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IN THIS ISSUE

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REVIEWS

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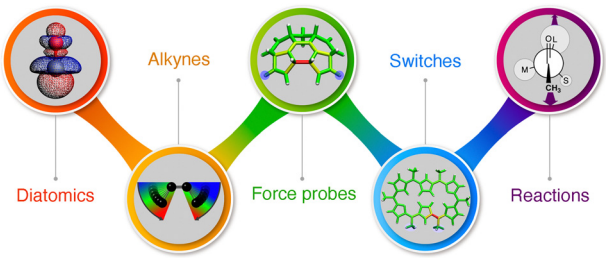
Wandering through quantum-mechanochemistry: from concepts to reactivity and switches

Mercedes Alonso,* Tom Bettens, Jochen Eeckhoudt, Paul Geerlings and Frank De Proft*



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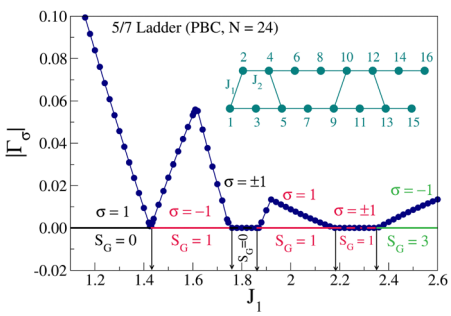
Quantum phase transitions in skewed ladder systems

Sambunath Das, Dayasindhu Dey, Rajamani Raghunathan, Zoltan G. Soos, Manoranjan Kumar* and S. Ramasesha*



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COMMUNICATIONS

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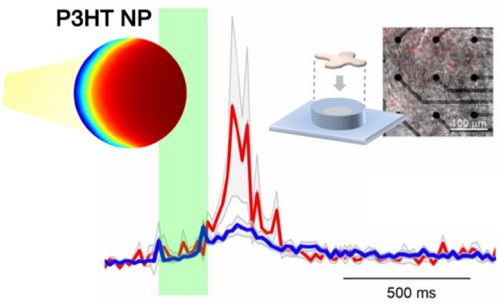
The light-dependent pseudo-capacitive charging of conjugated polymer nanoparticles coupled with the depolarization of the neuronal membrane

Greta Chiaravalli, Tiziana Ravasenga, Elisabetta Colombo, Jasnoor, Simona Francia, Stefano Di Marco, Riccardo Sacco, Grazia Pertile, Fabio Benfenati* and Guglielmo Lanzani*



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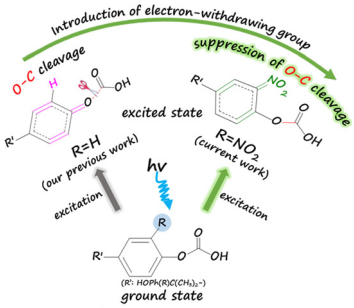
Theoretical design of durable and strong polycarbonates against photodegradation

Xiao Huang, Yuuichi Orimoto and Yuriko Aoki*



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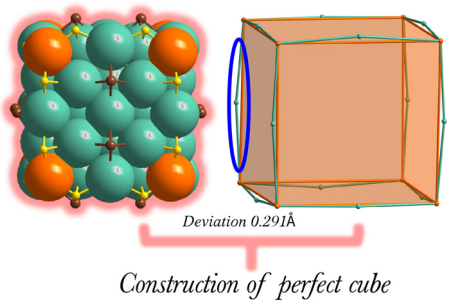
Constructing perfect cubic Ag–Cu alloyed nanoclusters through selective elimination of phosphine ligands

Li Tang, Qikai Han, Bin Wang, Zhonghua Yang, Chunyuan Song, Guanyu Feng and Shuxin Wang*



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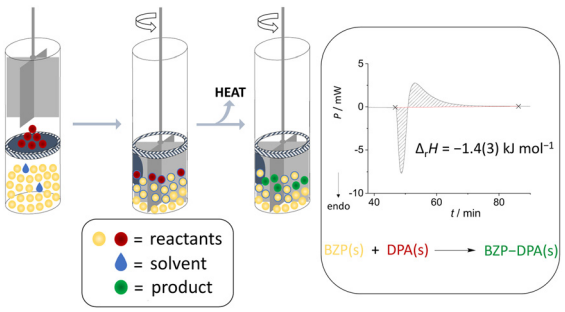
Direct thermodynamic characterization of solid-state reactions by isothermal calorimetry

Marija Cvetnić, Robert Šplajt, Edi Topić, Mirta Rubčić and Nikola Bregović*



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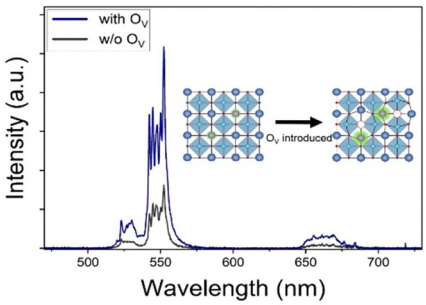

Enhancing the upconversion of Er^{3+} incorporated $BaTiO_3$ by introducing oxygen vacancies

Young Gwon Jung, Hyeongyu Bae and Kang Taek Lee*

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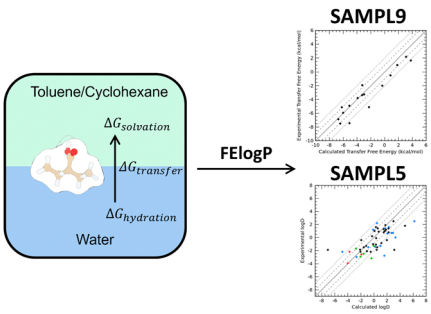

Development and test of highly accurate endpoint free energy methods. 3: partition coefficient prediction using a Poisson–Boltzmann method combined with a solvent accessible surface area model for SAMPL challenges

