakrishnan*



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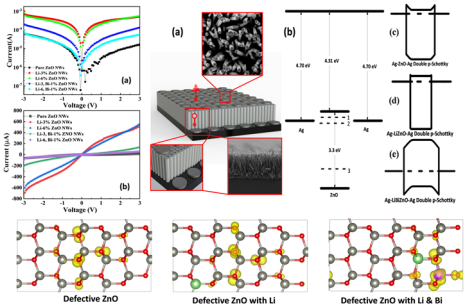
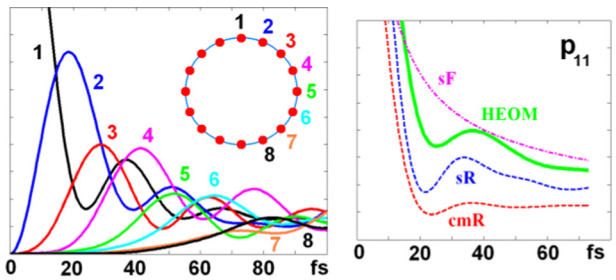
14206



Free carrier-mediated ferromagnetism in nonmagnetic ion (Bi–Li) codoped ZnO nanowires

Jamal Kazmi, Syed Raza Ali Raza,* Waqas Ahmad, Asad Masood, Abdul Jalil, A. A. Mohd Raub, Aumber Abbas, Md Khan Sobayel Rafiq and Mohd Ambri Mohamed*

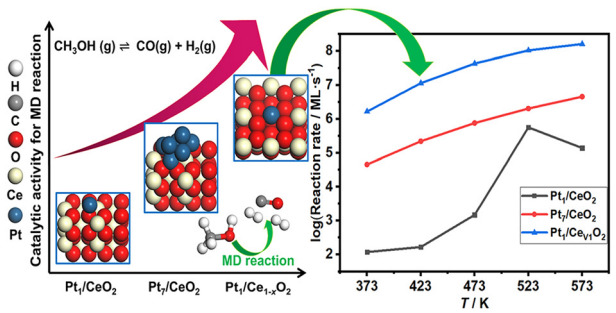
14219



Excitation dynamics in photosynthetic light-harvesting complex B850: exact solution *versus* Redfield and Förster limits

Vladimir I. Novoderezhkin

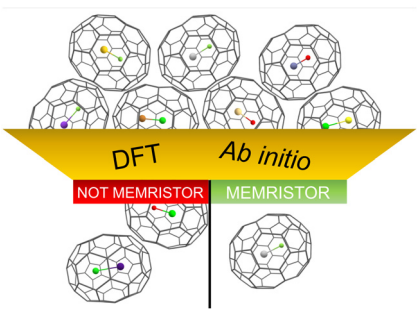
14232



A DFT study on methanol decomposition over single atom Pt/CeO_2 catalysts: the effect of the position of Pt

Hao Lu, Yuan Zhong, Yao Jie, Pan Yin, Xiao-Jie Zhao, Yu-Liang Feng, Tian-Yao Shen, Jing-Yi Guo, Wei Zhang, Min Pu and Hong Yan*

14245



A quest for ideal electric field-driven $MX@C_{70}$ endohedral fullerene memristors: which MX fits the best?

Lucie Tučková, Adam Jaroš, Cina Foroutan-Nejad* and Michal Straka*

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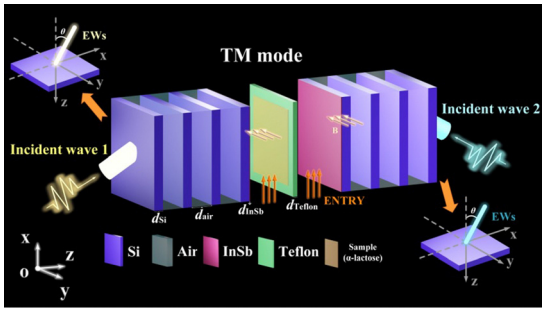
14257

Advanced optical terahertz fingerprint sensor based on coherent perfect absorption

