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IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 26(11) 8561–9076 (2024)

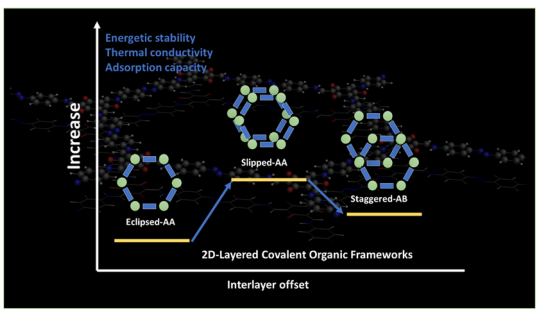
Cover
See Wei Ren, Silvia Picozzi *et al.*, pp. 8604–8612. Image reproduced by permission of Lei Qiao from *Phys. Chem. Chem. Phys.*, 2024, **26**, 8604.

REVIEW

8577

Effect of interlayer slipping on the geometric, thermal and adsorption properties of 2D covalent organic frameworks: a comprehensive review based on computational modelling studies

Hasnain Sajid

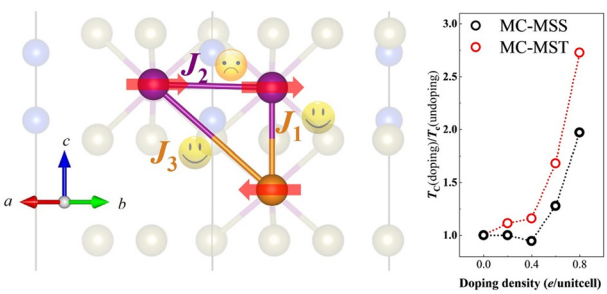


RESEARCH PAPERS

8604

Electron doping as a handle to increase the Curie temperature in ferrimagnetic $Mn_3Si_2X_6$ (X = Se, Te)

Lei Qiao, Paolo Barone, Baishun Yang, Phil D.C. King, Wei Ren* and Silvia Picozzi*



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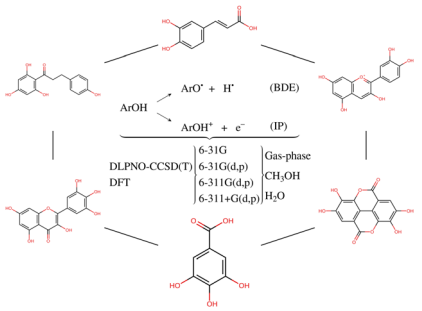
8613

A density functional theory benchmark on antioxidant-related properties of polyphenols

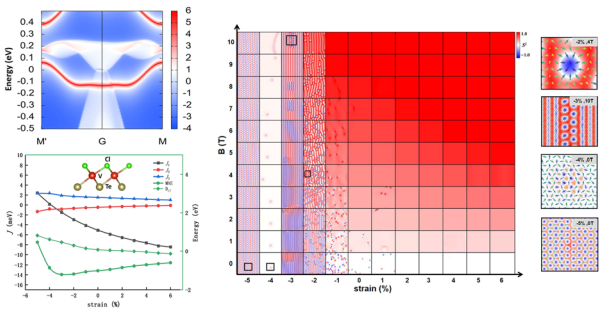
Rodrigo A. Mendes, Victor A. S. da Mata, Alex Brown and Gabriel L. C. de Souza*



8623

Intrinsic edge states and strain-tunable spin textures in the Janus 1T-VTeCl monolayer

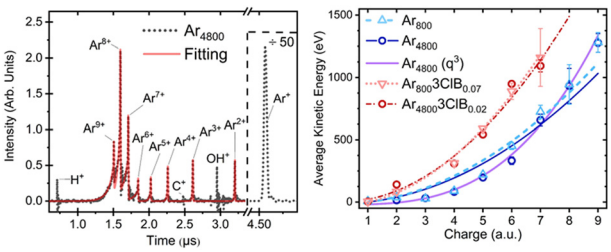
Zheng Chen, Hongliang Hu, Dushuo Feng, Zhihao Guan, Tingting Zhong, Xiaoping Wu and Changsheng Song*



8631

Kinetic energy distributions of atomic ions from disintegration of argon containing nanoclusters in moderately intense nanosecond laser fields: Coulomb explosion or hydrodynamic expansion

