

## IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 25(20) 13795–14644 (2023)



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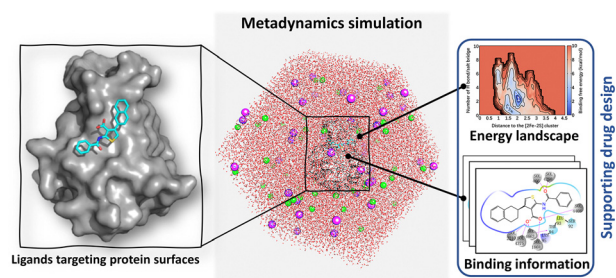
See Yu Wang and Kazuyuki Takeda, pp. 13838–13845. Image reproduced by permission of Art Action Inc. from *Phys. Chem. Chem. Phys.*, 2023, 25, 13838.

## PERSPECTIVES

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

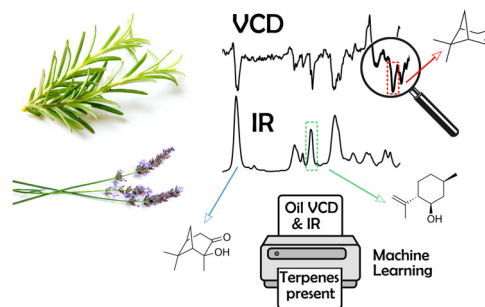
Ke Zuo, Agata Kranjc, Riccardo Capelli, Giulia Rossetti, Rachel Nechushtai and Paolo Carloni\*



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### 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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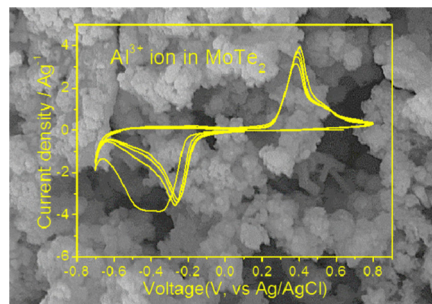


## COMMUNICATION

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### Investigation of reversible metal ion ( $\text{Li}^+$ , $\text{Na}^+$ , $\text{Mg}^{2+}$ , $\text{Al}^{3+}$ ) insertion in $\text{MoTe}_2$ 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

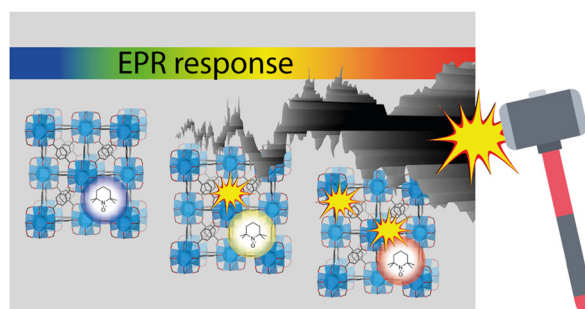
Yu Wang and Kazuyuki Takeda\*



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

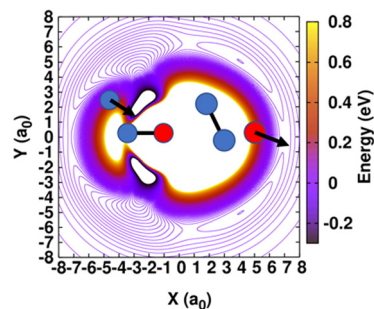
Artem S. Poryvaev,\* Kirill P. Larionov, Yana N. Albrekht, Alexander A. Efremov, Alexey S. Kiryutin, Kristina A. Smirnova, Vasily Y. Evtushok and Matvey V. Fedin\*



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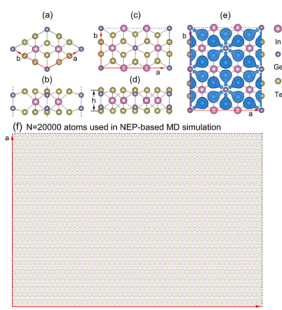
### Low-temperature kinetics for the $\text{N} + \text{NO}$ reaction: experiment guides the way

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



## RESEARCH PAPERS

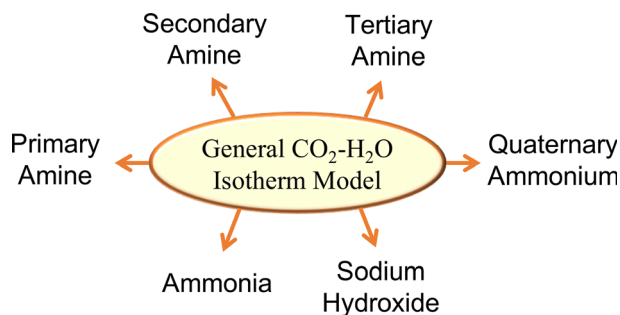
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### Investigation of the mechanical and transport properties of InGeX<sub>3</sub> (X = S, Se and Te) monolayers using density functional theory and machine learning

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\*

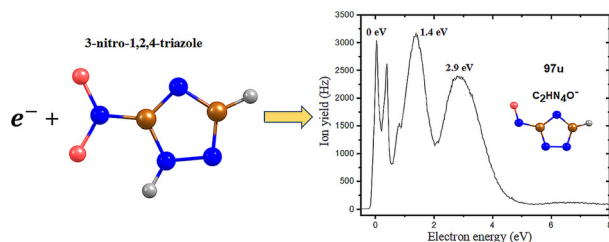
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### A general binary isotherm model for amines interacting with CO<sub>2</sub> and H<sub>2</sub>O

Yuta Kaneko\* and Klaus S. Lackner\*

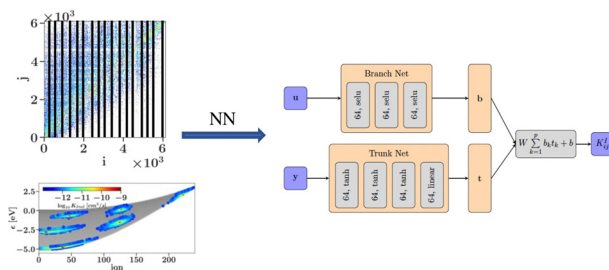
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### Decomposition of triazole and 3-nitrotriazole upon low-energy electron attachment

Muhammad Saqib, Farhad Izadi, Leon U. Isierhienhien, 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\*