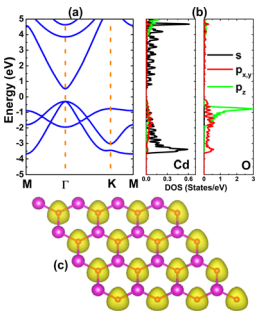
You Ran Wu, Rui Yang Dong, Jia Hao Zou and Hai Feng Zhang*



14266

Half-metallic and magnetic semiconductor behavior in CdO monolayer induced by acceptor impurities

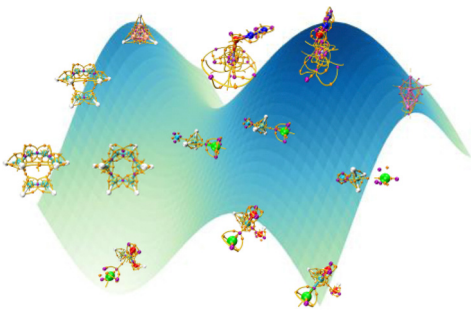
R. Ponce-Pérez, J. Guerrero-Sanchez and D. M. Hoat*



14274

A simple topology-based model for predicting the activation barriers of reactive processes at 0 K

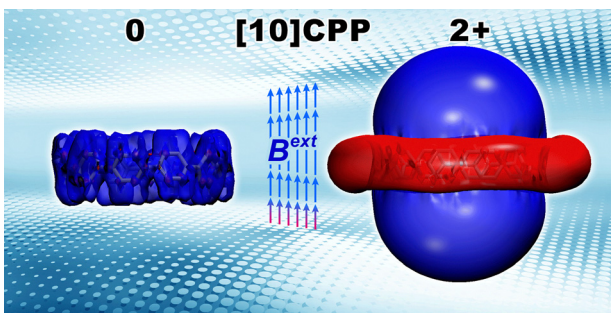
Leandro Ayarde-Henríquez,* Cristian Guerra, Mario Duque-Noreña and Eduardo Chamorro*



14285

Local and global aromaticity under rotation: analysis of two- and three-dimensional representative carbon nanostructures

Rafael Lingas, Nickolas D. Charistos* and Alvaro Muñoz-Castro*



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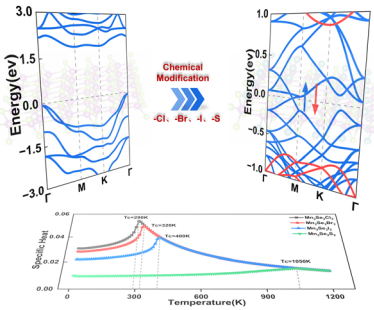
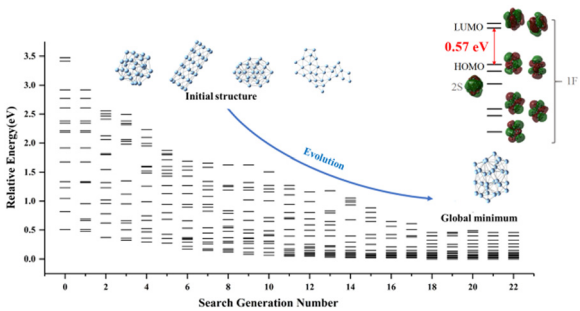


Room-temperature half-metals induced *via* chemical surface modification: 2D Mn_2Se_2 monolayer

Zhe Wang, Yanqiu Zheng, Ji Chen, Yun Wang, Yu Liang, Xiang Li and Fang Wu*

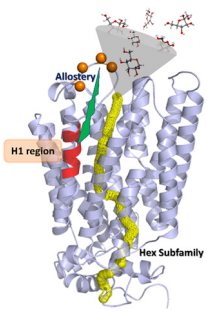
14303



The global minimum of Ag_{30}: a prolate spheroidal structure predicted using a genetic algorithm with incomplete local optimizations at the DFT level

Wen Liu, Lulu Huang, Lei Meng, Jin Hu and Xiaopeng Xing*

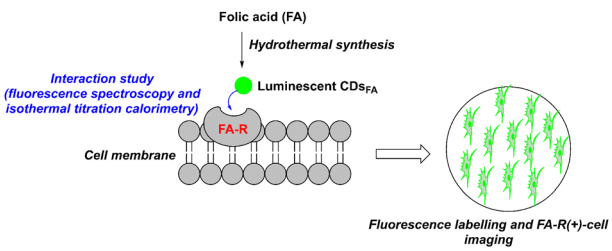
14311



Functional insight into *Cordyceps militaris* sugar transporters by structure modeling, network analysis and allosteric regulation