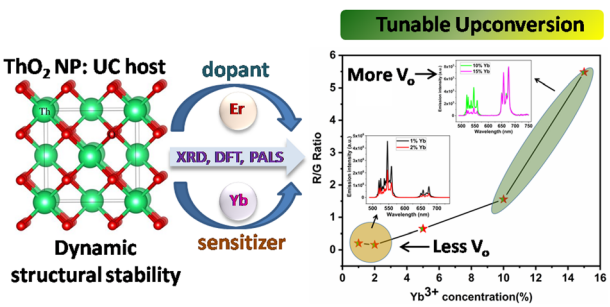
Steven Tran, Kim C. Tran, Axel Saenz Rodriguez and Wei Kong*



8641

Color tunable luminescence in ThO_2:Er^{3+},Yb^{3+} nanocrystals: a promising new platform for upconversion

Debarati Das, Santosh K. Gupta,* Reshmi T. Parayil, B. Modak and K. Sudarshan*



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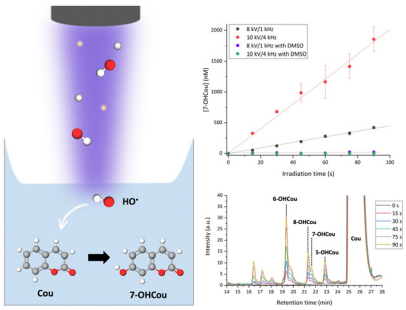
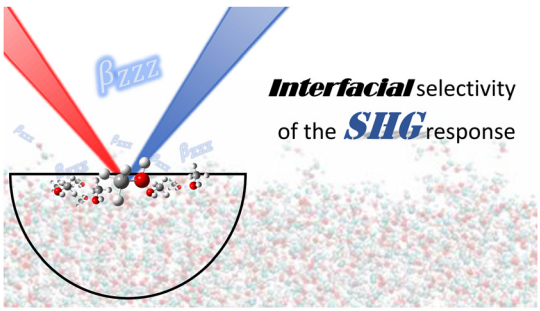


Quantifying hydroxyl radicals generated by a low-temperature plasma using coumarin: methodology and precautions

Florent Ducrozet, Amal Sebastian, Cecilia Julieta Garcia Villavicencio, Sylwia Ptasinska and Cécile Sicard-Roselli*

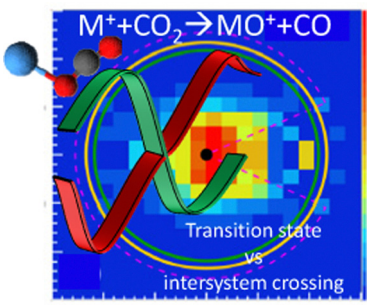
8658



Disentangling the molecular polarizability and first hyperpolarizability of methanol–air interfaces

Tárcius N. Ramos* and Benoît Champagne

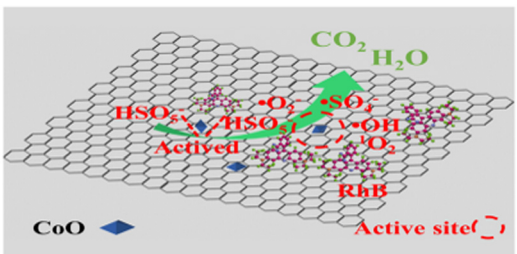
8670



Ta^+ and Nb^+ + CO_2: intersystem crossing in ion–molecule reactions

Maximilian E. Huber, Tucker W. R. Lewis, Marcel Meta, Shaun G. Ard, Yang Liu, Brendan C. Sweeny, Hua Guo, Milan Ončák, Nicholas S. Shuman* and Jennifer Meyer*

8681



CoO@graphene improves the Fenton-like reaction by adsorbing contaminants and activated species

Double pyramid stacked CoO nano-crystals induced by graphene at low temperatures as highly efficient Fenton-like catalysts

Kui Lu, Tao Ding, Mengxiang Zhu, Junjie Chen, Dongting Yue, Xing Liu, Xiaoqin Fang, Junfang Xia, Zhiyuan Qin, Minghong Wu* and Guosheng Shi*

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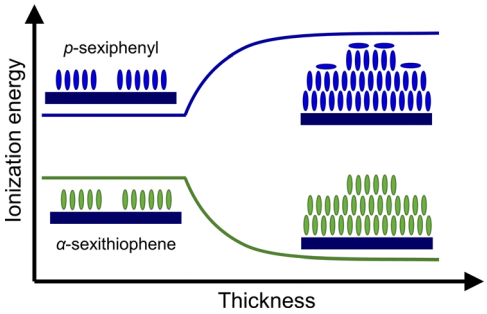
The ionization energy of α-sexithiophene and *p*-sexiphenyl in 2D and 3D thin films grown on silicon oxide surfaces