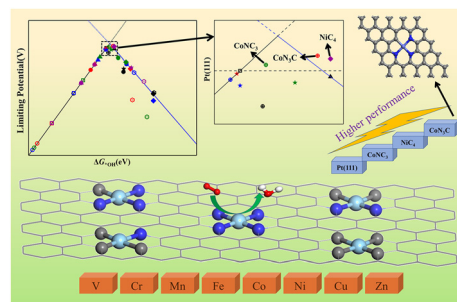




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### Exploring the catalytic activity of graphene-based TM-N<sub>x</sub>C<sub>4-x</sub> single atom catalysts for the oxygen reduction reaction *via* density functional theory calculation

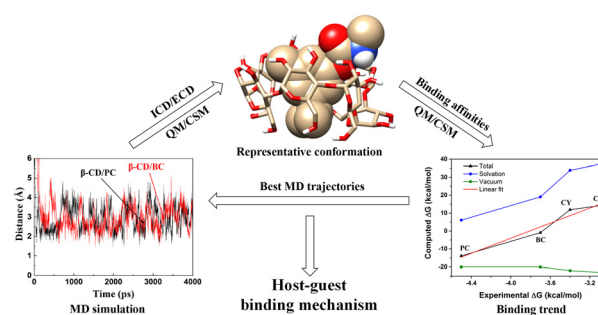
Zhengwei Du, Kaiming Deng, Erjun Kan and Cheng Zhan\*



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### How are *N*-methylcarbamates encapsulated by $\beta$ -cyclodextrin: insight into the binding mechanism

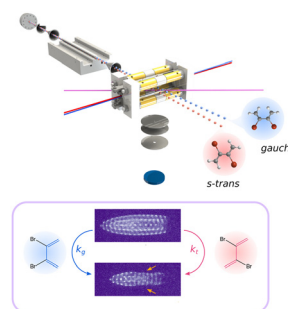
Xiaofang Bao, Xiao Liu, Ran Dou, Sen Xu, Dabin Liu, Jun Luo, Xuedong Gong, Chung F. Wong and Baojing Zhou\*



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

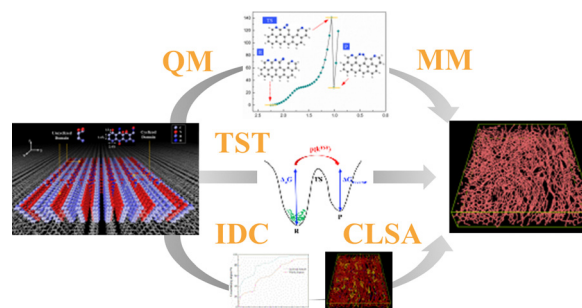
Ardita Kilaj, Silvan Käser, Jia Wang, Patrik Straňák, Max Schwilk, Lei Xu, O. Anatole von Lilienfeld, Jochen Küpper,\* Markus Meuwly\* and Stefan Willitsch\*



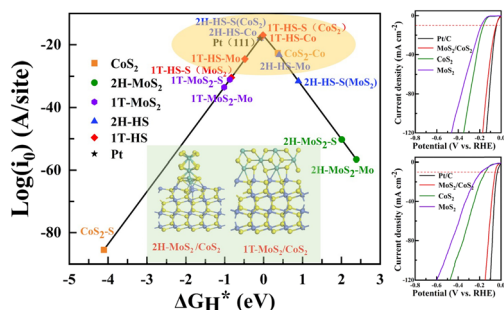
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### Insights into the carbonization mechanism of PAN-derived carbon precursor fibers and establishment of a kinetics-driven accelerated reaction template for atomistic simulation

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



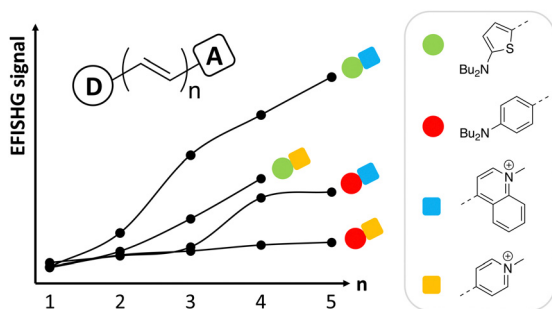
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### Interface prompted highly efficient hydrogen evolution of MoS<sub>2</sub>/CoS<sub>2</sub> heterostructures in a wide pH range

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

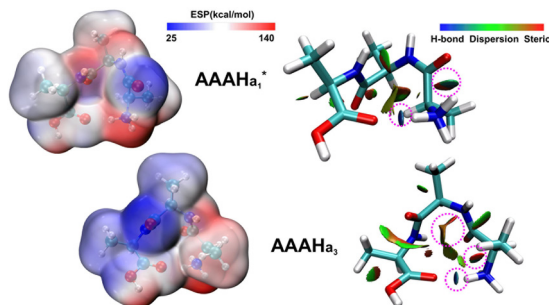
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### Electric-field induced second harmonic generation responses of push-pull polyenic dyes: experimental and theoretical characterizations

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

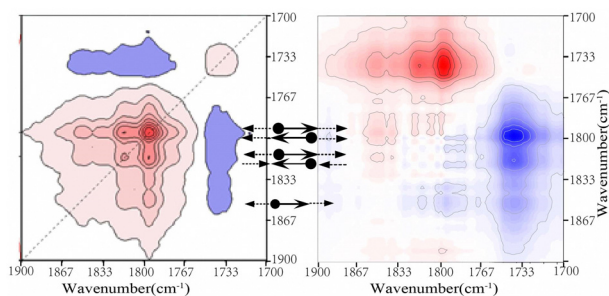
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### Identifying the protonation site and the scope of non-proline *cis*-peptide bond conformations: a first-principles study on protonated oligopeptides

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

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### 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\*

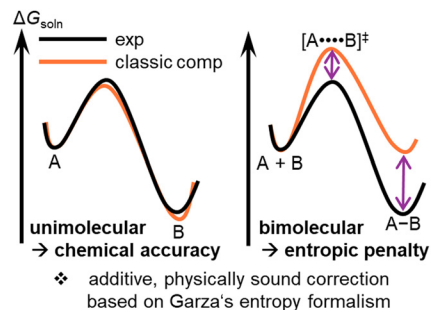


## RESEARCH PAPERS

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

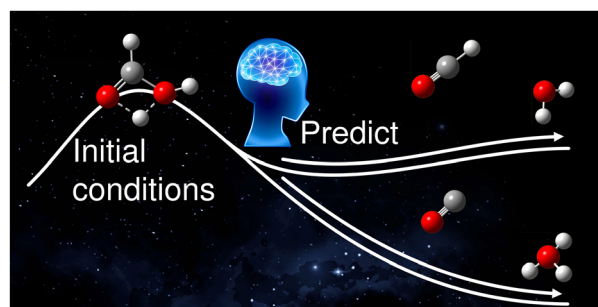
Jama Ariai\* and Urs Gellrich\*



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### Dynamics study of the post-transition-state-bifurcation process of the $(\text{HCOOH})\text{H}^+ \rightarrow \text{CO} + \text{H}_3\text{O}^+/\text{HCO}^+ + \text{H}_2\text{O}$ dissociation: application of machine-learning techniques