Xin Liu, Hanyang Zhang, Ziyun Zhou, Pranesha Prabhakaran, Wanwipa Vongsangnak,* Guang Hu* and Fei Xiao*

14324



Interaction between carbon dots from folic acid and their cellular receptor: a qualitative physicochemical approach

Erika Adhel, Nguyêt-Thanh Ha Duong, Thi Huyen Vu, Dario Taverna, Souad Ammar and Nawal Serradji*

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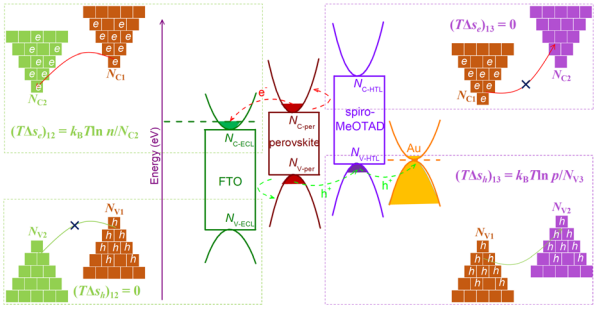
14334

Relating band edge DOS occupancy statistics associated excited state electron entropy generation to free energy loss and intrinsic V_{oc} deficit of solar cells

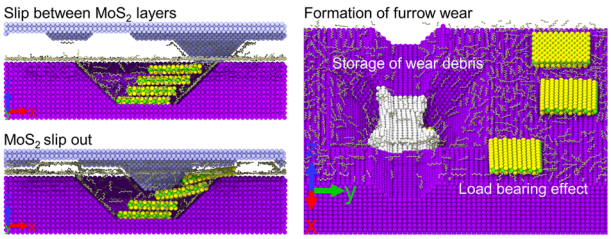
Like Huang



14348

Frictional properties of MoS_2 on a multi-level rough wall under starved lubrication

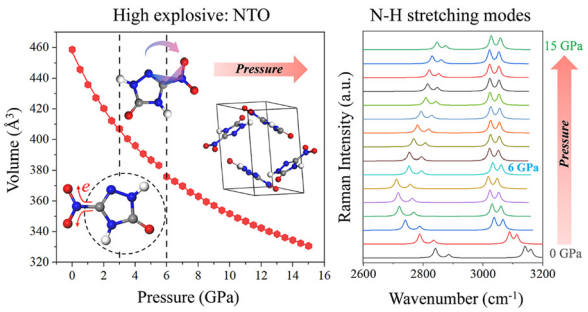
Changli Yi, Chengzhi Hu,* Lin Shi, Minli Bai, Yubai Li and Dawei Tang



14359

Pressure-dependent structure and electronic properties of energetic NTO crystals dominated by hydrogen-bonding interactions

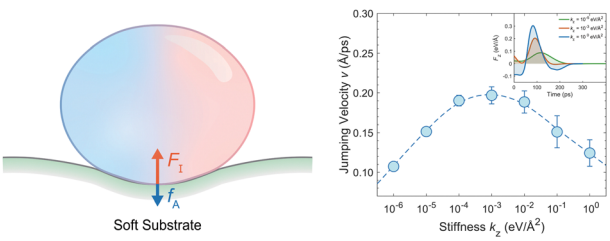
Junyu Fan, Pengju Wang and Nan Gao*



14368

Optimum substrate stiffness in coalescence-induced droplet jumping

Lianfu Qiu, Sheng Qian, Yifeng Ni and Qi Tong*



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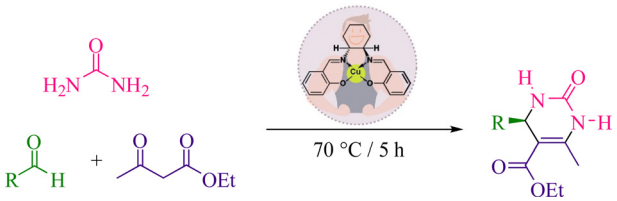
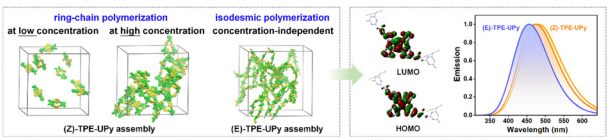