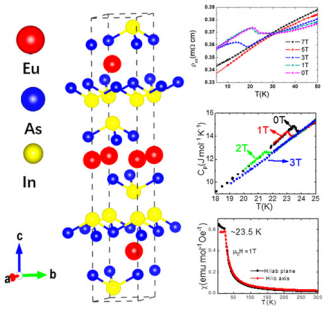
Keitaro Eguchi* and Hideyuki Murata*



8695

Single-crystal growth, structure and thermal transport properties of the metallic antiferromagnet Zintl-phase β-$EuIn_2As_2$

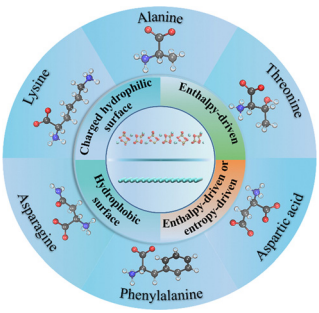
D. S. Wu,* S. H. Na, Y. J. Li, X. B. Zhou, W. Wu, Y. T. Song, P. Zheng, Z. Li and J. L. Luo*



8704

The impact of chemical properties of the solid–liquid–adsorbate interfaces on the entropy–enthalpy compensation involved in adsorption

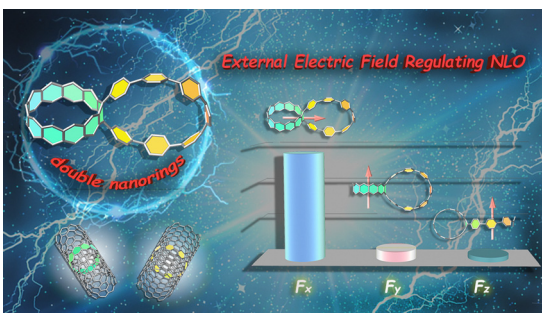
Jinling Xue, Mingyu Ji, Yuanyuan Lu, Dan Pan, Xiao Yang, Xiaoning Yang and Zhijun Xu*



8716

Tuning optical properties of π-conjugated double nanohoops under external electric field stimuli-responsiveness

Xiao Huang, Ping-yao Gan, Feng-wei Gao* and Zhong-min Su*



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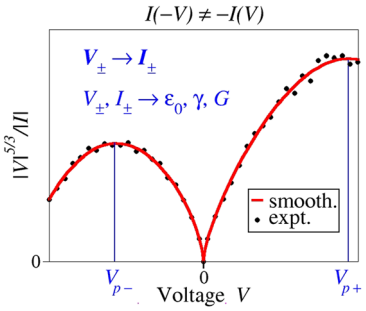
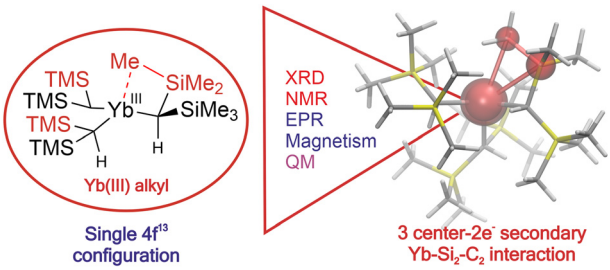


Gaining insight into molecular tunnel junctions with a pocket calculator without *I*–*V* data fitting. Five-thirds protocol

Ioan Bâldea

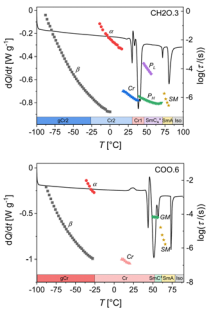
8734



Geometry and electronic structure of Yb(III)[CH(SiMe$_3$)$_2$]$_3$ from EPR and solid-state NMR augmented by computations

Anton Ashuiev, Florian Allouche, Md. Ashraful Islam, José P. Carvalho, Kevin J. Sanders, Matthew P. Conley, Daniel Klose, Giuseppe Lapadula, Michael Wörle, Dirk Baabe, Marc D. Walter, Andrew J. Pell,* Christophe Copéret,* Gunnar Jeschke,* Guido Pintacuda* and Richard A. Andersen

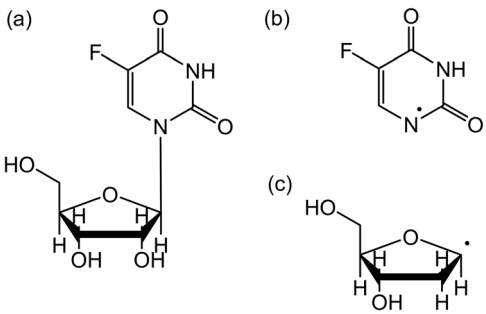
8748



Effect of the linking bridge type on the self-assembly behaviour of 2′,3′-difluoroterphenyl derivatives