Taoyu Niu, Xibing He, Fengyang Han, Luxuan Wang and Junmei Wang*

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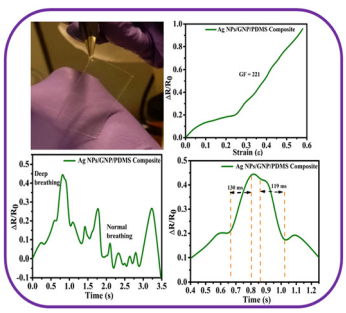

Flexible piezo-resistive strain sensors using all-polydimethylsiloxane based hybrid nanocomposites for wearable electronics

Rajib Mahato, Sk. Masiul Islam,* Ranjan Kumar Maurya, Sanjeev Kumar, Gaurav Purohit and Sumitra Singh*

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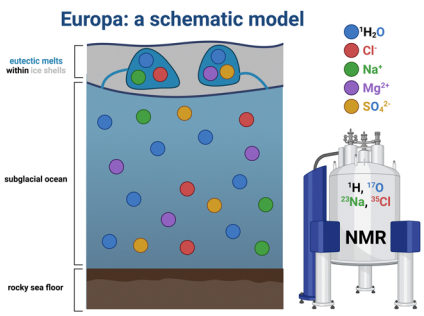

Water dynamics in eutectic solutions of sodium chloride and magnesium sulfate: implications for life in Europa's subsurface ocean and ice shell

Daniel Sieme and Nasrollah Rezaei-Ghaleh*

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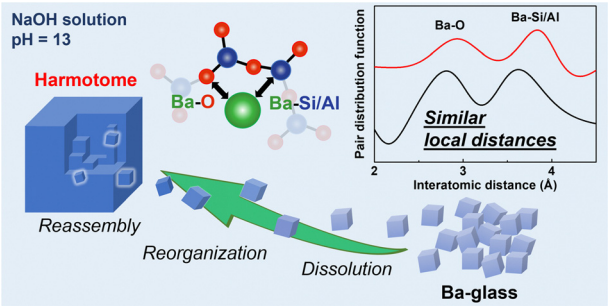
Revealing the evolution of local structures in the formation process of alkaline earth metal cation-containing zeolites from glasses

Peidong Hu, Makiko Deguchi, Hiroki Yamada, Kentaro Kobayashi, Koji Ohara, Sohei Sukenaga, Mariko Ando, Hiroyuki Shibata, Akihiko Machida, Yutaka Yanaba, Zhendong Liu,* Tatsuya Okubo and Toru Wakihara*



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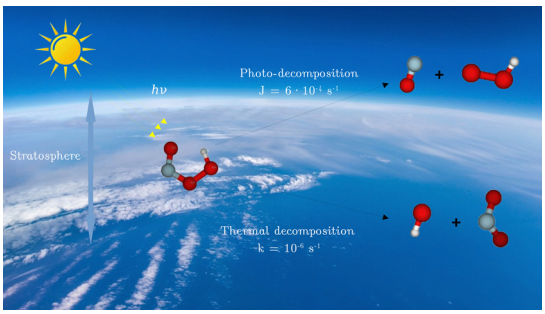
UV-spectrum and photodecomposition of peroxynitrous acid in the troposphere

Wiem Chebbi,* Najoua Derbel, Alexander Alijah and Thibaud Cours



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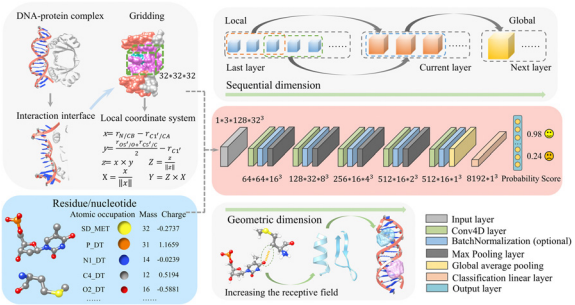
Evaluation of DNA–protein complex structures using the deep learning method

Chengwei Zeng, Yiren Jian, Chen Zhuo, Anbang Li, Chen Zeng and Yunjie Zhao*



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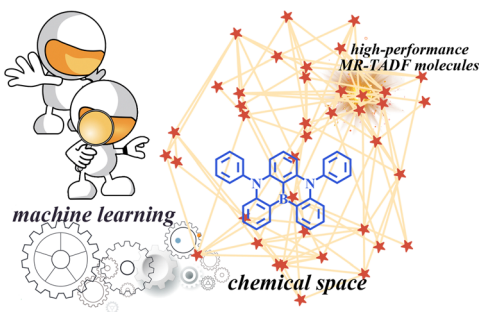
Machine-learning-assisted performance improvements for multi-resonance thermally activated delayed fluorescence molecules

Wanlin Cai, Cheng Zhong, Zi-Wei Ma, Zhuan-Yun Cai, Yue Qiu, Zubia Sajid and De-Yin Wu*



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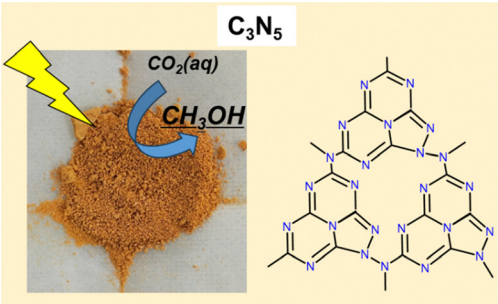

Highly efficient hydrogen production and selective CO_2 reduction by the C_3N_5 photocatalyst using only visible light

Kosei Ito and Kei Noda*

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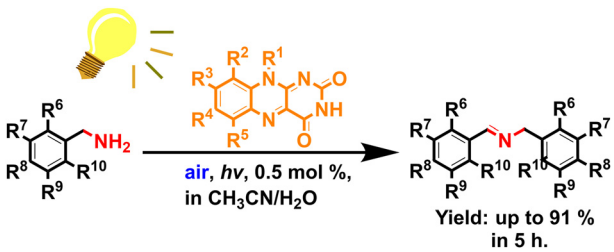

Tailoring flavin-based photosensitizers for efficient photooxidative coupling of benzylic amines