DFT stimulation and experimental insights of chiral Cu(II)–salen scaffold within the pocket of MWW-zeolite and its catalytic study

Pratikkumar Lakhani, Darshil Chodvadiya, Prafulla K. Jha, Vivek Kumar Gupta, Damian Trzybiński, Krzysztof Wozniak, Krzysztof Kurzydłowski, U. K. Goutam, Himanshu Srivastava and Chetan K. Modi*

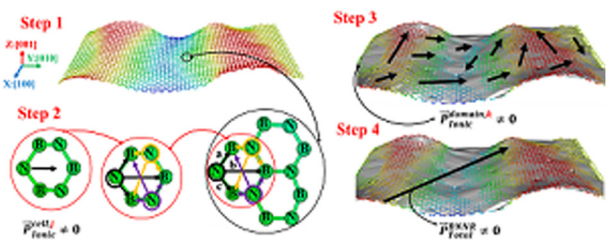
14387



Elucidation of the key role of isomerization in the self-assembly and luminescence properties of AIEgens

Hui Wang, Junfang Yang and Xiaoyan Zheng*

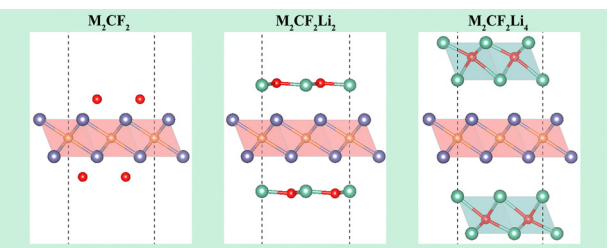
14400



Energy harvesting from mechanical vibrations: self-rectification effect

Gholamreza Ghashami, Maryam Mahnama, Mahdi Moghimi Zand,* S. Mehdi Vaez Allaei and Miquel López-Suárez

14406



Lithium storage performance enhanced by lithiation-induced structural phase transitions of fluorinated MXenes

Qinghua Wu, Zhe Wang, Qianku Hu,* Yuhuan Ji, Dandan Li, Junkai Wang, Qixun Xia, Libo Wang and Aiguo Zhou*

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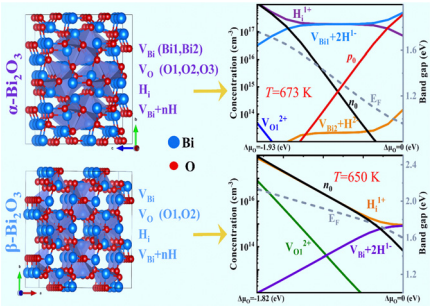
14417

Intrinsic point defects and the n- and p-type dopability in α- and β-Bi_2O_3 photocatalysts

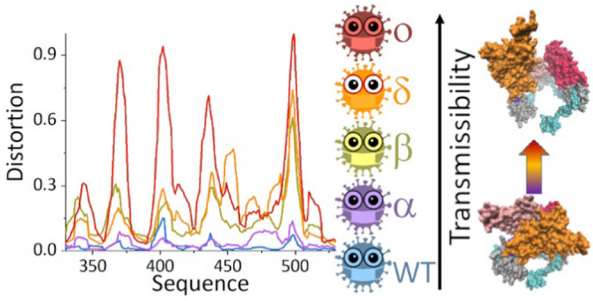
Jincheng Wang, Zuoyin Liu, Bo Kong,* Xinyou An, Min Zhang and Wentao Wang*