Anna Drzewicz,* Małgorzata Jasiurkowska-Delaporte, Przemysław Kula and Ewa Juszyńska-Gałązka

8761



Fragmentation of 5-fluorouridine induced by low energy (< 12 eV) electrons: insights into the radiosensitization of DNA

Paulina Wierzbicka, Hassan Abdoul-Carime and Janina Kopyra*

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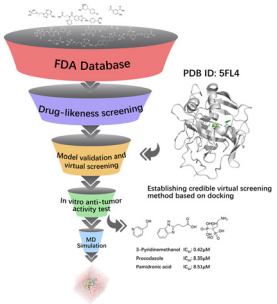
Discovery of non-sulfonamide carbonic anhydrase IX inhibitors through structure-based virtual screening

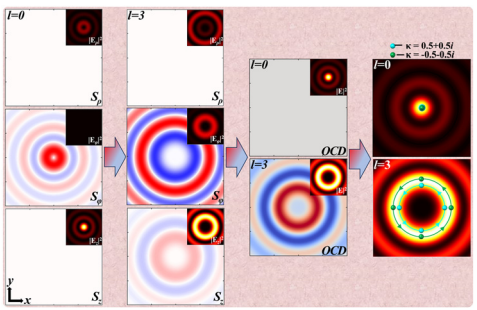
Tianheng Cheng, Nihan Wang, Rui Wen, Shizun Wang, Haoyu Zhang and Maosheng Cheng*



8775

Chiral nanoparticle separation and discrimination using radially polarized circular Airy vortex beams with orbital-induced spin angular momentum

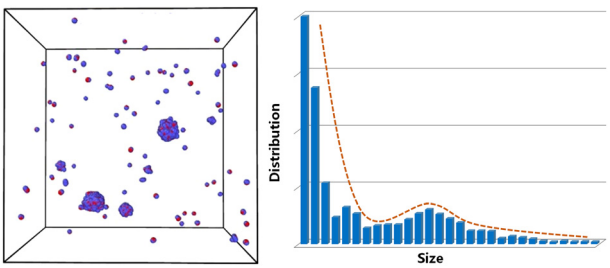
Hao Wu,* Tao Wang and Yi Hu*



8784

Abnormal condensation of water vapour at ambient temperature

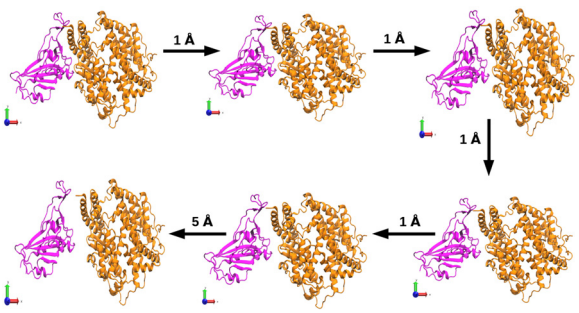
Chenchen Guo, Kun Yang, Hairong Qin, Yong Zhu, Min Chen and Yongjun Lü*



8794

Insights from *in silico* study of receptor energetics of SARS-CoV-2 variants

Lokendra Singh Dhami, Prabin Dahal, Bidhya Thapa, Narayan Gautam, Nurapati Pantha, Rameshwar Adhikari and Narayan Prasad Adhikari*



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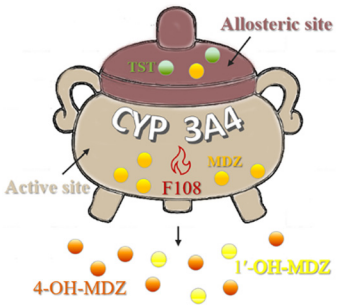
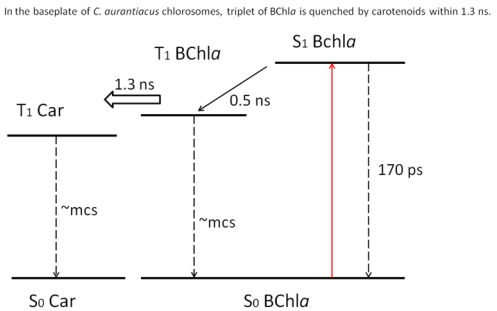


Assessing the role of residue Phe108 of cytochrome P450 3A4 in allosteric effects of midazolam metabolism