Huimin Guo,* Yang Qiu, Siyu Liu, Xiangyu Zhang and Jianzhang Zhao

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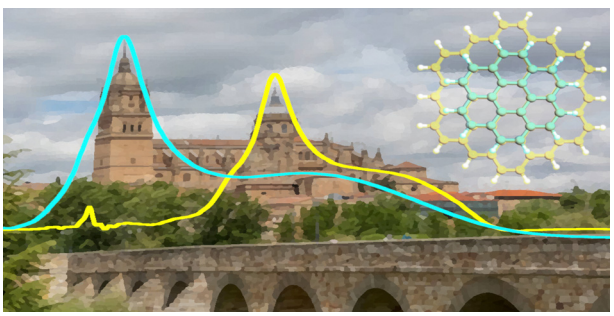

Coronene: a model for ultrafast dynamics in graphene nanoflakes and PAHs

Alberto Martín Santa Daría, Lola González-Sánchez and Sandra Gómez*

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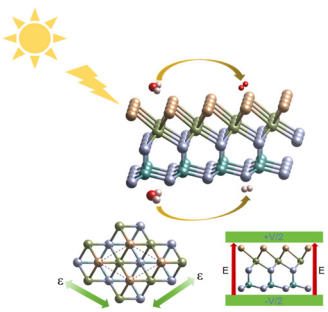

Two-dimensional $SPdAZ_2$ (A = Si, Ge; Z = N, P, As) monolayers with an intrinsic electric field for high-performance photocatalysis

Zhen Gao, Yao He* and Kai Xiong*

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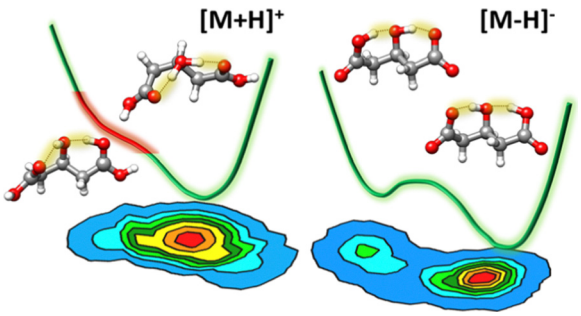
Correlated proton dynamics in hydrogen bonding networks: the benchmark case of 3-hydroxyglutaric acid

Bruno Martínez-Haya,* Juan Ramón Avilés-Moreno, Francisco Gámez, Jonathan Martens, Jos Oomens and Giel Berden



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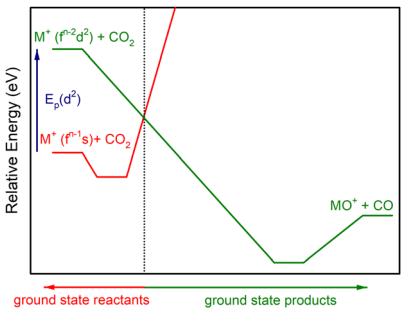
f-Block reactions of metal cations with carbon dioxide studied by inductively coupled plasma tandem mass spectrometry

Richard M Cox,* Kali M. Melby, Amanda D. French and Michael J. Rodriguez



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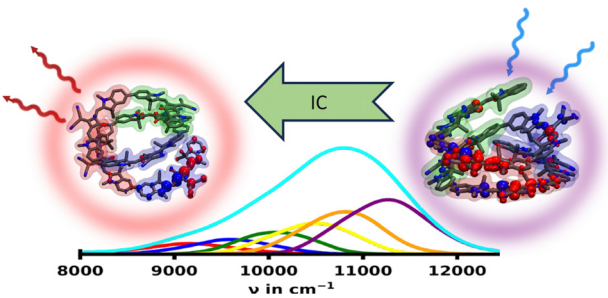
Simulation of exciton spectra in disordered supramolecular polymers: exciton localization in *cisoid* indolenine squaraine hexamers

David Fischermeier, Arthur Turkin, Joshua Selby, Christoph Lambert and Roland Mitrić*



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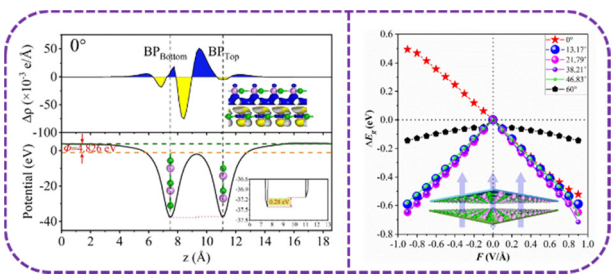
Twist angle and electric gating controllable electronic structure of the two-dimensional stacked BP homo-structure

Linwei Yao, Jiangni Yun,* Peng Kang, Hongyuan Zhao, Siyu Zhang, Liru Zeng, Zhisong Bi, Junfeng Yan, Wu Zhao and Zhiyong Zhang



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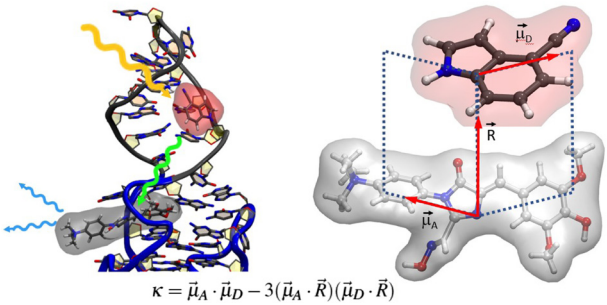

Conformational preferences of modified nucleobases in RNA aptamers and their effect on Förster resonant energy transfer

David Fischermeier, Christian Steinmetzger, Claudia Höbartner and Roland Mitrić*

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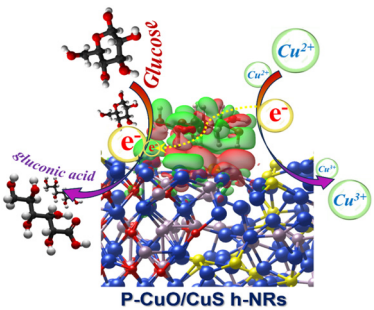