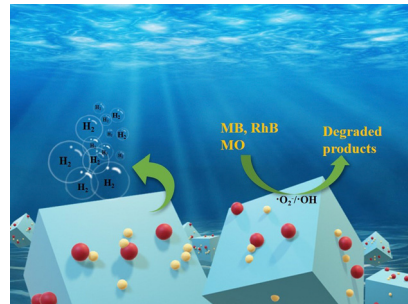
Tatsuhiko Murakami,\* Shunichi Ibuki, Yu Hashimoto, Yuya Kikuma and Toshiyuki Takayanagi



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### Synthesis and highly efficient photocatalysis applications of CdS QDs and Au NPs Co-modified $\text{KTaO}_3$ perovskite cubes

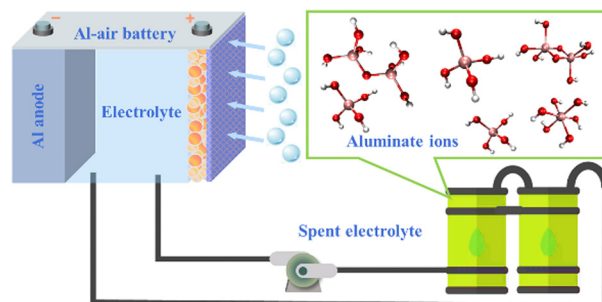
Niuniu Zhang, Xia Wu, Kangjia Lv, Yujie Chu, Guan Wang\* and Dongdi Zhang\*



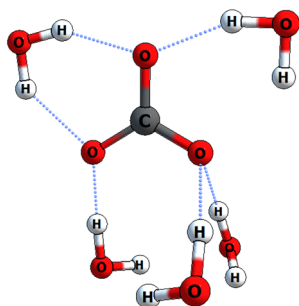
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### Properties and composition of the spent electrolyte for premium circulation mediated by Al-air batteries

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



14046

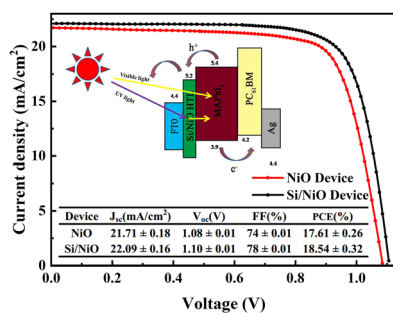


Do I exist?

### On the existence of $\text{CO}_3^{2-}$ microsolvated clusters: a theoretical study

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

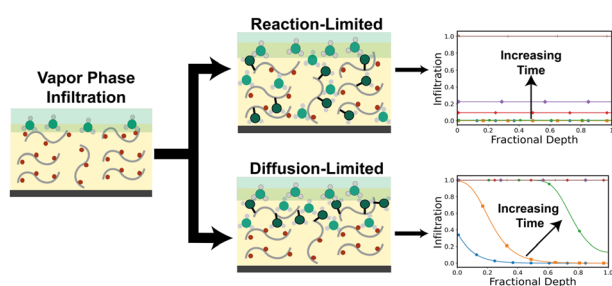
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### Silicon/nickel oxide core/shell nanospheres as a hole transport layer for high efficiency and light-stable perovskite solar cells

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

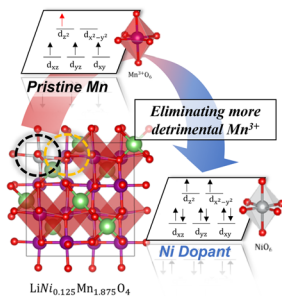
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### Interpreting inorganic compositional depth profiles to understand the rate-limiting step in vapor phase infiltration processes

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

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### Dopant-induced electronic design of redox-active elements in $\text{LiMn}_2\text{O}_4$ spinel structures

Jae Seung Seol, Seungho Yu and Ki Chul Kim\*



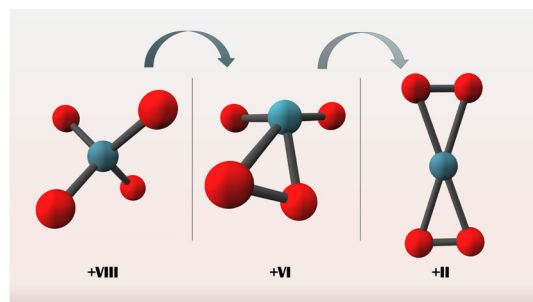


## RESEARCH PAPERS

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

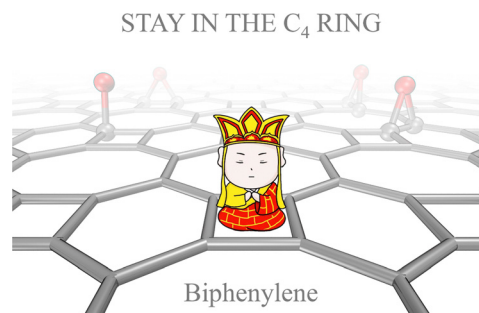
Nuno A. G. Bandeira\* and Joaquim Marçalo



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**Locally spontaneous dynamic oxygen migration on biphenylene: a DFT study**

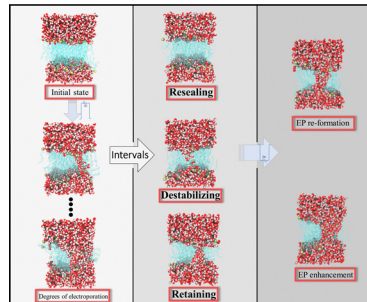
Boyi Situ, Zihan Yan, Rubin Huo, Kongbo Wang, Liang Chen, Zhe Zhang, Liang Zhao\* and Yusong Tu\*