Tingting Fu, Hongxing Zhang and Qingchuan Zheng*

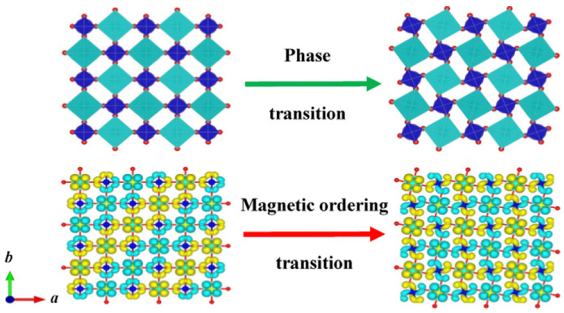
8815



Quenching of bacteriochlorophyll *a* triplet state by carotenoids in the chlorosome baseplate of green bacterium *Chloroflexus aurantiacus*

Andrei G. Yakovlev* and Alexandra S. Taisova

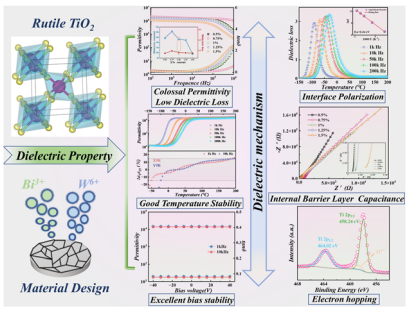
8824



Pressure-induced structural and magnetic ordering transitions in the J_1–J_2 square lattice antiferromagnets $AMoOPO_4Cl$ (A = K, Rb)

Yuanhui Xu,* Rui Cui, Hongping Jiang, Yixuan Du, Yongchao Jia, Keju Sun and Xianfeng Hao*

8834



Giant dielectric response and relaxation behavior of Bi^{3+}/W^{6+} co-doped TiO_2 ceramics

Guoyan Yang, Zhanhui Peng,* Huan Liu, Di Wu, Pengfei Liang, Linling Wei, Xiaolian Chao* and Zupei Yang*

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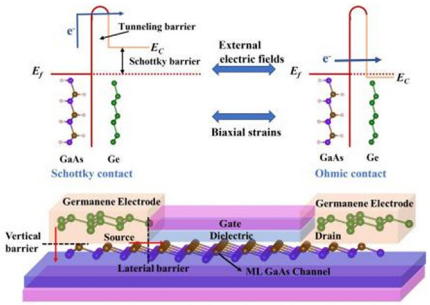
Transition from Schottky to Ohmic contacts in 2D Ge/GaAs heterostructures with high tunneling probability

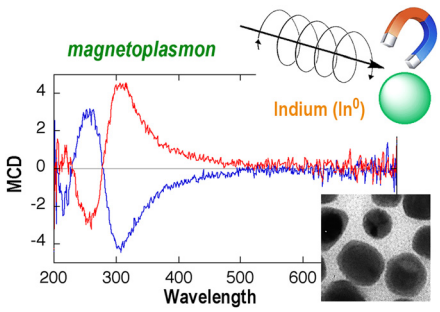
Yang Shen,* Jianfeng Zhu, Qihao Zhang, Hua Zhu, Qianglong Fang, Xiaodong Yang and Baolin Wang



8850

UV-resonant magnetoplasmonic properties of chemically synthesized indium nanoparticles

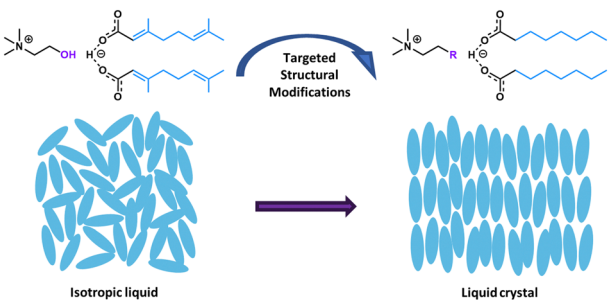
Ririka Matsuda and Hiroshi Yao*



8858

Understanding the effects of targeted modifications on the 1 : 2 Choline And GEranate structure

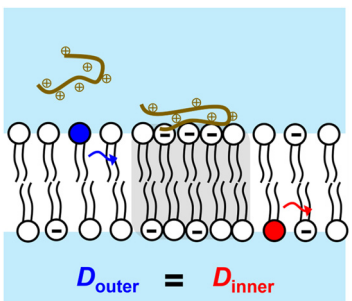
Ana Dobre, Spyridon Koutsoukos, Frederik Philippi, Daniel Rauber, Christopher W. M. Kay, Oriele Palumbo, Maxie M. Roessler and Tom Welton*