P-incorporated CuO/Cu_2S heteronanorods as efficient electrocatalysts for the glucose oxidation reaction toward highly sensitive and selective glucose sensing

L. L. D. Thi,* Thi H. Ho, Tuan V. Vu, Dang L. T. Nguyen, Minh Xuan Tran, Sonny H. Rhim and C.-D. Nguyen*

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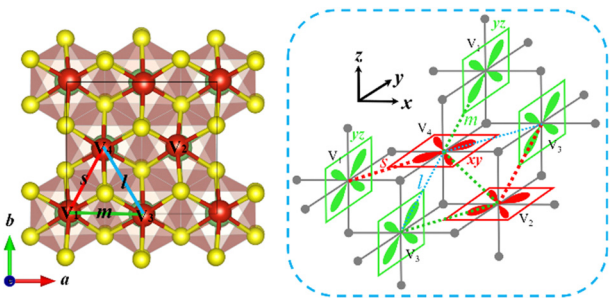

Structural dimerization and charge-orbital ordering in a ferromagnetic semiconductor LiV_2S_4 monolayer

Rui Song, Bili Wang, Kai Feng, Jia Yao, Mengjie Lu, Jing Bai, Shuai Dong and Ming An*

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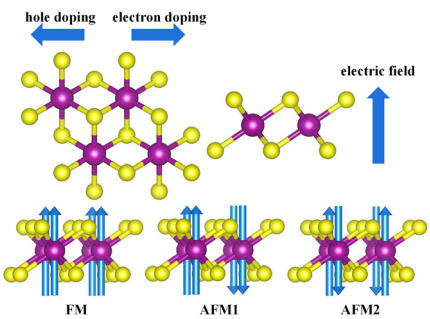

Charge doping and electric field tunable ferromagnetism and Curie temperature of the MnS_2 monolayer

Jing Xie,* Dongni Wu, Yangfang Liao, Xiaolong Cao and Shiyou Zhou

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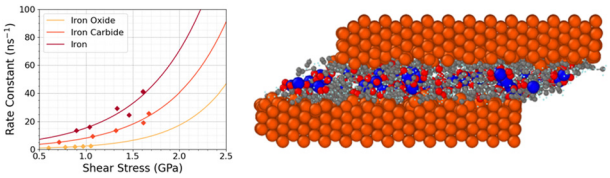
Effects of surface chemistry on the mechanochemical decomposition of tricresyl phosphate

Egheosa Ogbomo,* Fakhrul H. Bhuiyan, Carlos Ayestarán Latorre, Ashlie Martini and James P. Ewen*



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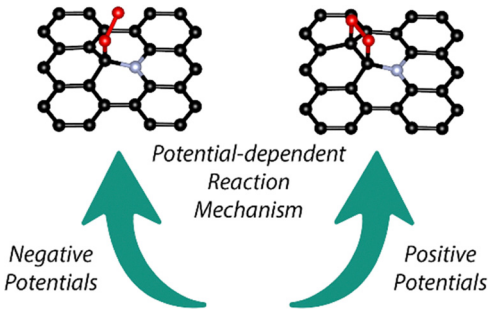
Revision of the oxygen reduction reaction on N-doped graphenes by grand-canonical DFT

Vitaliy A. Kislenko, Sergey V. Pavlov, Victoria A. Nikitina and Sergey A. Kislenko*



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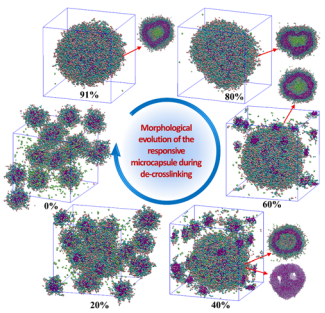
A dissipative particle dynamics simulation of controlled loading and responsive release of theranostic agents from reversible crosslinked triblock copolymer vesicles

Zhikun Wang, Fengting Li, Li Wang, Yueqi Liu, Miantuo Li, Nannan Cui, Chunling Li, Shuangqing Sun* and Songqing Hu*



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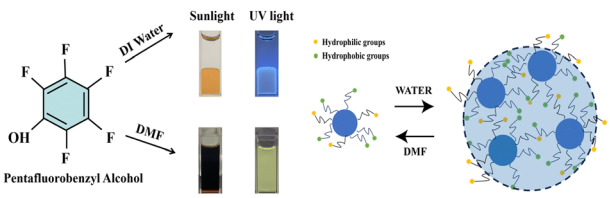
Solvent-controlled synthesis of hydrophilic and hydrophobic carbon dots

Chenhan Zhang, Zhihua Ying,* Yuan Jiang,* Haiyang Wang, Xuebin Zhou, Weipeng Xuan and Peng Zheng



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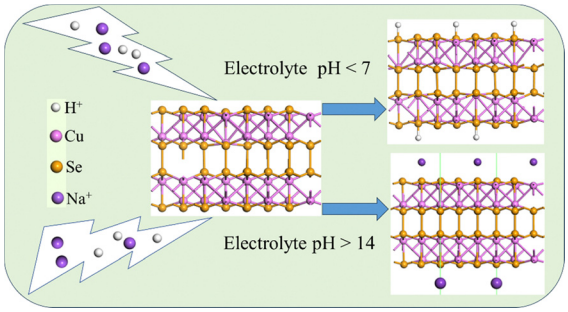

Theoretical insights into surface-phase transition and ion competition during alkali ion intercalation on the Cu_4Se_4 nanosheet

Yang-Xin Yu*

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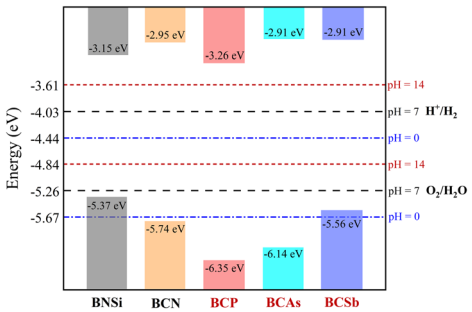

