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Andreas W. Hauser, Martina Havenith, Markus Koch and Martin Sterrer

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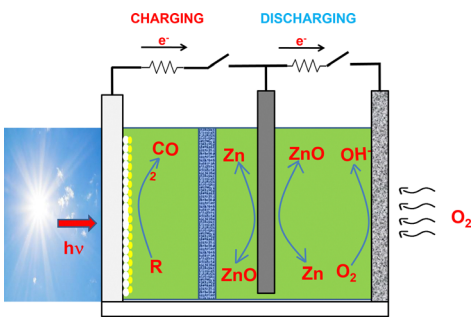

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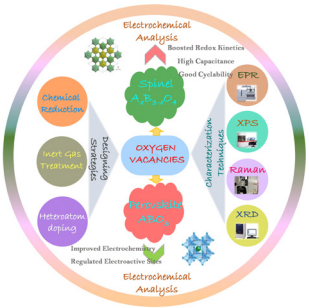
Overview of the oxygen vacancy effect in bimetallic spinel and perovskite oxide electrode materials for high-performance supercapacitors

Sk. Khaja Hussain and Jin Ho Bang*



PERSPECTIVE

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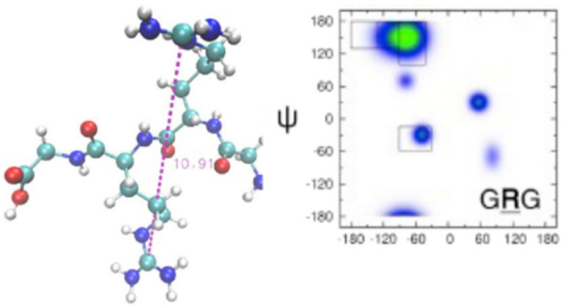
The relevance of short peptides for an understanding of unfolded and intrinsically disordered proteins

Reinhard Schweitzer-Stenner



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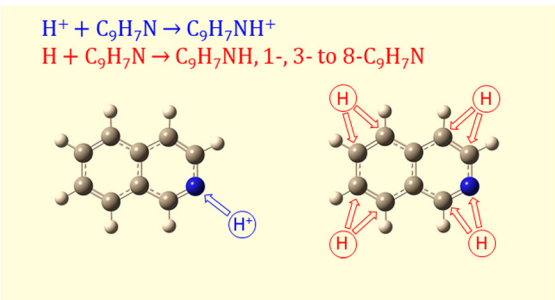
Infrared spectra of isoquinolinium (iso-$C_9H_7NH^+$) and isoquinolinyl radicals (iso-C_9H_7NH and 1-, 3-, 4-, 5-, 6-, 7- and 8-iso-HC_9H_7N) isolated in solid *para*-hydrogen

Prasad Ramesh Joshi,* Masashi Tsuge,* Chih-Yu Tseng and Yuan-Pern Lee*



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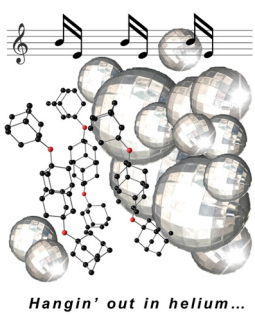
Diamondoid ether clusters in helium nanodroplets

Jasna Alić, Roman Messner, Marija Alešković, Florian Küstner, Mirta Rubčić, Florian Lackner,* Wolfgang E. Ernst* and Marina Šekutor*



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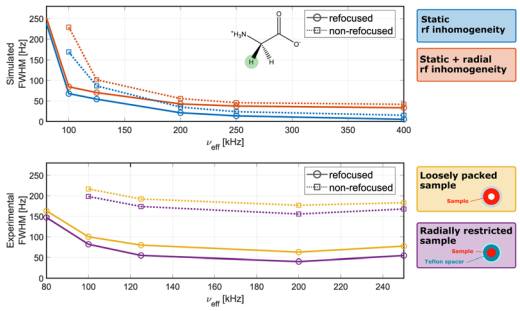
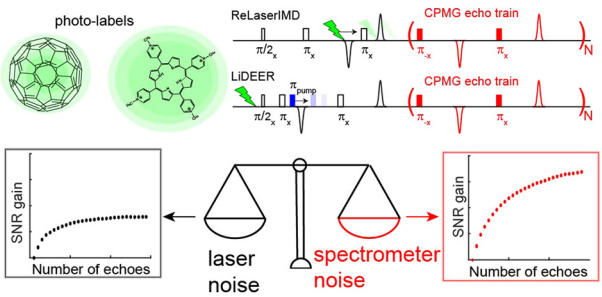


Residual proton line width under refocused frequency-switched Lee-Goldburg decoupling in MAS NMR

Kathrin Aebischer and Matthias Ernst*

11971



Sensitivity optimization in pulse EPR experiments with photo-labels by multiple-echo-integrated dynamical decoupling

Natalya E. Sannikova, Anatoly R. Melnikov, Sergey L. Veber, Olesya A. Krumkacheva* and Matvey V. Fedin*

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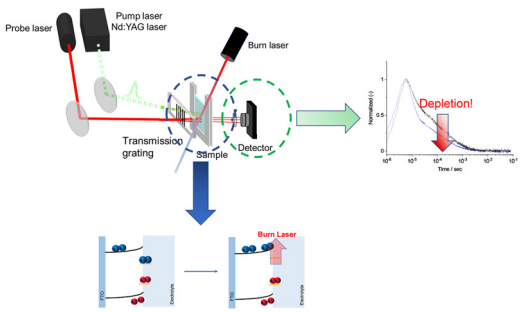

Development of charge carrier-selective heterodyne transient grating spectroscopic technique and its application in the distinction of surface trap states in hematite