8873

Peripheral adsorption of polylysine on one leaflet of a lipid bilayer reduces the lipid diffusion of both leaflets

Kosei Shimizu, Miyuki Sakaguchi, Shoichi Yamaguchi and Takuhiro Otosu*



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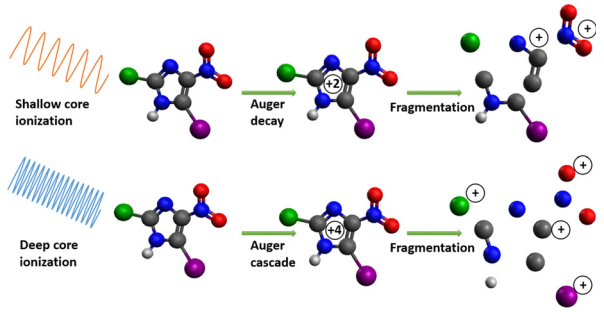
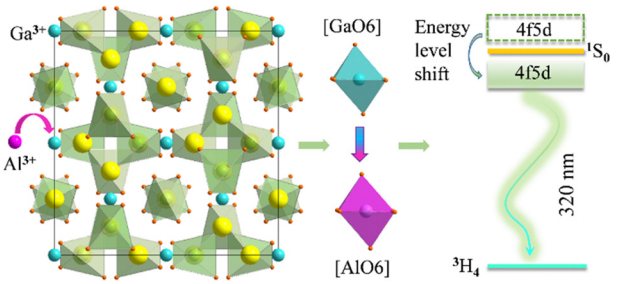


Shell-dependent photofragmentation dynamics of a heavy-atom-containing bifunctional nitroimidazole radiosensitizer

Lassi Pihlava,* Pamela H. W. Svensson, Edwin Kukk, Kuno Kooser, Emiliano De Santis, Arvo Tõnisoo, Tanel Käämbre, Tomas André, Tomoko Akiyama, Lisa Hessenthaler, Flavia Giehr, Olle Björneholm, Carl Caleman and Marta Berholts*

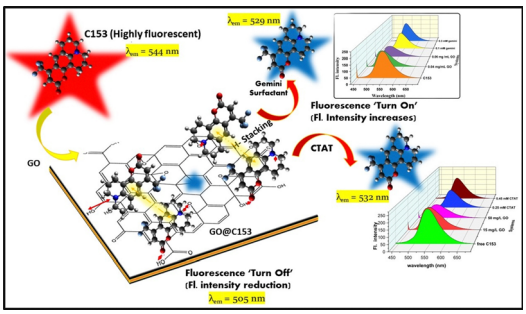
8891



Adjustable ultraviolet and white light dual emission phosphor $Y_2Sr(Ga_{1-y}Al_y)_4SiO_{12}:xPr^{3+}$ for health lighting

Qihui Yu, Huan Zheng, Jiajun He, Xu Yang, Yingnan Guo,* Li Guan, Xu Li* and Fenghe Wang*

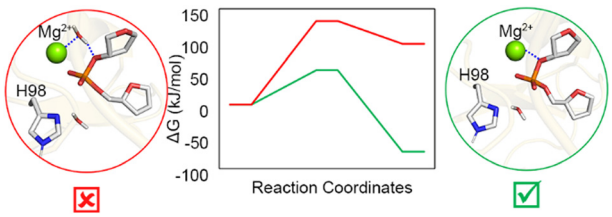
8900



Exploration of the impact of graphene oxide, acetylenic gemini, and CTAT on the photophysical and aggregation properties of dipolar coumarin 153

Raju Sardar, Sourav Das, Rajesh Banik, Sayani Bhunia and Soumen Ghosh*

8919



Elucidation of the catalytic mechanism of a single-metal dependent homing endonuclease using QM and QM/MM approaches: the case study of I-*Ppo*I

Rajwinder Kaur, Angela Frederickson and Stacey D. Wetmore*

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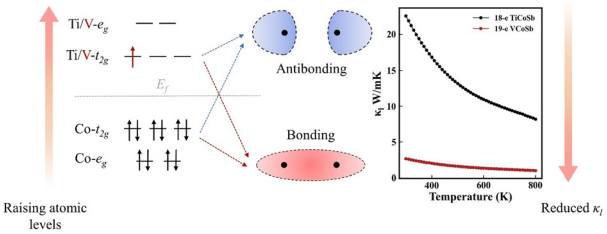
Strong electron–phonon coupling and high lattice thermal conductivity in half-Heusler thermoelectric materials