Two-dimensional ternary pentagonal BCX (X = P, As, and Sb): promising photocatalyst semiconductors for water splitting with strong piezoelectricity

Luqi Liu, Xuxin Kang, Shan Gao* and Xiangmei Duan*

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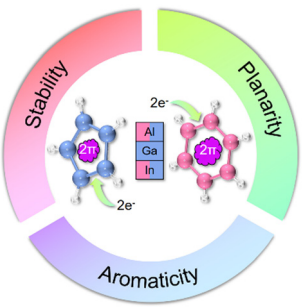

Group 13 five- and six-membered rings with rare 2π aromaticity

Yutong Huo, Xiaojiao Gu, Xinde Li and Peng Jin*

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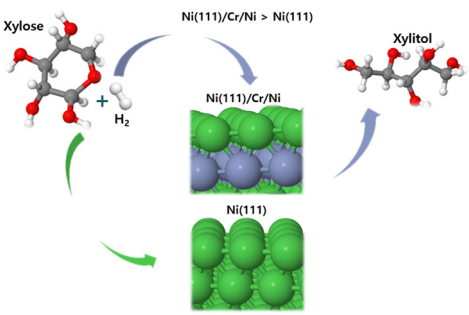

First-principles study on the design of nickel based bimetallic catalysts for xylose to xylitol conversion

Shedrack G. Akpe, Sun Hee Choi and Hyung Chul Ham*

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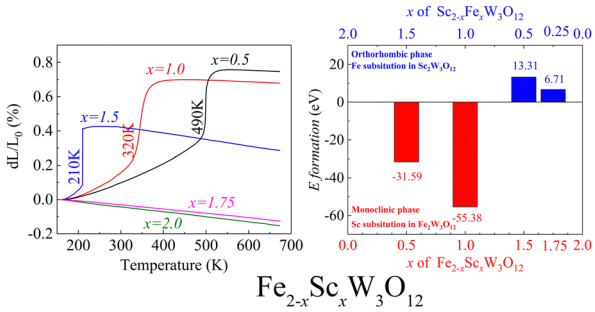
The formation energy, phase transition, and negative thermal expansion of $Fe_{2-x}Sc_xW_3O_{12}$

Gaojie Zeng, Chunyan Wang, Huanli Yuan, Xi Zhen, Qilong Gao, Juan Guo, Mingju Chao, Xiansheng Liu* and Erjun Liang*



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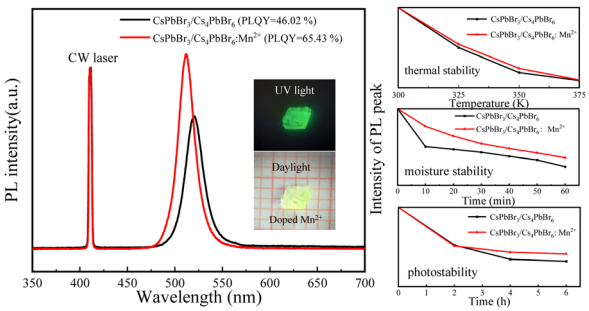
Solution-grown millimeter-scale Mn-doped $CsPbBr_3/Cs_4PbBr_6$ crystals with enhanced photoluminescence and stability for light-emitting applications

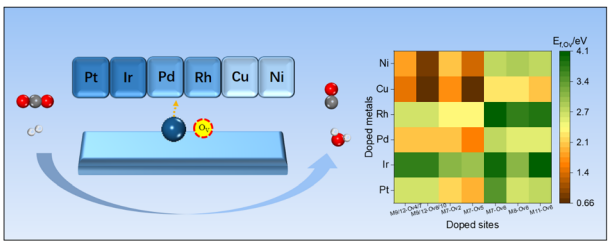
Wenfang Peng, Rongrong Hu,* Bobo Yang, Qiaoyun Wu, Pan Liang, Lin Cheng, Xixi Cheng, Yuefeng Li* and Jun Zou*



381

Computational screening of single-atom doped In_2O_3 catalysts for the reverse water gas shift reaction

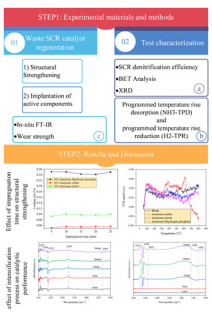
Yuchen Wang and Shenggang Li*



390

Research on structural strengthening technology for regenerative denitration catalysts

Dongliang Ji, Dongxue Jiang, Yang Li, Huan Zhang, Haiyun Zhou, Zhaoqin Huang* and Jianzhong Zhu*



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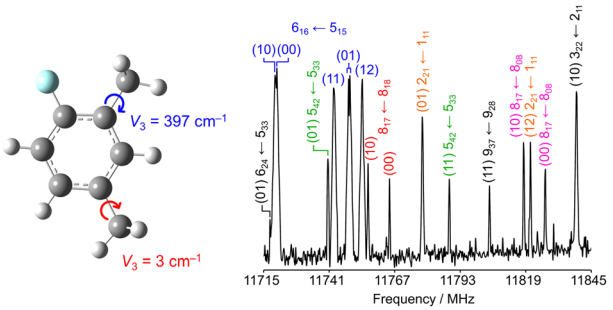
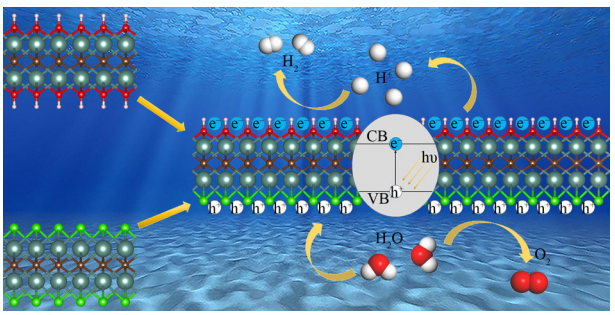
402