Young Hyun Kim, Yu Gyeong Bae and Woon Yong Sohn*

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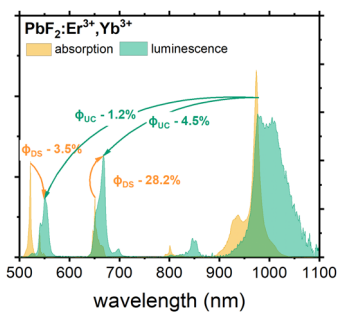

Absolute quantum yield for understanding upconversion and downshift luminescence in $PbF_2:Er^{3+},Yb^{3+}$ crystals

Eduard Madirov, Dmitry Busko, Ian A. Howard, Bryce S. Richards and Andrey Turshatov*

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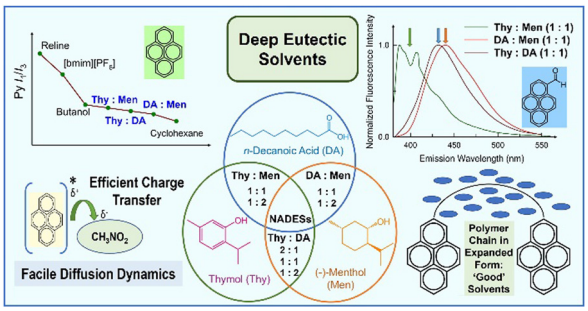
Fluorescence of pyrene and its derivatives to reveal constituent and composition dependent solvation within hydrophobic deep eutectic solvents

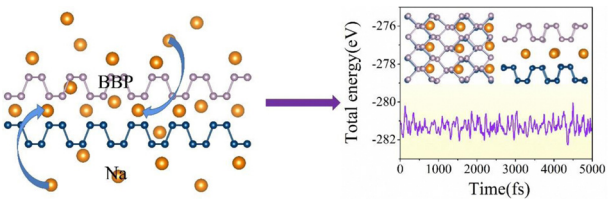
Deepika, Shreya Juneja and Siddharth Pandey*



12013

A first-principles study of bilayered black phosphorene as a potential anode material for sodium-ion batteries

Jiaxin Li, Weiling Chen, Xian Lin, Guigui Xu, Kehua Zhong,* Jian-Min Zhang* and Zhigao Huang*



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Transport coefficients from Einstein–Helfand relations using standard and energy-conserving dissipative particle dynamics methods

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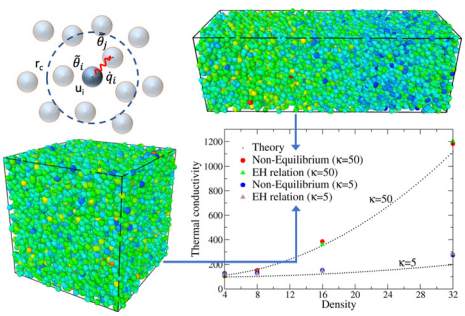

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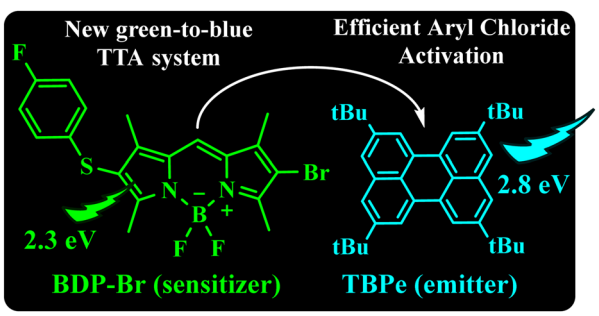
A new green-to-blue upconversion system with efficient photoredox catalytic properties

Jorge Castellanos-Soriano, Till J. B. Zähringer, Jorge C. Herrera-Luna, M. Consuelo Jiménez, Christoph Kerzig* and Raúl Pérez-Ruiz*



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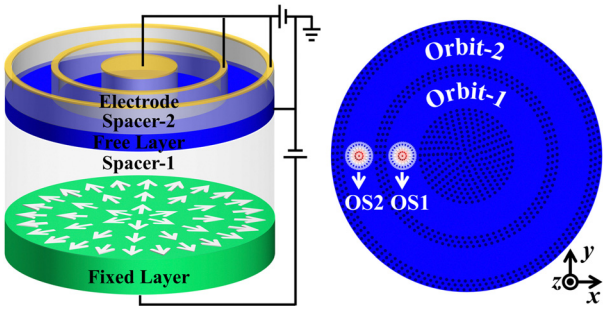
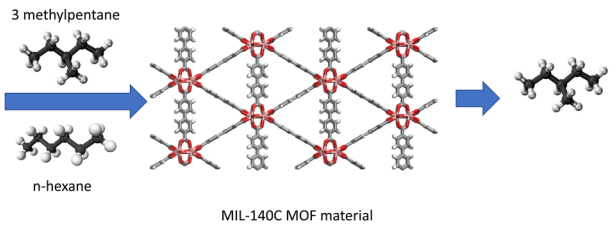


Dynamics of orbital skyrmions in a circular nanodisk

Youhua Feng, Xi Zhang* and Gang Xiang*

12057



Adsorption and dynamics of linear and mono-branched hexane isomers in MIL-140 metal–organic frameworks

Hengli Zhao, José A. C. Silva, Adriano Henrique, Farid Nouar, Christian Serre, Guillaume Maurin and Aziz Ghoufi*

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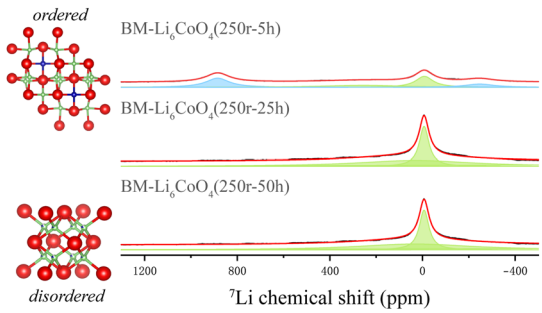