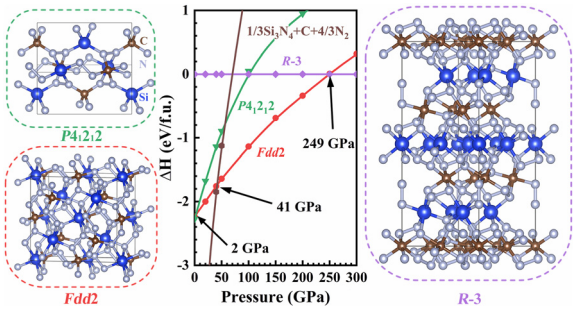
Ruoyu Wang, Jianfeng Cai, Qiang Zhang, Xiaojian Tan, Jiehua Wu, Guoqiang Liu* and Jun Jiang*



8938

A pressure-induced superhard $SiCN_4$ compound uncovered by first-principles calculations

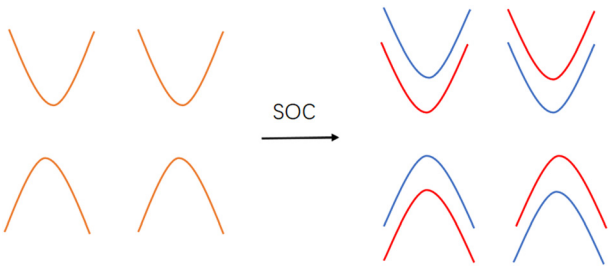
Chengyu Wang, Guoliang Yu, Shoutao Zhang, Yu Zhao, Hui Chen, Taimin Cheng* and Xinxin Zhang*



8945

Large valley splitting induced by spin–orbit coupling effects in monolayer W_2NSCl

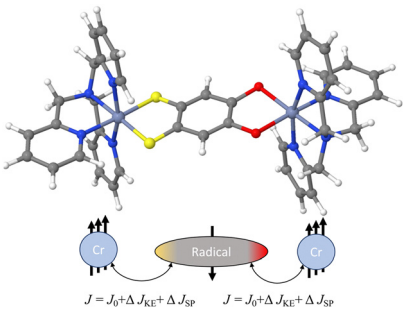
Mengxian Lan, Suen Wang, Xiaoyu Liu, Sai Ma, Shiqian Qiao, Ying Li, Hong Wu, Feng Li* and Yong Pu*



8952

What governs magnetic exchange couplings in radical-bridged dinuclear complexes?

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



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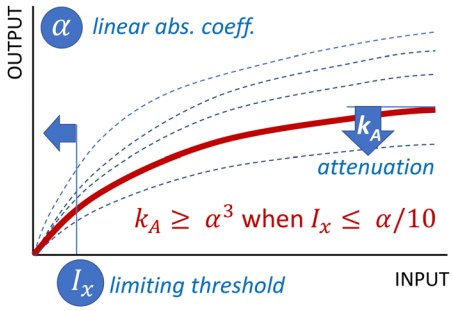
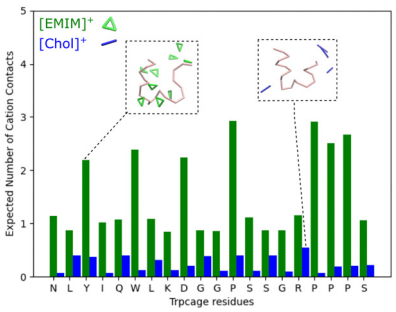
8965



Conditions for the efficiency of optical limiting based on experiment and quantum chemical calculations

Alexander Yu. Tolbin,* Mikhail S. Savelyev, Pavel N. Vasilevsky and Alexander Yu. Gerasimenko

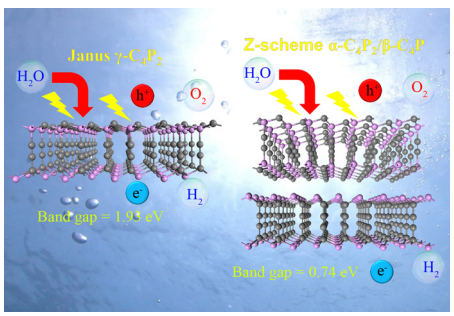
8973



Opposing roles of organic salts on mini-protein structure

Pei-Yin Lee, Onkar Singh, Neha Nanajkar, Harry Bermudez* and Silvina Matysiak*

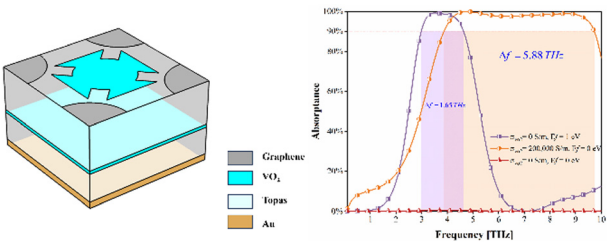
8982



Novel C_4P_2 monolayers: forming Z-scheme heterojunction and Janus structure for high-efficiency metal-free photocatalytic water splitting