14430

The SARS-CoV-2 spike protein structure: a symmetry tale on distortion trail

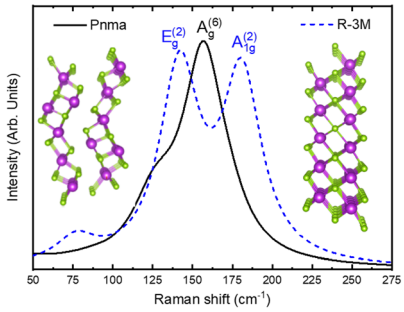
Inbal Tuvi-Arad* and Yaffa Shalit



14440

Vibrational properties of metastable orthorhombic Bi_2Se_3

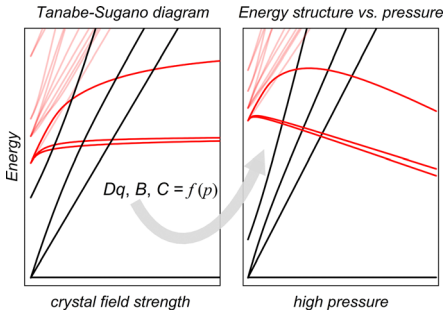
Paloma B. Souza, Milton A. Tumelero,* Ricardo Faccio, Rasin Ahmed, Cristiani C. Plá Cid, Giovanni Zangari and Andre A. Pasa



14449

Evolution of the full energy structure of Mn^{4+} in fluoride phosphors under high pressure conditions

Tadeusz Leśniewski



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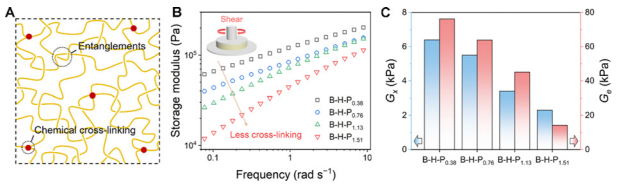
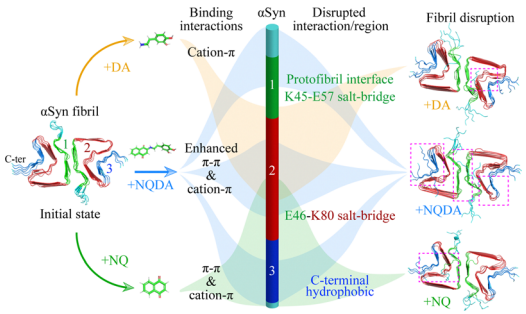
14463



How chemical cross-linking and entanglements in polybutadiene elastomers cope with tearing

Xiangliang Zeng, Xinnian Xia,* JianFeng Fan, Rong Sun and Xiaoliang Zeng*

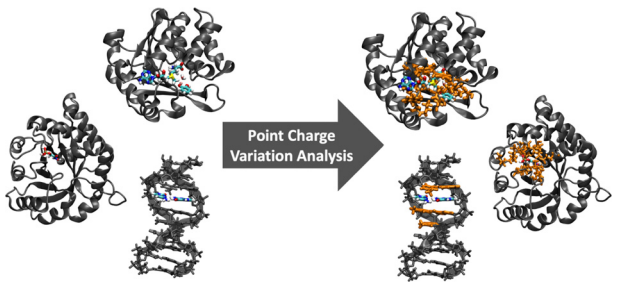
14471



Naphthoquinone–dopamine hybrids disrupt α-synuclein fibrils by their intramolecular synergistic interactions with fibrils and display a better effect on fibril disruption

Yun Zhou, Yifei Yao, Zhongyuan Yang, Yiming Tang and Guanghong Wei*

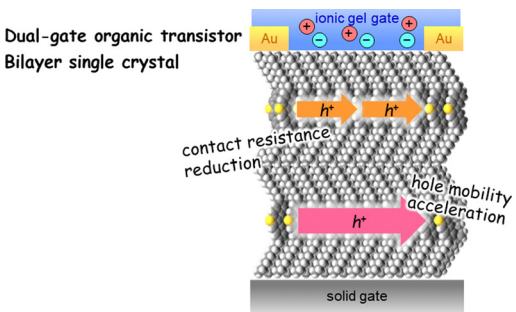
14484



Efficient automatic construction of atom-economical QM regions with point-charge variation analysis

Felix Brandt and Christoph R. Jacob*

14496



Individual and synergetic charge transport properties at the solid and electrolyte interfaces of a single ultrathin single crystal of organic semiconductors

Taehyun Won, Shohei Kumagai,* Naotaka Kasuya,* Yu Yamashita, Shun Watanabe, Toshihiro Okamoto and Jun Takeya*