Measuring T_1 relaxation in paramagnetic solids with solid-state NMR: a case study on the milling induced phase transition in Li_6CoO_4

Nianrui Guo, Fushan Geng, Guozhong Lu, Xinbiao Jiang, Chao Li, Bingwen Hu and Ming Shen*

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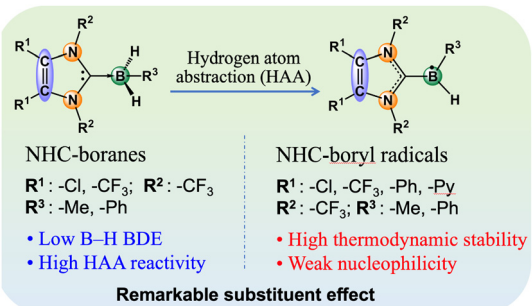

Formation and reactivity of NHC-boryl radicals: insight into substituent effect from theoretical calculations

Lin Zhang and Zexing Cao*

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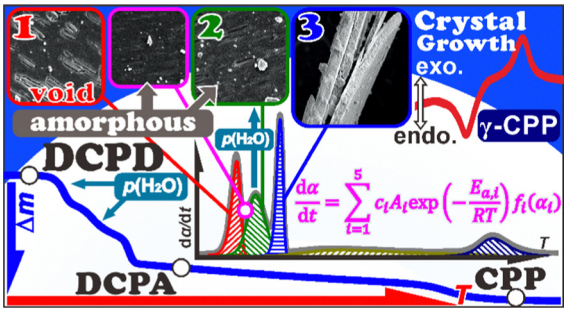
Physico-geometrical kinetic insight into multistep thermal dehydration of calcium hydrogen phosphate dihydrate

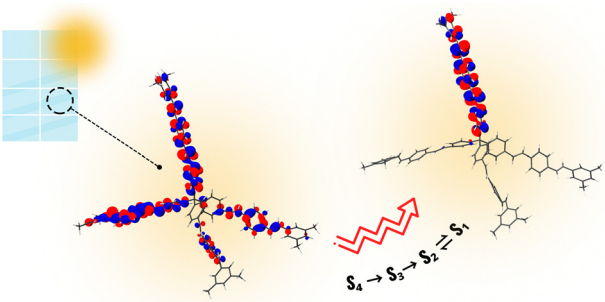
Masami Hara and Nobuyoshi Koga*



12097

Impact of the core on the inter-branch exciton exchange in dendrimers

Valeria Bonilla, Victor M. Freixas, Sebastian Fernandez-Alberti and Johan Fabian Galindo*



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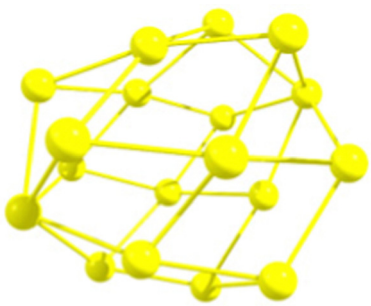
Engineering magic number Au_{19} and Au_{20} cage structures using electron withdrawing atoms

Heather M. Gaebler, Julianna R. Castiglione and Ian P. Hamilton*



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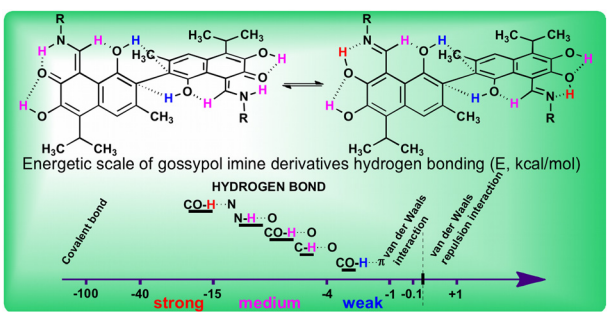
Intramolecular hydrogen bonds of gossypol imine derivatives

Oleksii M. Dykun,* Viktor M. Anishchenko, Andrii M. Redko and Volodymyr I. Rybachenko



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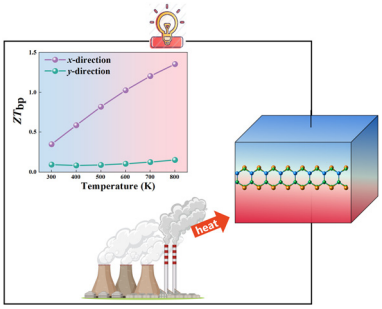

Electron–phonon coupling, bipolar effects, and thermoelectric performance of the $CuSbS_2$ monolayer

Ao-Dong Chen, Chuan-Lu Yang,* Mei-Shan Wang and Xiao-Guang Ma

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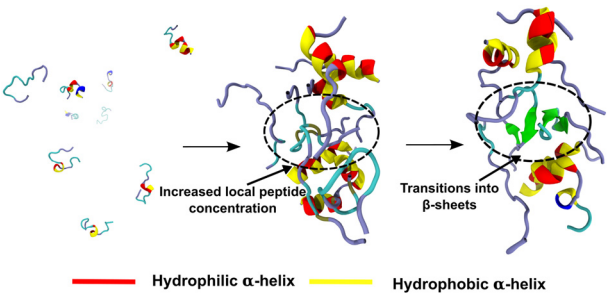

Helical intermediate formation and its role in amyloids of an amphibian antimicrobial peptide