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

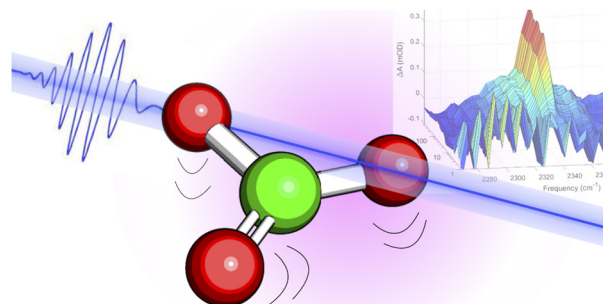
Fei Guo,\* Jiong Zhou, Ji Wang, Kun Qian and Hongchun Qu



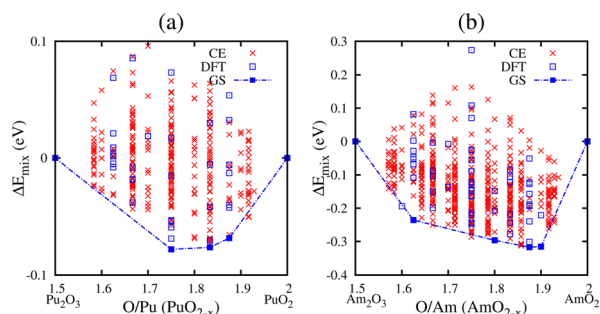
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**The primary photolysis of aqueous carbonate di-anions**

Jan Thøgersen, Tobias Weidner and Frank Jensen\*



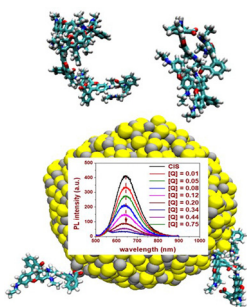
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### Evidence of vacancy ordered structures in $\text{PuO}_{2-x}$ and $\text{AmO}_{2-x}$ from first-principles calculations

P. S. Ghosh\* and A. Arya

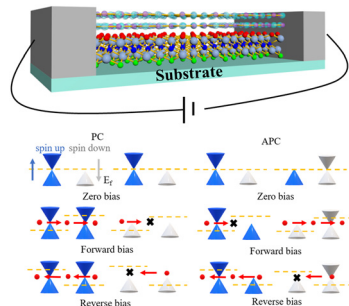
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### Dye-induced photoluminescence quenching of quantum dots: role of excited state lifetime and confinement of charge carriers

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

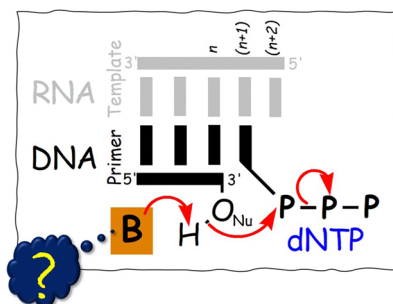
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### Spin-gapless van der Waals heterostructure for spin gating through magnetic injection devices

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

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

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

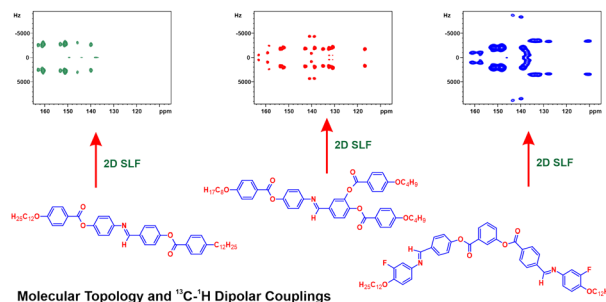


## RESEARCH PAPERS

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

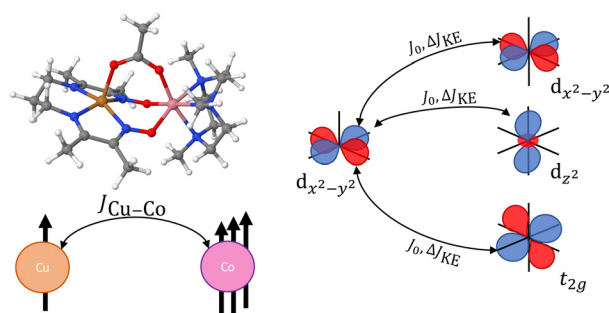
M. Kesava Reddy, P. Jaya Shalini, Nitin P. Lobo, Arun Roy and T. Narasimhaswamy\*



14170

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

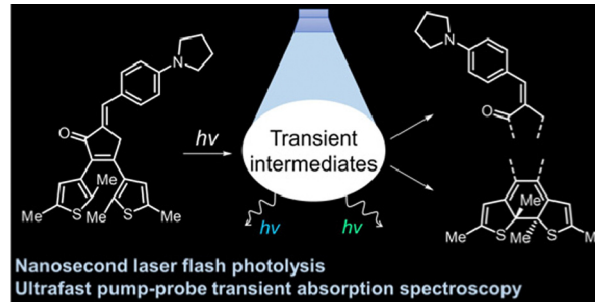
Gwenhaël Duplaix-Rata, Boris Le Guennic and Grégoire David\*



14179

## Multifunctional fluorescent diarylethene: time-resolved study of photochemistry

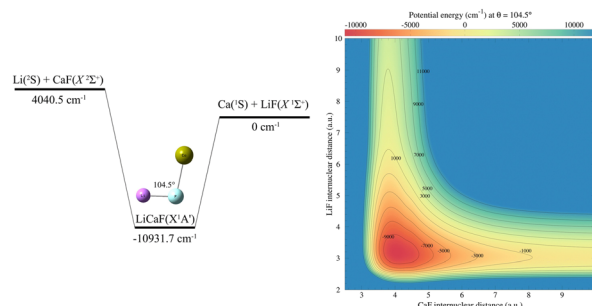
Veronica V. Semionova, Ivan P. Pozdnyakov, Vjacheslav P. Grivin, Victor F. Plyusnin, Yuri P. Tsentalovich, Valerii Z. Shirinian, Alexei A. Melnikov, Sergei V. Chekalin, Andrey G. Lvov\* and Evgeni M. Glebov\*



14193

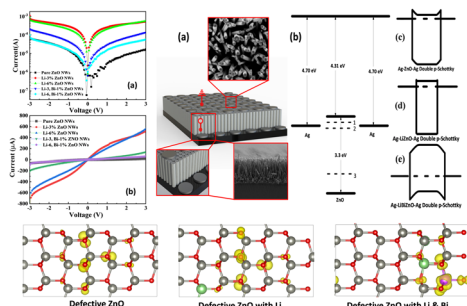
The  $\text{Li} + \text{CaF} \rightarrow \text{Ca} + \text{LiF}$  chemical reaction under cold conditions