Approaching the free rotor limit: extremely low methyl torsional barrier observed in the microwave spectrum of 2,4-dimethylfluorobenzene

Safa Khemissi,* Martin Schwell, Isabelle Kleiner and Ha Vinh Lam Nguyen*

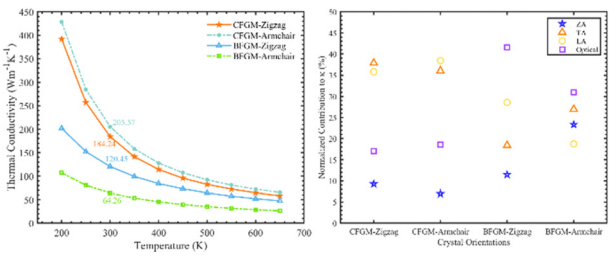
412



First-principles studies on the electronic and photocatalytic water splitting properties of surface functionalized Y_2C-based MXenes

Sheng-Yi Zhang, Ni-Ping Shi, Chuan-Kui Wang* and Guang-Ping Zhang*

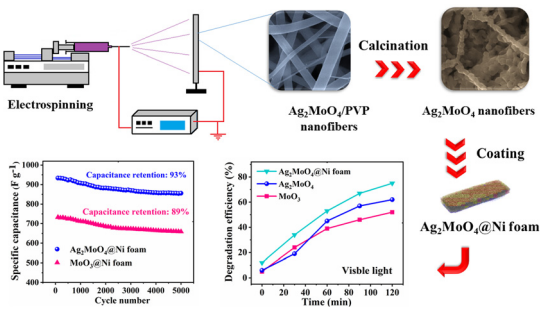
421



First-principles prediction of the thermal conductivity of two configurations of difluorinated graphene monolayer

Ao Chen, Hua Tong, Cheng-Wei Wu, Shi-Yi Li, Pin-Zhen Jia* and Wu-Xing Zhou*

430



Novel electrospun bead-like Ag_2MoO_4 nanofibers coated on Ni foam for visible light-driven heterogeneous photocatalysis and high-performance supercapacitor electrodes

Amirreza Safartoobi, Jamal Mazloom* and Farhad Esmaeili Ghodsi

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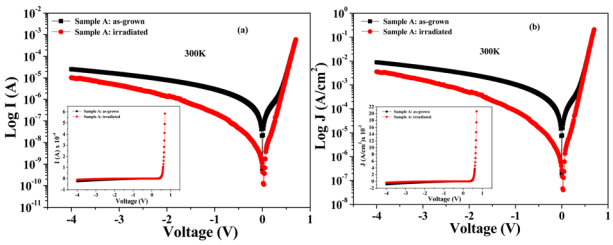
Effects of gamma radiation on the electrical properties of InAs/InGaAs quantum dot-based laser structures grown on GaAs and Si substrates by molecular beam epitaxy

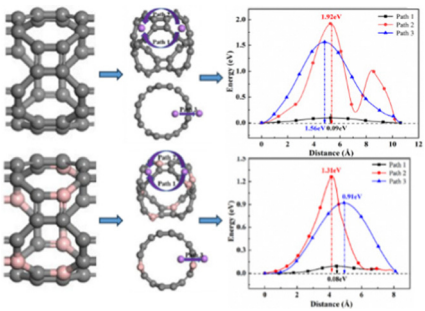
M. Al Huwayz, D. A. Jameel,* Walter M. de Azevedo, Jorlandio F. Felix, N. Al Saqri, O. M. Lemine, S. Abu Alrub and M. Henini



455

Exploring the structural stability and electrochemical performance of B doped T-graphene nanotubes from first-principles calculations

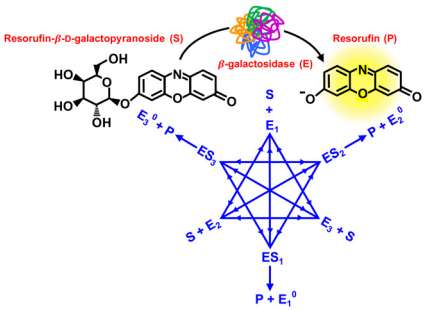
Ruyan Zhang, Yuhua Hou,* Xialei Guo, Xinyu Li, Wei Li, Xiaoma Tao and Youlin Huang*



463

A minimal kinetic model for the interpretation of complex catalysis in single enzyme molecules

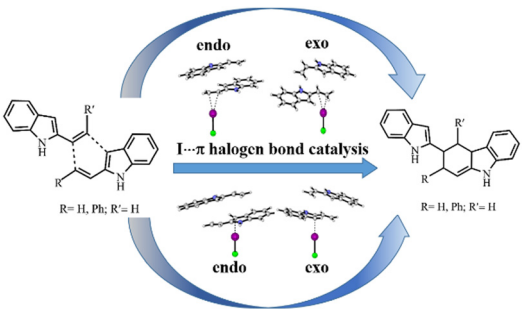
Prasanta Kundu, Soma Saha* and Gautam Gangopadhyay



477

Halogen bond catalysis of the [4+2] cycloaddition reaction of 2-alkenylindoles: catalytic modes and stereoselectivity

Ying Li, Chang Zhao, Huaiyu Zhang* and Yanli Zeng*



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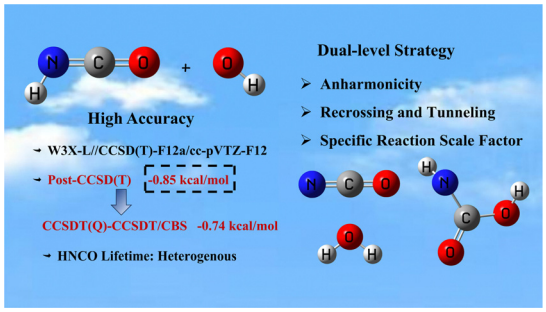
485



Quantitative kinetics of the atmospheric reaction between isocyanic acid and hydroxyl radicals: post-CCSD(T) contribution, anharmonicity, recrossing effects, torsional anharmonicity, and tunneling