Anup Kumar Prasad, Lisandra L. Martin and Ajay S. Panwar*

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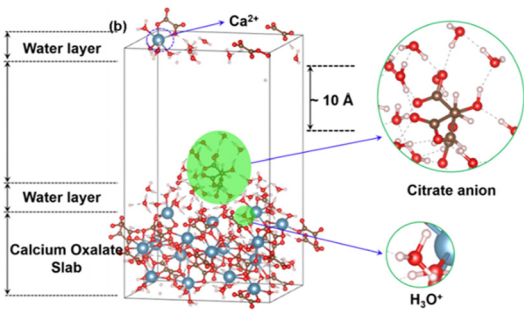
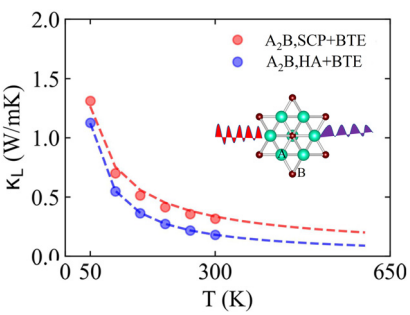


A molecular understanding of citrate adsorption on calcium oxalate polyhydrates

Yangyang Su, Jelle Vekeman, Flavio Siro Brigiano, Etienne Paul Hessou, Yuheng Zhao, Diane Sorgeloos, Marc Raes, Tom Hauffman, Kehzi Li and Frederik Tielens*

12157



Ultralow lattice thermal conductivity of binary compounds A_2B (A = Cs, Rb & B = Se, Te) with higher-order anharmonicity correction

Shuming Zeng,* Lei Fang, Yusong Tu, M. Zulfiqar* and Geng Li*

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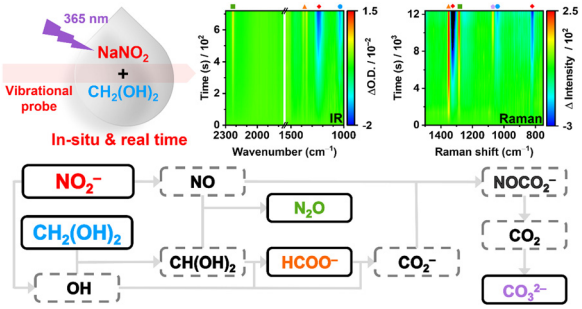
12165

***In situ* and real-time vibrational spectroscopic characterizations of the photodegradation of nitrite in the presence of methanediol**

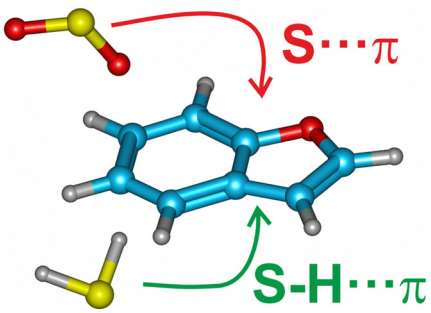
Chiao-Mi Cheng, Cheng-Zong Lu, Chun-Yao Hou, Yuan-Jyun Jhao, Yi-Fen Lai, I-Chia Chen, Yi-Hsueh Chuang and Li-Kang Chu*



12174

Sulfur–arene interactions: the S···π and S–H···π interactions in the dimers of benzofuran···sulfur dioxide and benzofuran···hydrogen sulfide

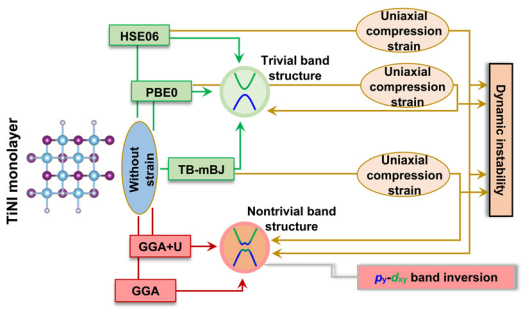
Yan Jin, Wenqin Li, Rizalina Tama Saragi, Marcos Juanes, Cristóbal Pérez, Alberto Lesarri* and Gang Feng*



12182

New insights into band inversion and topological phase of TiNI monolayer

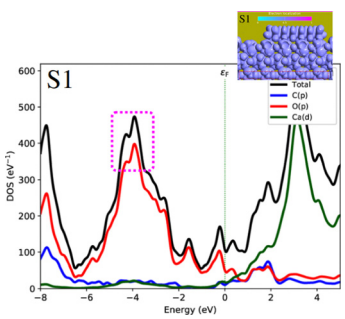
Shahram Yalameha, Zahra Nourbakhsh, Mohammad Saeed Bahramy and Daryoosh Vashaee*



12192

Unravelling the impact of oily alkane molecules on the optical properties of the calcite(10.4) surface

Junais Habeeb Mokkath



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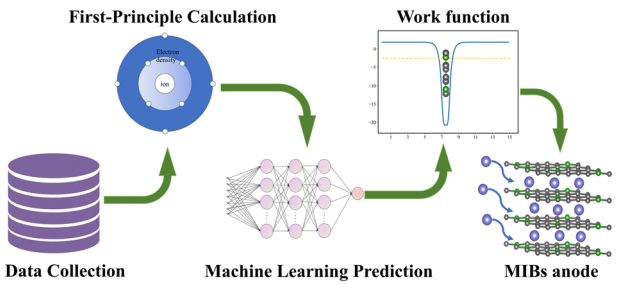
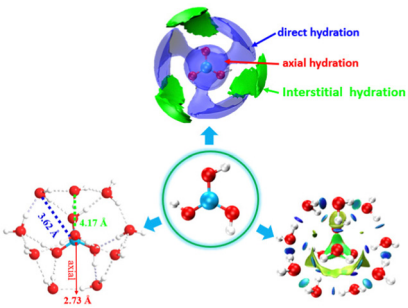
12200



Machine-learning-assisted discovery of boron-doped graphene with high work function as an anode material for Li/Na/K-ion batteries