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



## RESEARCH PAPERS

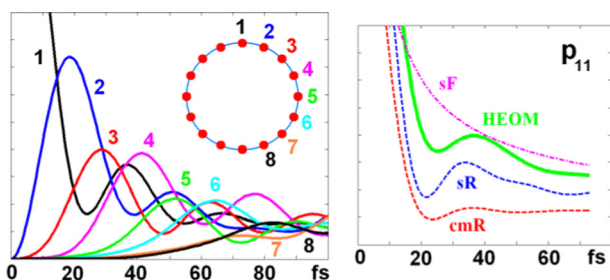
14206



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

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

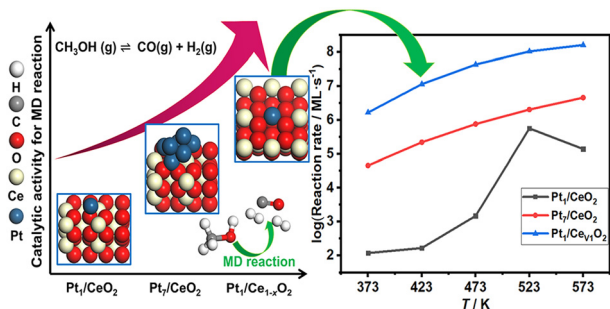
14219



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

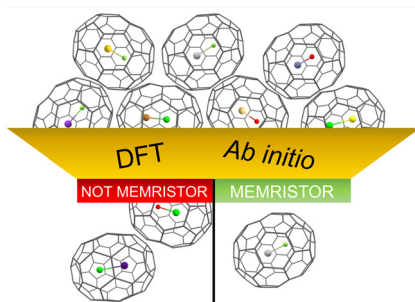
Vladimir I. Novoderezhkin

14232

A DFT study on methanol decomposition over single atom Pt/CeO<sub>2</sub> 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<sub>70</sub> endohedral fullerene memristors: which MX fits the best?

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

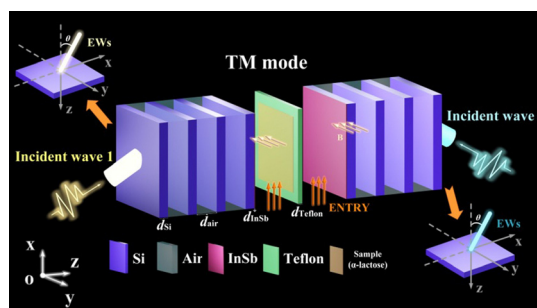




14257

### Advanced optical terahertz fingerprint sensor based on coherent perfect absorption

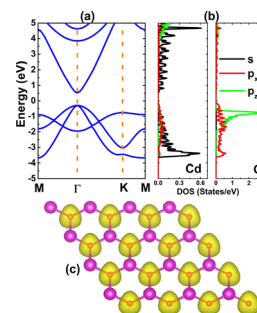
You Ran Wu, Rui Yang Dong, Jia Hao Zou and Hai Feng Zhang\*



14266

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

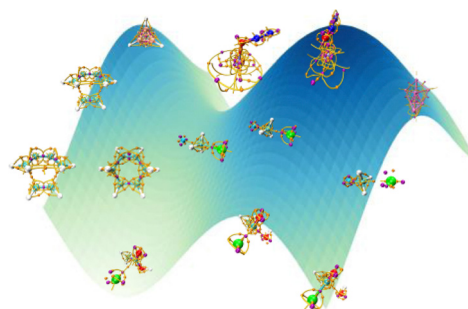
R. Ponce-Pérez, J. Guerrero-Sanchez and D. M. Hoat\*



14274

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

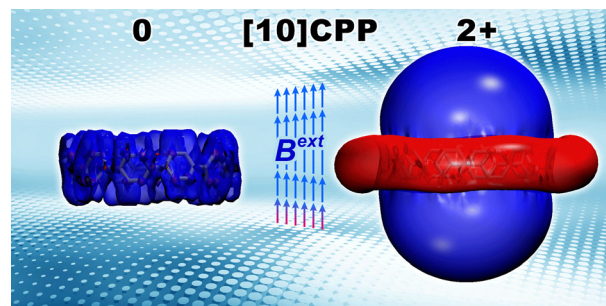
Leandro Ayarde-Henriquez,\* Cristian Guerra, Mario Duque-Noreña and Eduardo Chamorro\*