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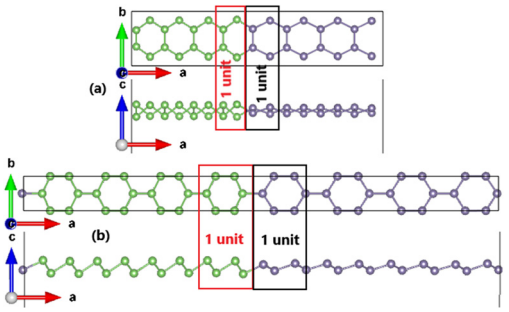
14502

Novel germanene–arsenene and germanene–antimonene lateral heterostructures: interline-dependent electronic and magnetic properties

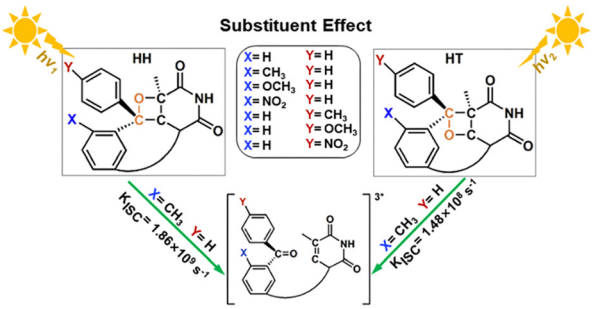
Chu Viet Ha, Bich Ngoc Nguyen Thi, Pham Quynh Trang, R. Ponce-Pérez, J. Guerrero-Sanchez and D. M. Hoat*



14511

Controlling the repair mechanisms of oxetanes through functional group substitution

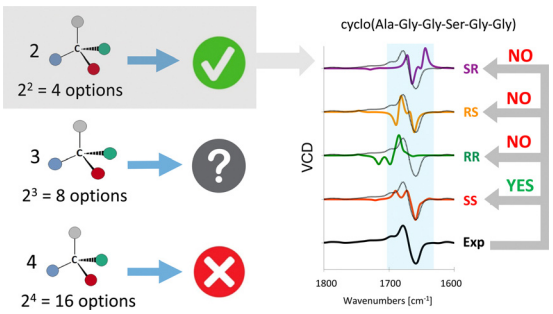
Yan Shen, Shaoqin Zhang, Yingli Su, Zexing Qu* and Haisheng Ren*



14520

Can the absolute configuration of cyclic peptides be determined with vibrational circular dichroism?

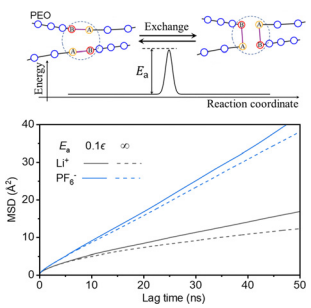
Karolina Di Remigio Eikås,* Monika Krupová, Tone Kristoffersen, Maarten T. P. Beerepoot and Kenneth Ruud*



14530

Structure and dynamics of dynamic covalent cross-linked PEOs and PEO/$LiPF_6$ electrolytes: a coarse-grained simulation study

Tongfei Wu* and Ping Zhang



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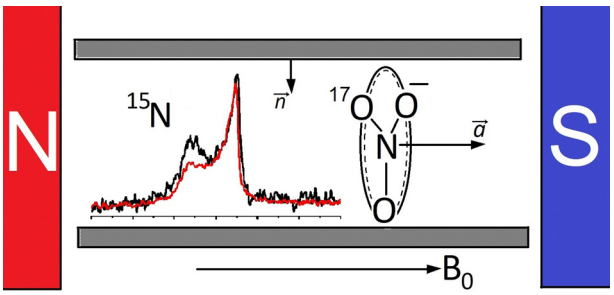
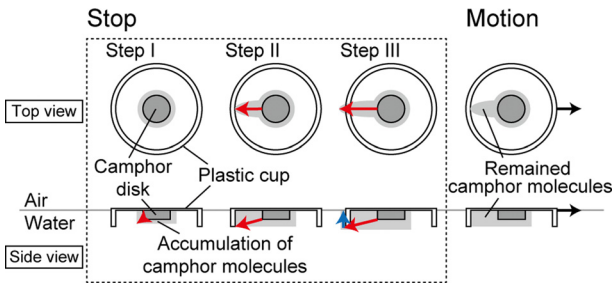
14538