Yi Luo, Haiyuan Chen,* Jianwei Wang and Xiaobin Niu

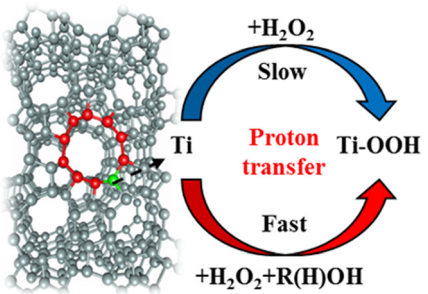
12207



Structural analysis of potassium borate solutions

Fayan Zhu, Daniel T. Bowron, Sabrina Gärtner, Chunhui Fang, Yongquan Zhou, Hongyan Liu and Alex C. Hannon*

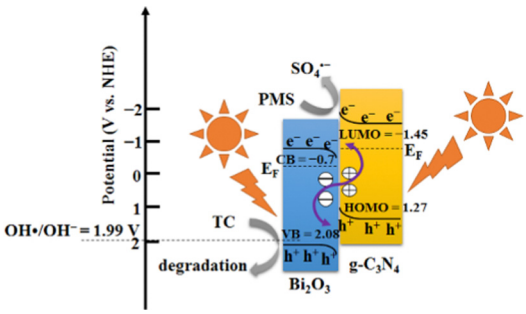
12220



Evidence of solvent-mediated proton transfer during H_2O_2 activation in titanosilicate-catalyzed oxidation systems

Yunkai Yu, Jianhao Wang, Nan Fang, Zhen Chen, Dongxu Liu, Yueming Liu* and Mingyuan He

12231



A 1D/2D Bi_2O_3/g-C_3N_4 step-scheme photocatalyst to activate peroxymonosulfate for the removal of tetracycline hydrochloride: insight into the mechanism, reactive sites, degradation pathway and ecotoxicity

Mingyang Long, Di Li,* Qianqian Zhao, Hongmiao Li, Qi Wen, Li Wang, Lei Wu, Fang Song and Jun Zhou

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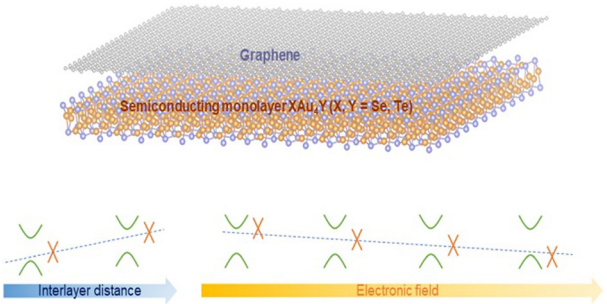
12245

Tunable Schottky contacts in graphene/XAu_4Y (X, Y = Se, Te) heterostructures

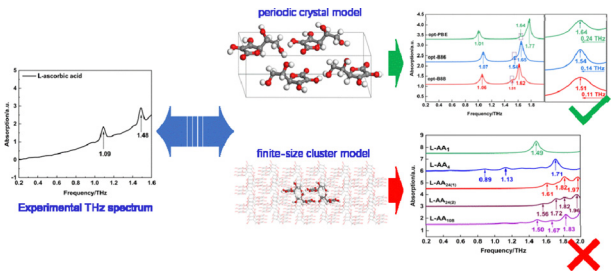
Yufei Xue, Lei Gao,* Weina Ren, Xuxia Shai, Tingting Wei, Chunhua Zeng* and Hua Wang*



12252

First principles terahertz spectroscopy of molecular crystals: the crucial role of periodic boundary conditions benchmarked with experimental L-ascorbic acid spectra

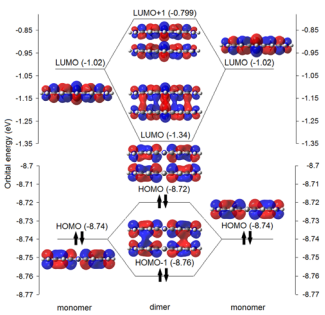
Ying Wang, Huifang Ma, Yanzhao Yang, Jiantao Qi, Guiming Zhang, Hao Ren* and Wenyue Guo*



12259

Theoretical study of the excitation of proflavine H-dimers in an aqueous solution: the effect of functionals and dispersion corrections

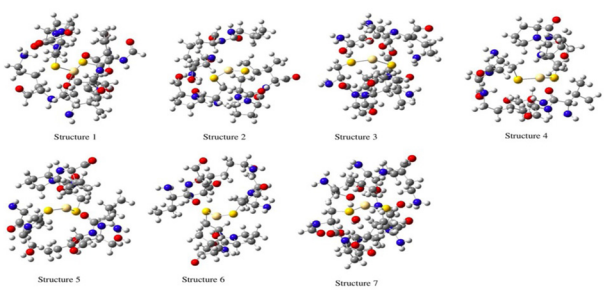
Evgeniy S. Savenko and Victor V. Kostjukov*



12277

Calculation of electric field gradients in Cd(II) model complexes of the CueR protein metal site

Catriona A. O'Shea, Rasmus Fromsejer, Stephan P. A. Sauer, Kurt V. Mikkelsen* and Lars Hemmingsen*



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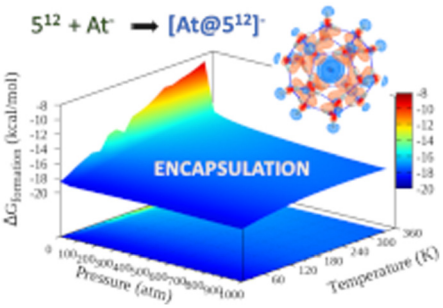
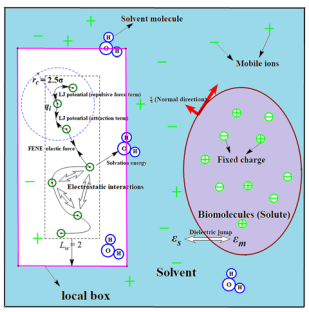
12284