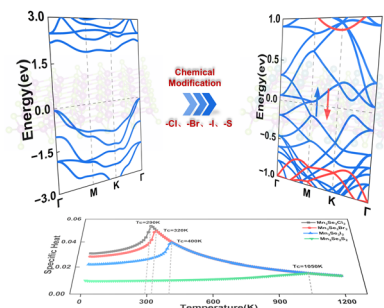
14285

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

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



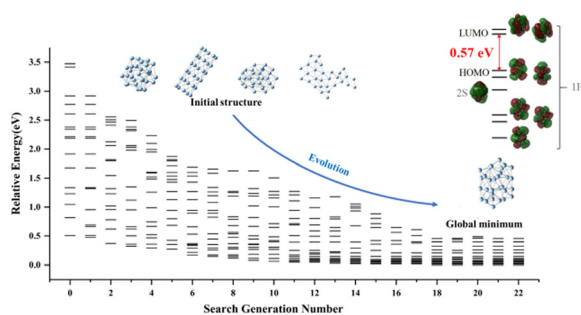
14294



### Room-temperature half-metals induced via chemical surface modification: 2D $\text{Mn}_2\text{Se}_2$ monolayer

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

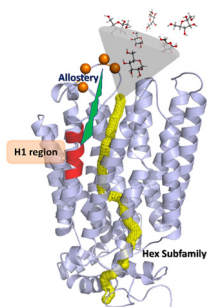
14303



### The global minimum of $\text{Ag}_{30}$ : 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\*

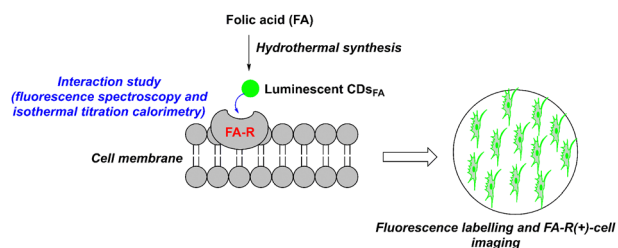
14311



### 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\*

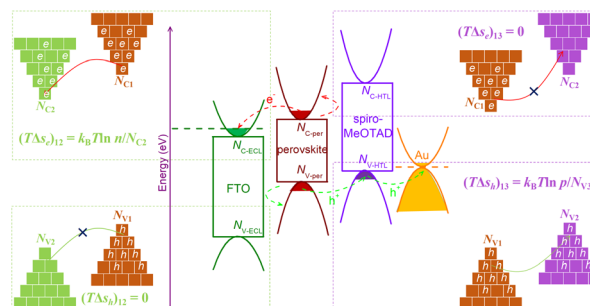


## RESEARCH PAPERS

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

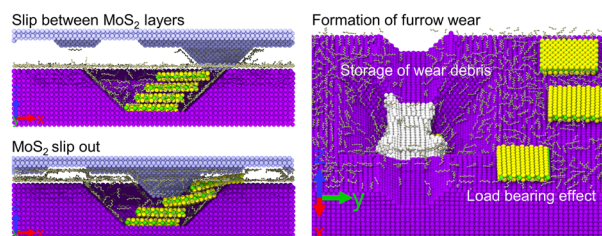
Like Huang



14348

### Frictional properties of MoS<sub>2</sub> on a multi-level rough wall under starved lubrication

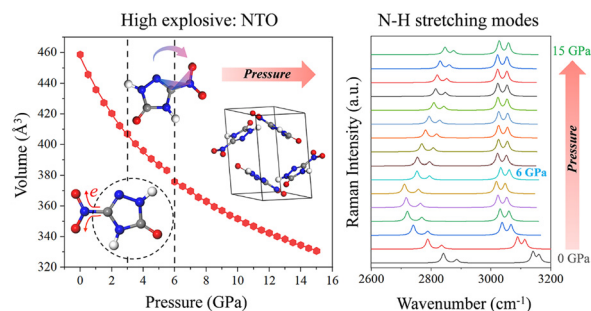
Changli Yi, Chengzhi Hu,\* Lin Shi, Minli Bai, Yubai Li and Dawei Tang



14359

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

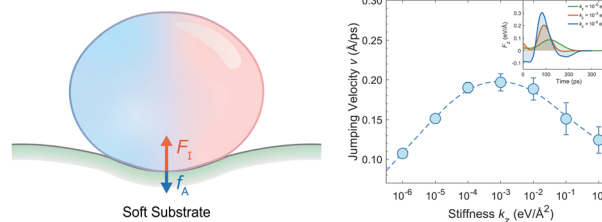
Junyu Fan, Pengju Wang and Nan Gao\*



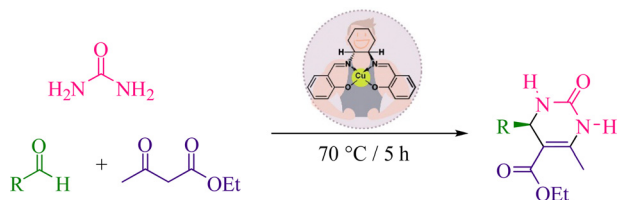
14368

### Optimum substrate stiffness in coalescence-induced droplet jumping

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



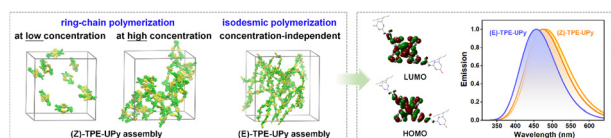
14374



### 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\*

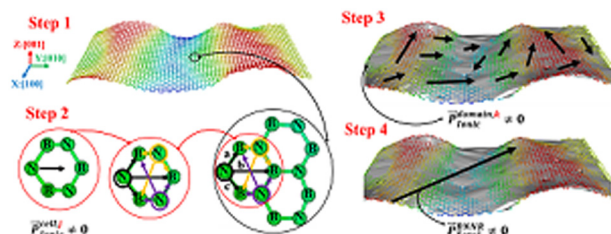
14387



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

Hui Wang, Junfang Yang and Xiaoyan Zheng\*

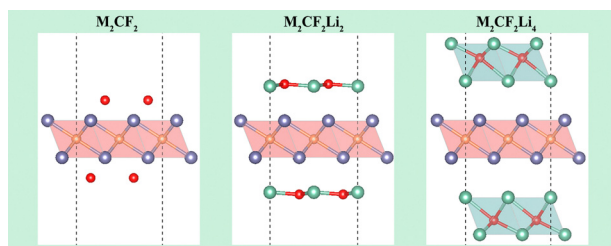
14400



### 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\*

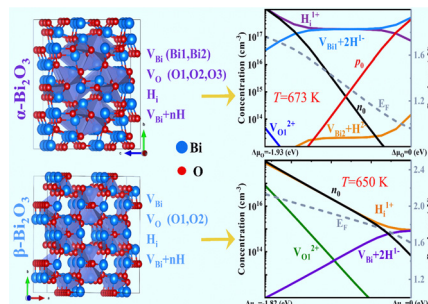




14417

### Intrinsic point defects and the n- and p-type dopability in $\alpha$ - and $\beta$ - $\text{Bi}_2\text{O}_3$ photocatalysts

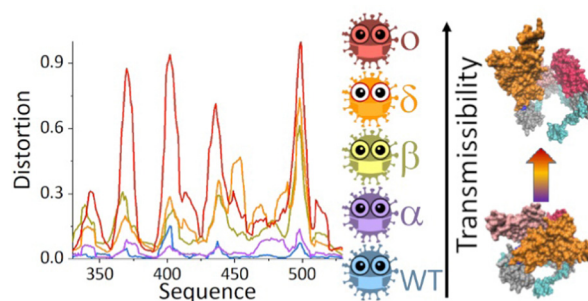
Jincheng Wang, Zuoyin Liu, Bo Kong,\* Xinyou An, Min Zhang and Wentao Wang\*