State of anion in ethylammonium nitrate enclosed between micrometer-spaced glass plates as studied by ^{17}O and ^{15}N NMR

Andrei Filippov* and Oleg N. Antzutkin

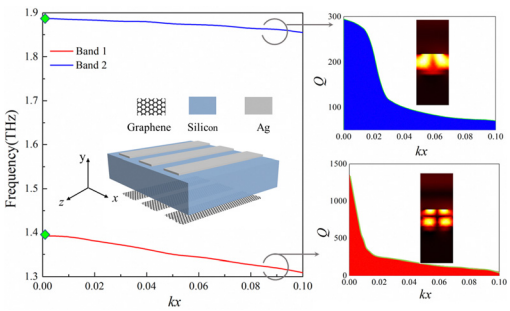
14546



Height-dependent oscillatory motion of a plastic cup with a camphor disk floated on water

Risa Fujita, Nami Takayama, Muneyuki Matsuo, Makoto Iima and Satoshi Nakata*

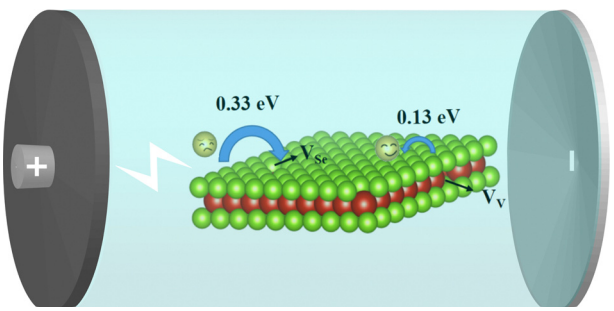
14552



Generation of symmetry-protected bound states in the continuum in a graphene plasmonic waveguide system for optical switching

Min Li, Banxian Ruan, Baihui Zhang, Enduo Gao, Zhenbin Zhang, Xia Chang and Hongjian Li*

14558



Mechanisms of adsorption and diffusion of Na on a VSe_2 monolayer with engineering-induced vacancies

Xuerui Shi, Jialin Li, Xiaojiao Zhang, Mingjun Li, Qun Jing, Guozhao Fang and Mengqiu Long*

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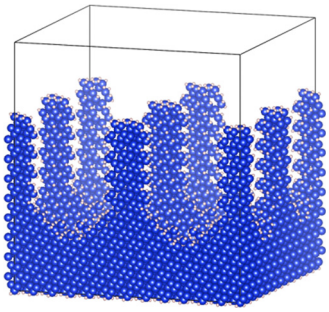
14566

Clarifying the effects of nanoscale porosity of silicon on the bandgap and alignment: a combined molecular dynamics–density functional tight binding computational study

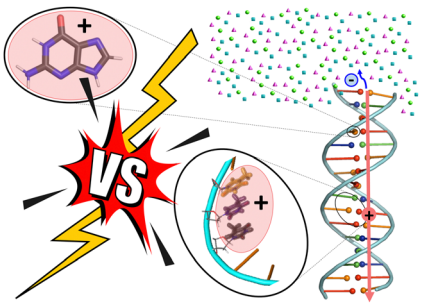
Panus Sundarapura, Sergei Manzhos* and Manabu Ihara*



14578

Intramolecular and intermolecular hole delocalization rules the reducer character of isolated nucleobases and homogeneous single-stranded DNA

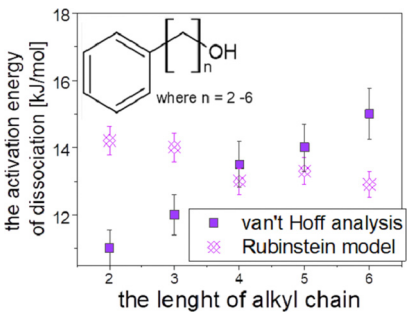
Jesús Lucia-Tamudo,* Sergio Díaz-Tendero* and Juan J. Nogueira*