Encapsulation of Astatide by a water cage

Sara Gómez,* Elizabeth Flórez, Nancy Acelas, Cacier Hadad and Albeiro Restrepo*

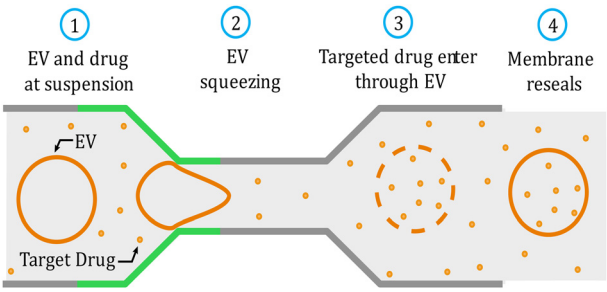
12290



An energy minimization strategy based on an improved nonlinear conjugate gradient method for accelerating the charged polymer dynamics simulation

Hao Lin, Yiwei Shi, Enlong Shang and Shuyang Dai*

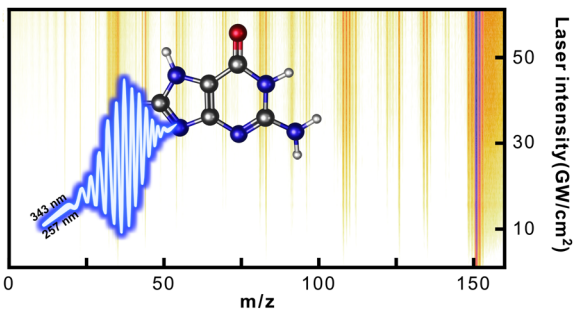
12308



Coarse-grained molecular simulation of extracellular vesicle squeezing for drug loading

Khayrul Islam, Meghdad Razizadeh and Yaling Liu*

12322



High-throughput UV-photofragmentation studies of thymine and guanine

Siwen Wang, Yerbolat Dauletyarov, Peter Krüger and Daniel A. Horke*

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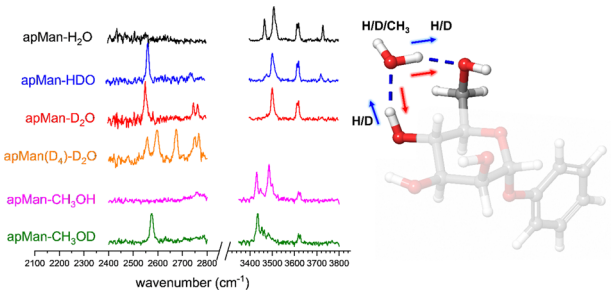
12331

Isotopic dependence of intramolecular and intermolecular vibrational couplings in cooperative hydrogen bond networks: singly hydrated phenyl-α-D-mannopyranoside as a case study

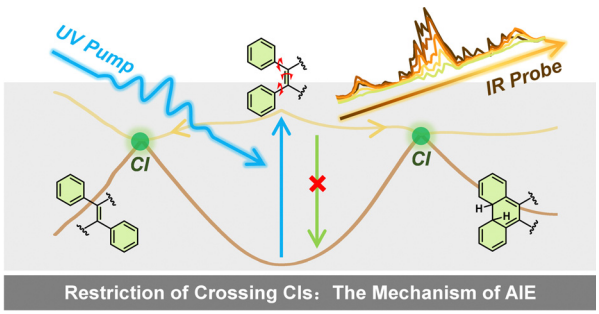
Ander Camiruaga, Gildas Goldsztejn and Pierre Çarçabal*



12342

Restriction of crossing conical intersections: the intrinsic mechanism of aggregation-induced emission

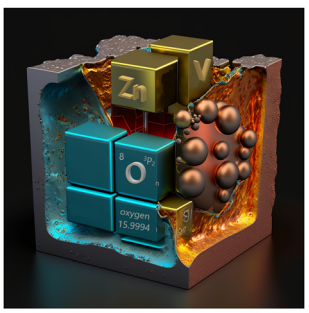
Jie Peng, Xin He, Yao Li, Jianxin Guan, Baihua Wu, Xinmao Li, Zhihao Yu, Jian Liu* and Junrong Zheng*



12352

First principles calculation of the ZnV_2O_6(001) surface terminations: the thermodynamic stability and electronic structure study

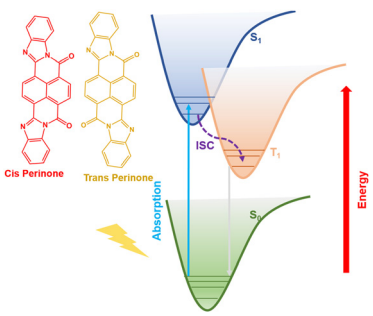
Anqi Yang, Jiaolian Luo,* Zhenyu Xie, Qian Chen* and Quan Xie



12363

Probing the excited state dynamics in perinone molecules for photovoltaic applications using transient absorption spectroscopy

Suman Dhami, Yogesh Kumar, Chaitrali Sengupta and Ravindra Pandey*



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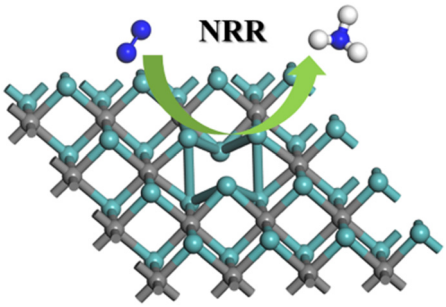
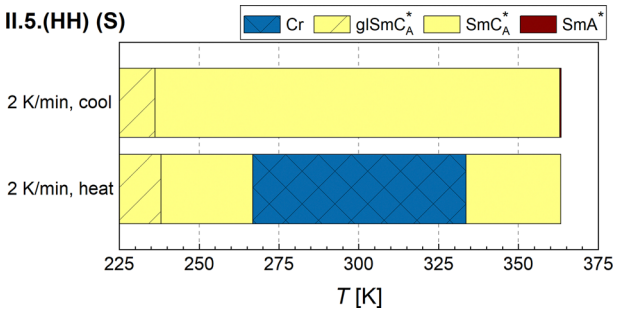
12371