14430

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

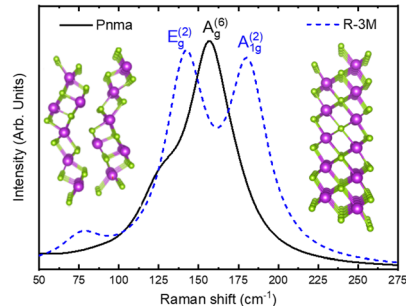
Inbal Tuvi-Arad\* and Yaffa Shalit



14440

### Vibrational properties of metastable orthorhombic $\text{Bi}_2\text{Se}_3$

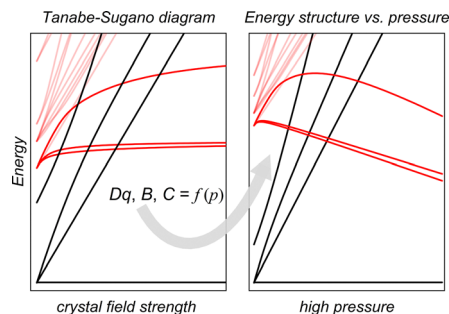
Paloma B. Souza, Milton A. Tumelero,\* Ricardo Faccio, Rasin Ahmed, Cristian C. Plá Cid, Giovanni Zangari and Andre A. Pasa



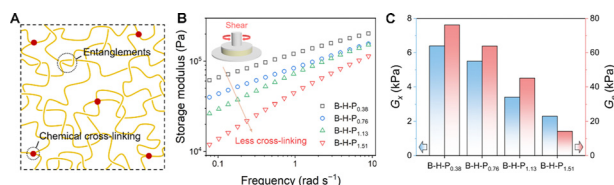
14449

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

Tadeusz Leńniewski



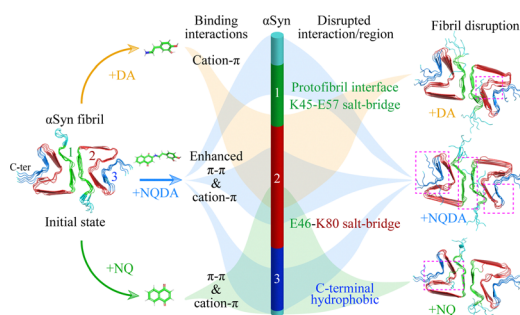
14463



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

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

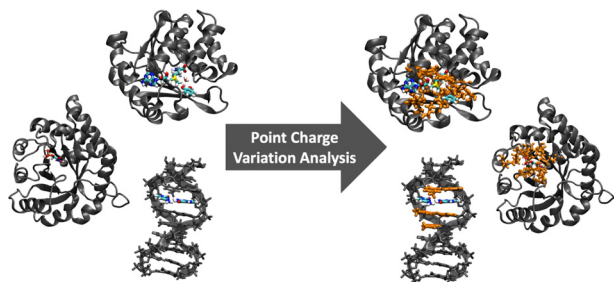
14471



## Naphthoquinone–dopamine hybrids disrupt $\alpha$ -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\*

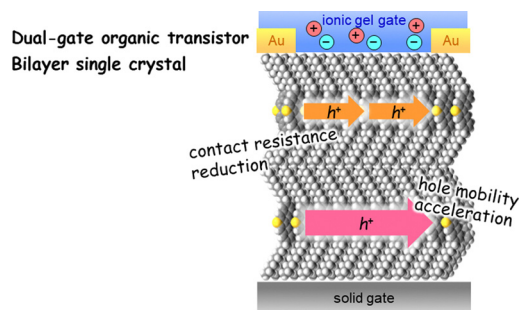
14484



## 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\*

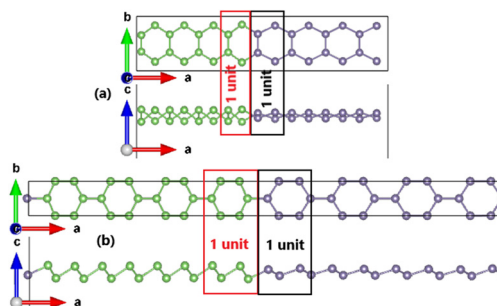


## RESEARCH PAPERS

14502

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

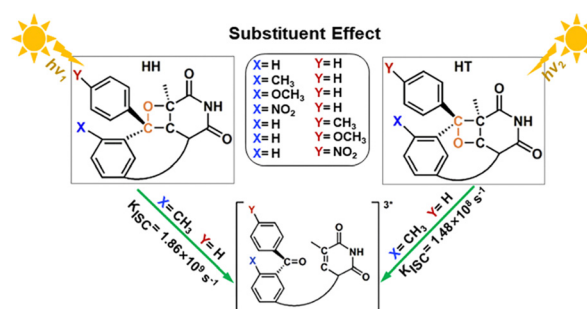
Chu Viet Ha, Bich Ngoc Nguyen Thi, Pham Quynh Trang, R. Ponce-Pérez, J. Guerrero-Sanchez and D. M. Hoat\*



14511

### Controlling the repair mechanisms of oxetanes through functional group substitution

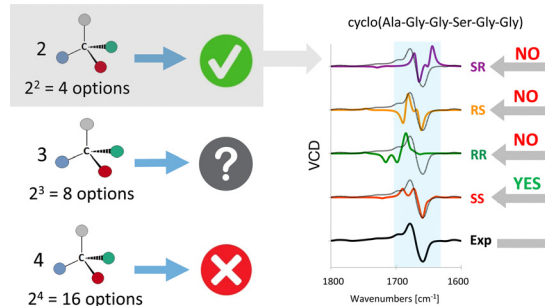
Yan Shen, Shaoqin Zhang, Yingli Su, Zexing Qu\* and Haisheng Ren\*



14520

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

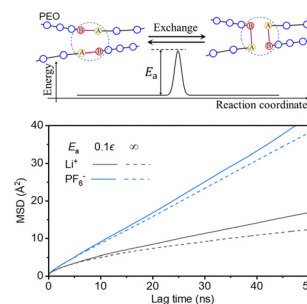
Karolina Di Remigio Eikás\*, Monika Krupová, Tone Kristoffersen, Maarten T. P. Beerepoot and Kenneth Ruud\*



14530

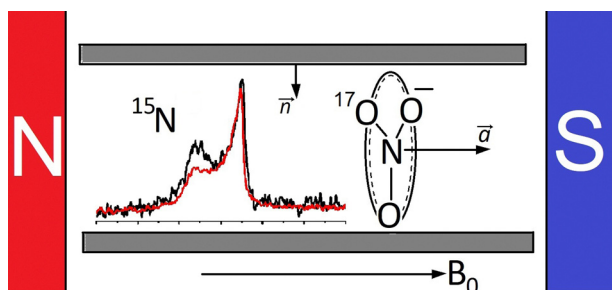
### Structure and dynamics of dynamic covalent cross-linked PEOs and PEO/LiPF<sub>6</sub> electrolytes: a coarse-grained simulation study