14590

On the relationship between the Debye process in dielectric response and a dissociation–association phenomenon in phenyl alcohols

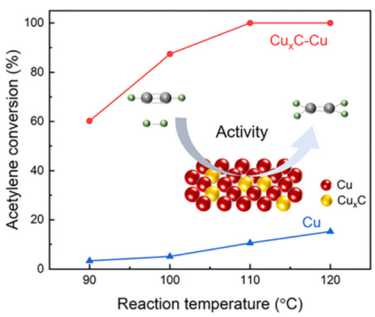
Anna Czaderna-Lekka,* Magdalena Tarnacka,* Zaneta Wojnarowska, Barbara Hachuła, Marian Paluch and Kamil Kamiński



14598

A highly active catalyst derived from CuO particles for selective hydrogenation of acetylene in large excess ethylene

Aonan Zeng, Chenyang Lu, Bo Xu, Anjie Wang,* Ying-Ya Liu, Zhichao Sun and Yao Wang*



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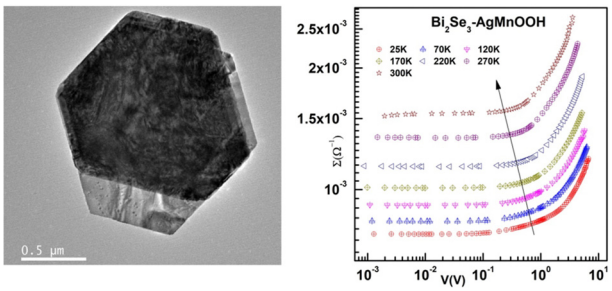
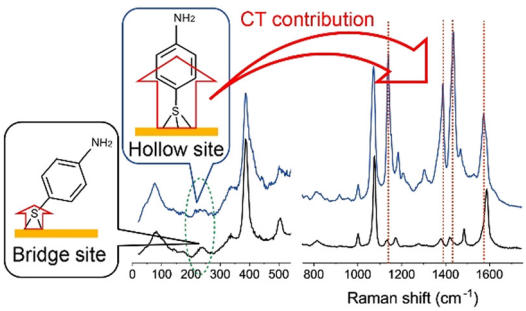
14606



Investigation of electrical transport properties in solution-processed Bi_2Se_3–AgMnOOH nanocomposite

Rishika Chakraborty, Sutanu Das, Siddheswar Rudra, Arpan Kumar Nayak, Pradip K. Maji, Upendranath Nandi* and Mukul Pradhan*

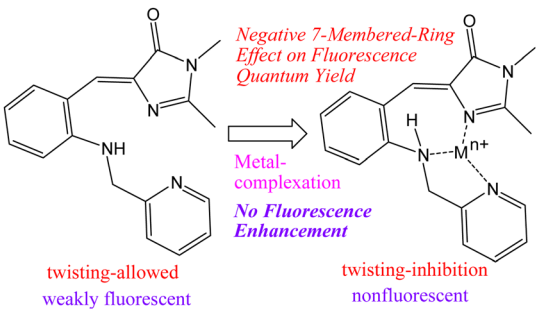
14618



Revisit of the plasmon-mediated chemical transformation of *para*-aminothiophenol

Toshiki Kondo, Motoharu Inagaki, Shohei Tanaka, Shinya Tsukiji, Kenta Motobayashi and Katsuyoshi Ikeda*

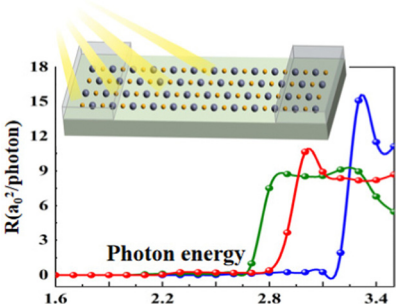
14627



7-membered-ring effect on fluorescence quantum yield: does metal-complexation-induced twisting-inhibition of an amino GFP chromophore derivative enhance fluorescence?

Hao-Wei Ke and Kuangsen Sung*

14635



Electronic transport properties of two-dimensional tetragonal zinc chalcogenides

Yaoyun Zhu, Shuang Meng and Jia Zhou*

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