Defective Mo_2C as a promising electrocatalyst for the nitrogen reduction reaction

Xuanyue Zhang, Tingting Zhao, Likai Yan* and Zhongmin Su

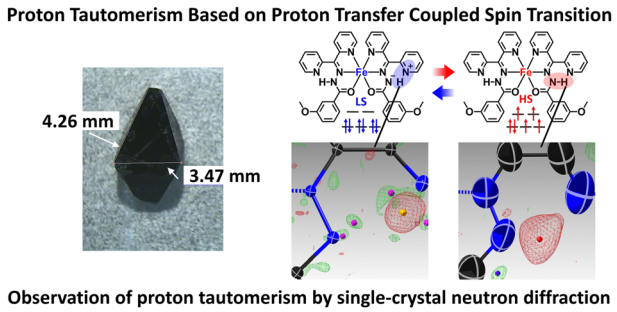
12379



Vitrification of the smectic C_A* phase and kinetics of cold crystallization investigated for a fluorinated compound with a chiral centre based on (*S*)-(+)-3-octanol

Aleksandra Deptuch,* Artur Lelito, Ewa Juszyńska-Gałązka, Małgorzata Jasiurkowska-Delaporte and Magdalena Urbańska

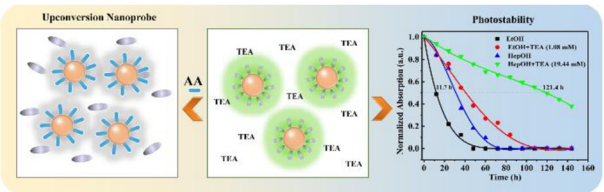
12394



Observation of proton-transfer-coupled spin transition by single-crystal neutron-diffraction measurement

Takumi Nakanishi, Yuta Hori, Yasuteru Shigeta, Hiroyasu Sato, Shu-Qi Wu, Ryoji Kiyanagi, Koji Munakata, Takashi Ohhara and Osamu Sato*

12401



The effect of triethylamine on dye-sensitized upconversion luminescence and its application in nanoprobes and photostability

Xiao-Bo Zhang, Zuo-Qin Liang,* Xu Yan, Mao-Mao Li, Chang-Qing Ye, Xiao-Mei Wang and Xu-Tang Tao

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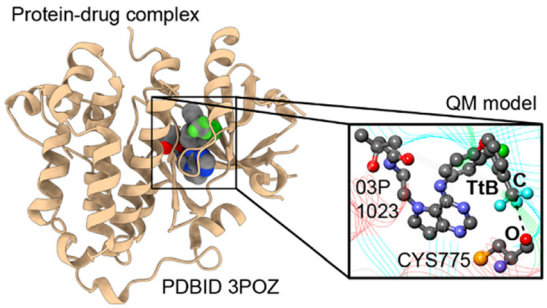
12409

Tetrel bonds involving a CF_3 group participate in protein–drug recognition: a combined crystallographic and computational study

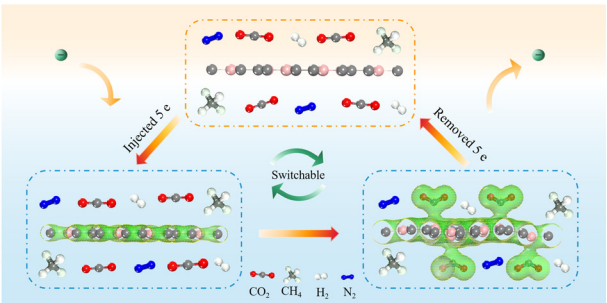
María de las Nieves Piña, Akshay Kumar Sahu, Antonio Frontera, Himansu S. Biswal* and Antonio Bauzá*



12420

Charge-controlled switchable CO_2 capture and gas separation using BC_3 nanosheets

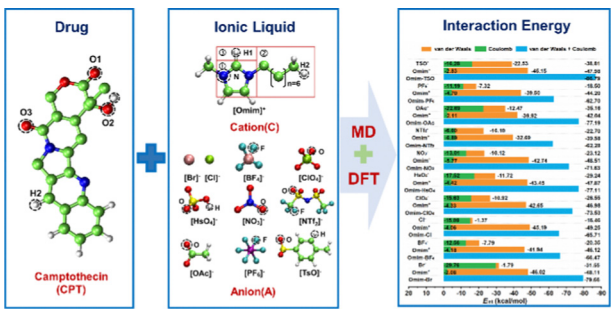
Yiqun Guo, Xuxin Kang, Shan Gao* and Xiangmei Duan*



12426

Theoretical study on the solvation mechanism of camptothecin in ionic liquids

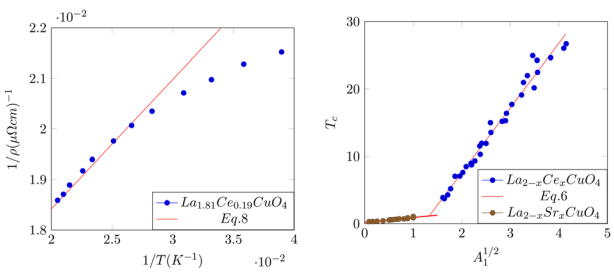
Xiaotong Zhu, Yiping Huang and Yuanhui Ji*



12443

Universal correlation of the superconducting transition temperature with the linear-in-T coefficient, electron packing parameter, and the numbers of valence and conduction electrons