Tongfei Wu\* and Ping Zhang



## RESEARCH PAPERS

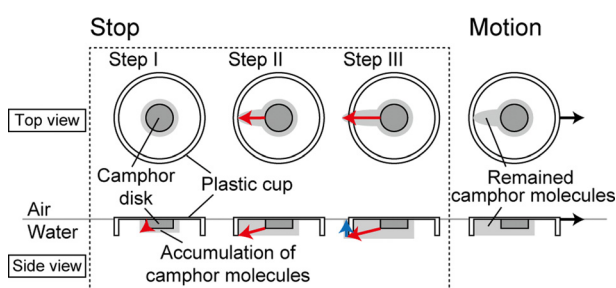
14538



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

Andrei Filippov\* and Oleg N. Antzutkin

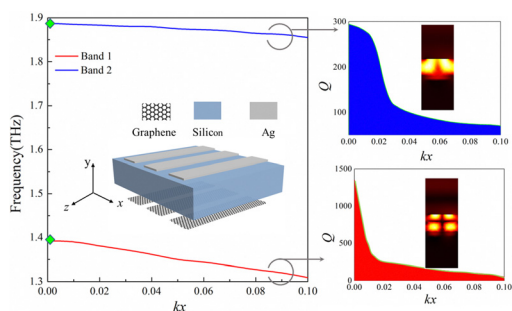
14546



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

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

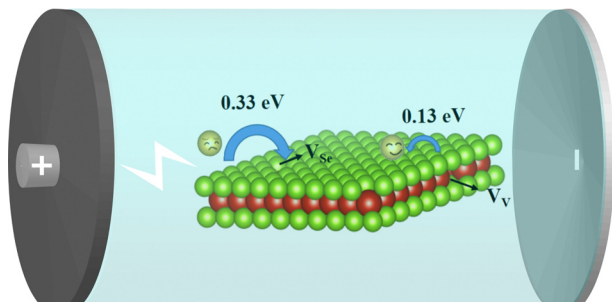
14552



### 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 $\text{VSe}_2$ monolayer with engineering-induced vacancies

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



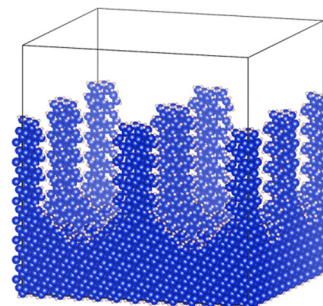


## RESEARCH PAPERS

14566

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

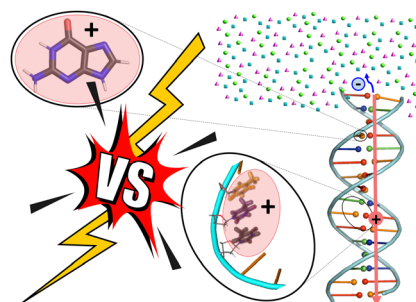
Panus Sundarapura, Sergei Manzhos\* and Manabu Ihara\*



14578

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

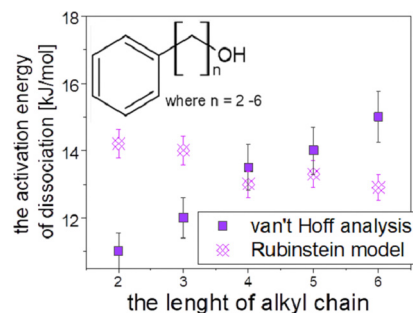
Jesús Lucia-Tamudo,\* Sergio Díaz-Tendero\* and Juan J. Nogueira\*



14590

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

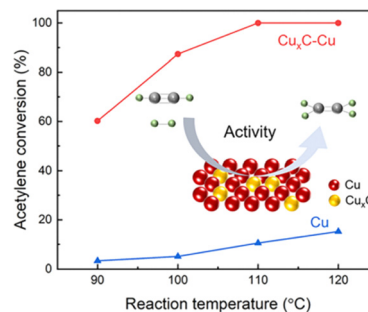
Anna Czaderna-Lekka,\* Magdalena Tarnacka,\* Zaneta Wojnarowska, Barbara Hachuta, Marian Paluch and Kamil Kamiński



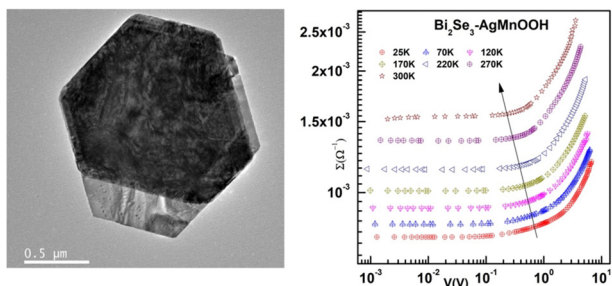
14598

### 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\*



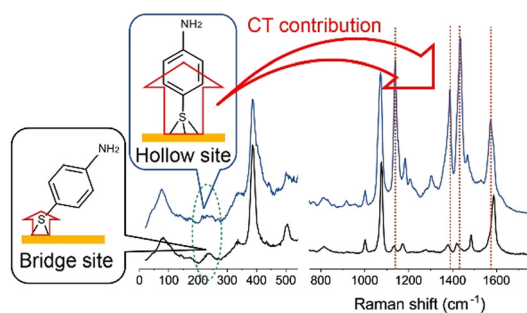
14606



### Investigation of electrical transport properties in solution-processed $\text{Bi}_2\text{Se}_3$ -AgMnOOH nanocomposite

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

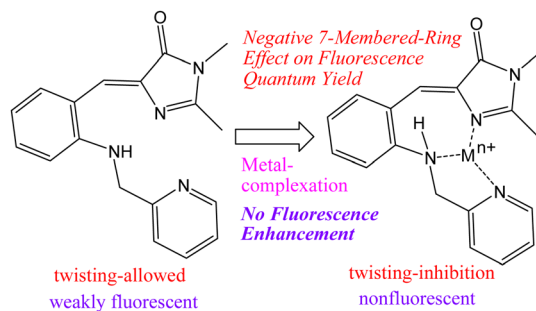
14618



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

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

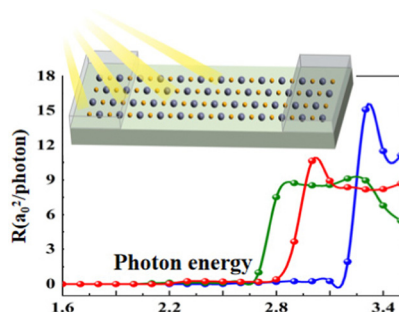
14627



### 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\*