Dai-Dan Deng and Bo Long*

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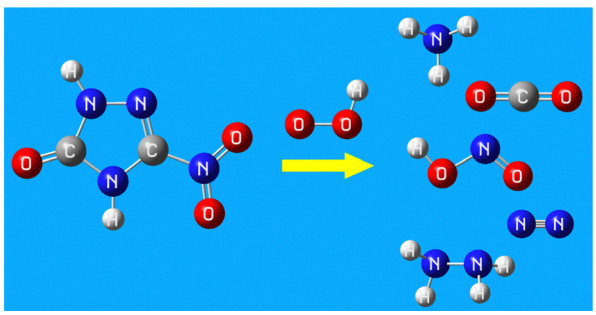

Degradation of NTO induced by superoxide and hydroperoxyl radicals: a comprehensive DFT study

Liudmyla K. Sviatenko, Leonid Gorb and Jerzy Leszczynski*

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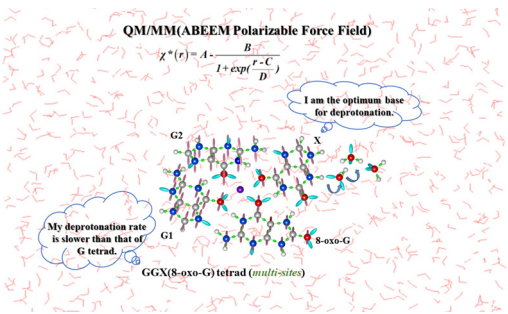

Development of a QM/MM(ABEEM) method for the deprotonation of neutral and cation radicals in the G-tetrad and GGX(8-oxo-G) tetrad

Yue Wang, Linlin Liu, Yue Gao, Jiayue Zhao, Cui Liu,* Lidong Gong* and Zhongzhi Yang

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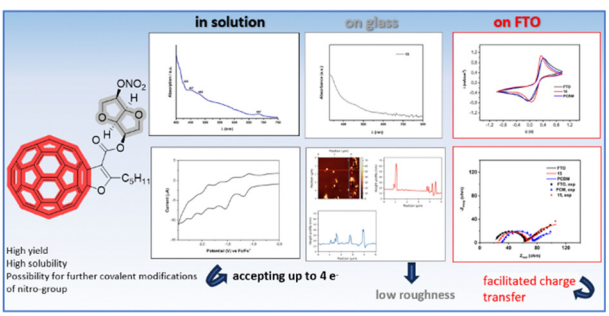

Exploring fullerene derivatives for optoelectronic applications: synthesis and characterization study

Jovana Jakšić, Evgenija Milinković, Katarina Cvetanović, Zorana Tokić Vujošević, Vladislav Jovanov, Aleksandra Mitrović* and Veselin Maslak*

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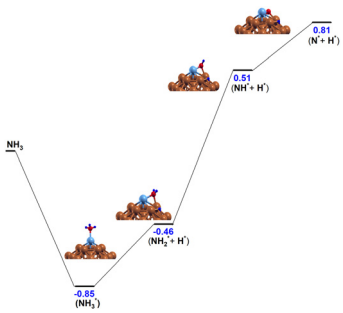
524

Adsorption and dehydrogenation of ammonia on Ru_{55}, Cu_{55} and $Ru@Cu_{54}$ nanoclusters: role of single atom alloy catalyst

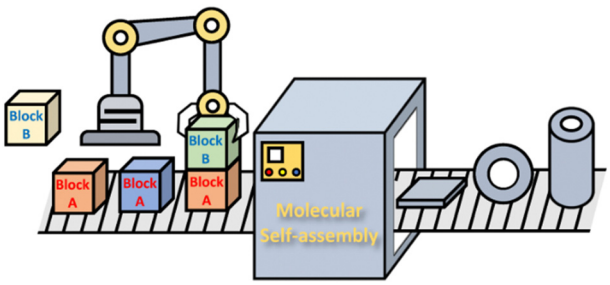
D. Chattaraj* and C. Majumder



533

Self-assembly morphology transition mechanism of similar amphiphilic molecules

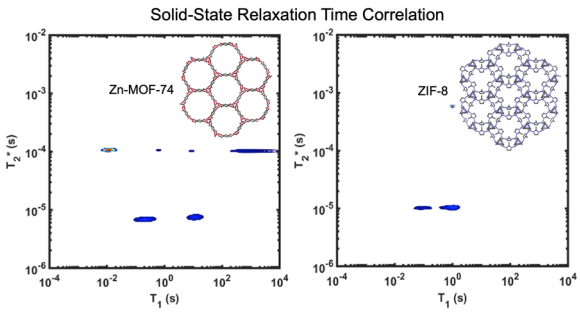
Junben Weng, Haojiang Yao, Junfeng Wang* and Guohui Li*



543

***In situ* monitoring of mechanochemical MOF formation by NMR relaxation time correlation**

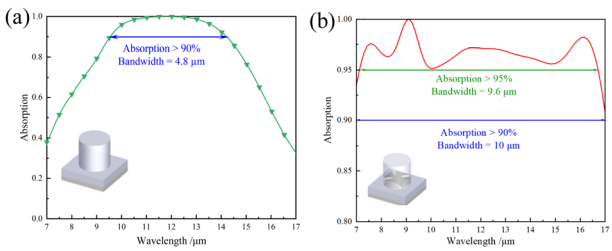
Madeleine E. Leger, Jiangfeng Guo, Bryce MacMillan, Hatem M. Titi, Tomislav Friščić, Bruce Balcom* and Barry A. Blight*



551

Design of metamaterial perfect absorbers in the long-wave infrared region

Yang Wang, Xiu Li, Shenbing Wu, Changjun Hu and Yuanyuan Liu*



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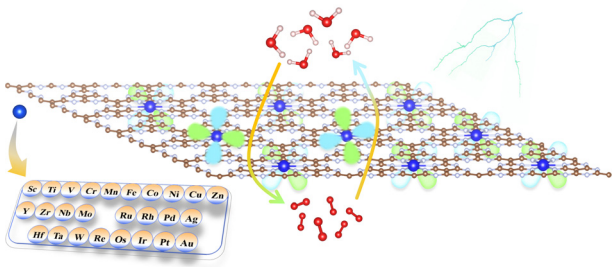