Tian Hao



(a) Data fitted with Eq. 8 (b) Data fitted with Eq. 6

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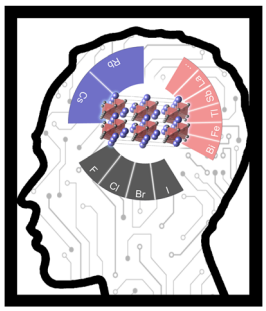
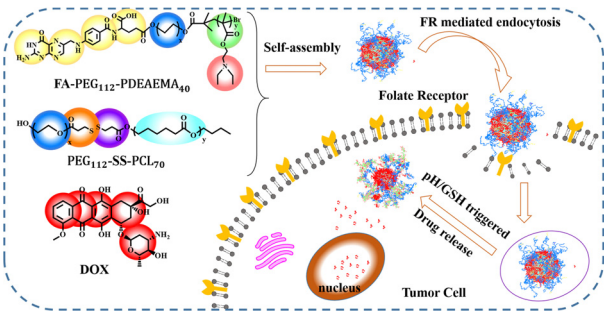
12450



Substitution engineering of lead-free halide perovskites for photocatalytic applications assisted by machine learning

Tao Wang, Shuxin Fan, Hao Jin,* Yunjin Yu and Yadong Wei*

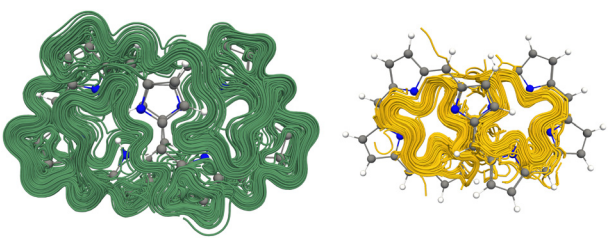
12458



Folate modified dual pH/reduction-responsive mixed micelles assembled using FA-PEG-PDEAEMA and PEG-SS-PCL for doxorubicin delivery

Chufen Yang, Delin Wang, Wenyao Liu, Zexiong Yang, Teng He, Fang Chen and Wenjing Lin*

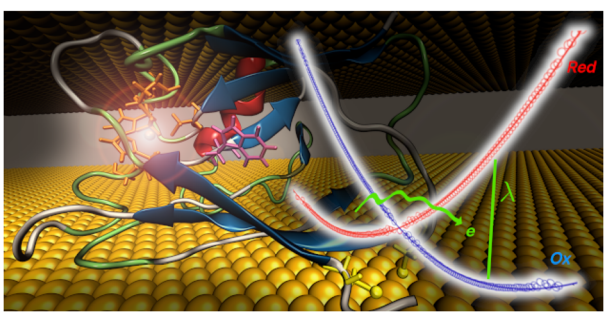
12469



Current-density pathways in figure-eight-shaped octaphyrins

Qian Wang, Jaakko Pyykkö, Maria Dimitrova, Stefan Taubert and Dage Sundholm*

12479



Applicability of perturbed matrix method for charge transfer studies at bio/metallic interfaces: a case of azurin

Outi Vilhelmiina Kontkanen, Denys Biriukov and Zdenek Futera*

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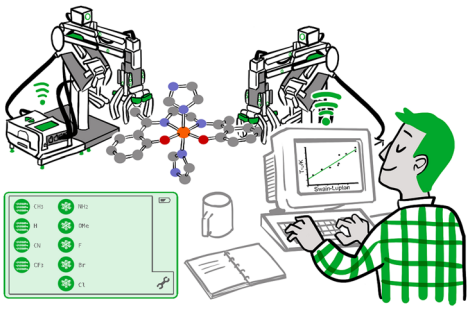
12490

Fine-tuning of the spin-crossover properties of Fe(III) complexes *via* ligand design

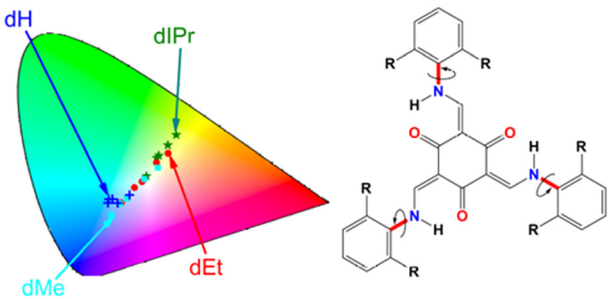
Daniel Vidal, Jordi Cirera* and Jordi Ribas-Arino*



12500

Magnifying the ESIPT process in tris(salicylideneanilines) *via* the steric effect – a pathway to the molecules with panchromatic fluorescence

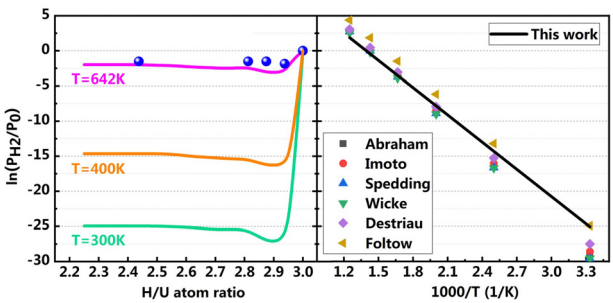
Pawel Gawrys, Olaf Morawski,* Marzena Banasiewicz and Cristina A. Barboza*



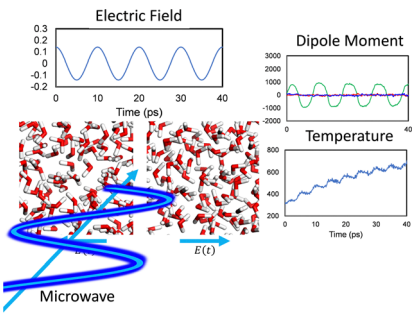
12515

Initial decomposition mechanisms and the inverse effects of temperature and P_{H_2} on the thermodynamic stability of UH_3

Le Zhang, Yanhong Zhao, Hongzhou Song, Xingyu Gao, Qili Zhang, Yu Liu, Bo Sun,* Mingfeng Tian, Haifeng Song and Haifeng Liu*



12522

The selective heating effect of microwave irradiation on a binary mixture of water and polyethylene oxide: a molecular dynamics simulation approach

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