The regulatory function of the d-orbital structure in TM@g-t-C_4N_3 for bifunctional catalysis of the oxygen evolution/reduction reaction

Zhenduo Wang, Meichen Wu, Yuhong Huang, Jianmin Zhang* and Xiumei Wei*

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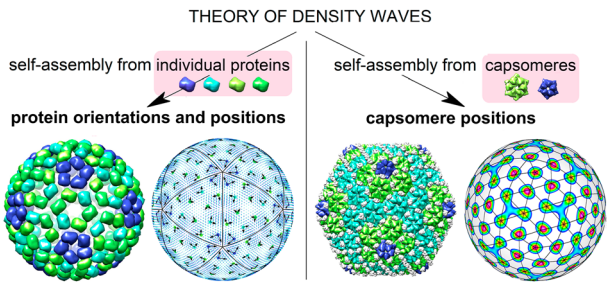

Theory of density waves and organization of proteins in icosahedral virus capsids

Olga V. Konevtsova, Dmitrii V. Chalin and Sergei B. Rochal*

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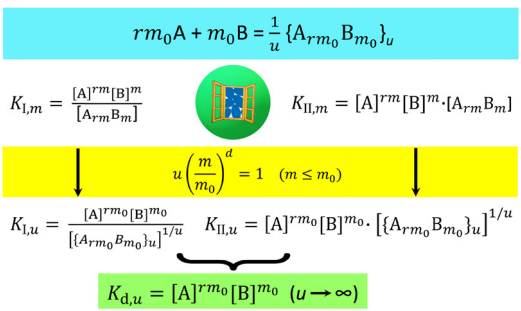

Pseudo-equilibrium equations for calcium phosphate precipitation with multi-unit particles

Tian-Lan Zhang

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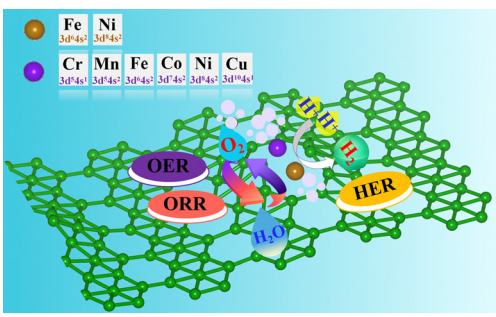

Bifunctional diatomic site catalysts supported by β_{12}-borophene for efficient oxygen evolution and reduction reactions

Jia Liu, Minjing Zhang, Si-Dian Li* and Yuewen Mu*

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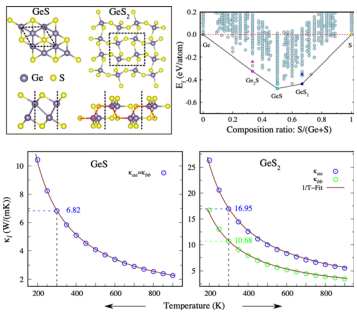
602

Prediction of novel ground-state structures and analysis of phonon transport in two-dimensional Ge_xS_y compounds

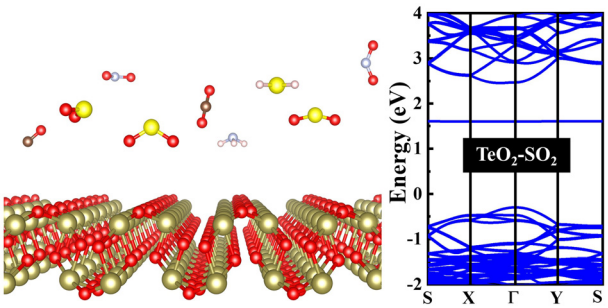
Asad Ali and Young-Han Shin*



612

Adsorption and sensing performance of air pollutants on a β-TeO_2 monolayer: a first-principles study

Ying Wang, Shiying Guo,* Xiaoyong Xu, Jing Pan, Jingguo Hu and Shengli Zhang*



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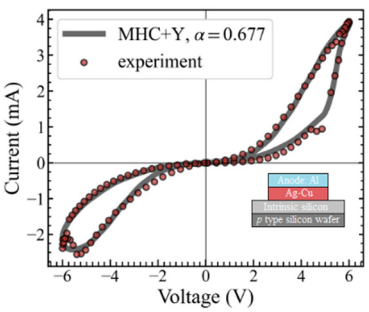
Fractional Marcus–Hush–Chidsey–Yakopcic current–voltage model for redox-based resistive memory devices

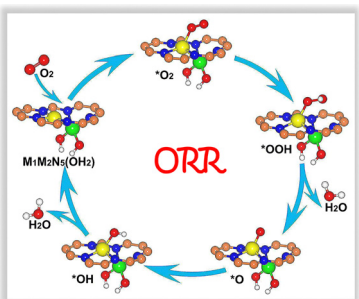
G. V. Paradezhenko,* D. V. Prodan, A. A. Pervishko, D. Yudin and A. Allagui



628

Boosting the oxygen reduction reaction activity of dual-atom catalysts on N-doped graphene by regulating the N coordination environment

Lei Li,* Xiaoxia Wu, Qiuying Du, Narsu Bai and Yuhua Wen*



CORRECTION

635

Correction: Structural, electronic, optical, elastic, thermodynamic and thermal transport properties of $Cs_2AgInCl_6$ and $Cs_2AgSbCl_6$ double perovskite semiconductors using a first-principles study

Keqing Zhang, Lijun Zhang, S. K. S. Saravana Karthikeyan, Chang Yi Kong, Fuchun Zhang, Xiang Guo,* Nam Nguyen Dang, Sankar Ganesh Ramaraj* and Xinghui Liu*

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