Jiahe Lin* and Bofeng Zhang*

8993



A tri-functional, independently tunable terahertz absorber based on a vanadium dioxide–graphene hybrid structure

Guozheng Wu, Chao Li,* Dong Wang, Song Gao, Wenya Chen, Shijing Guo and Jiaran Xiong

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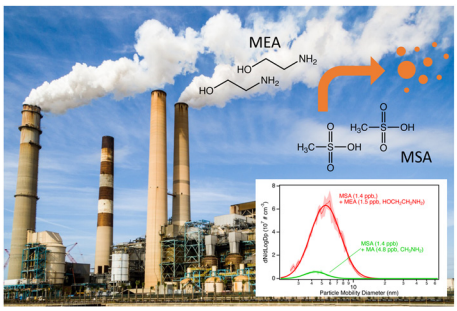
9005

Implications for new particle formation in air of the use of monoethanolamine in carbon capture and storage

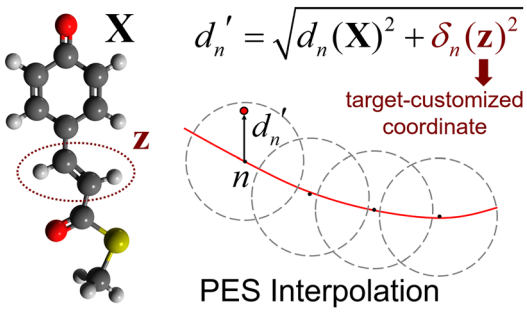
Véronique Perraud,* Kanuri Roundtree, Patricia M. Morris, James N. Smith* and Barbara J. Finlayson-Pitts



9021

Potential energy interpolation with target-customized weighting coordinates: application to excited-state dynamics of photoactive yellow protein chromophore in water

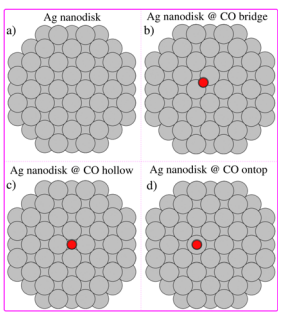
Seung Soo Kim and Young Min Rhee*



9037

Plasmon-induced hot carrier distribution in a composite nanosystem: role of the adsorption site

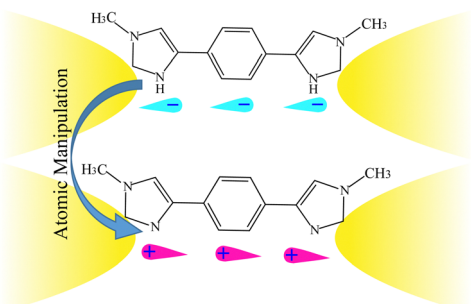
Mufasila Mumthaz Muhammed and Junais Habeeb Mokkath*



9051

Tuning the polarity of charge carriers in N-heterocyclic carbene-based single-molecule junctions *via* atomic manipulation

Minglang Wang* and Guang-Ping Zhang



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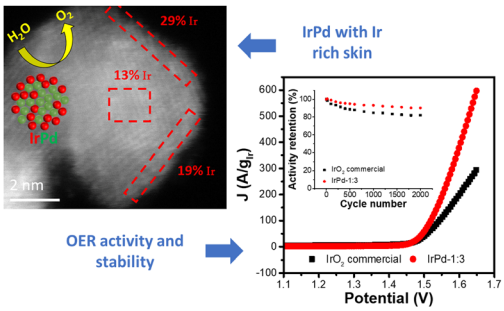
9060



Tailoring iridium–palladium nanoparticles with Ir-rich skin: a highly durable anode electrocatalyst for acidic water electrolysis *via* a facile microwave-assisted chemical reduction method

Swapnil Sanjay Karade, Raghunandan Sharma,* Per Morgen, Darko Makovec, Sašo Gyergyek and Shuang Ma Andersen*

CORRECTIONS

9073

Correction: Pericyclic reaction benchmarks: hierarchical computations targeting CCSDT(Q)/CBS and analysis of DFT performance

Pascal Vermeeren, Marco Dalla Tiezza, Mark E. Wolf, Mitchell E. Lahm, Wesley D. Allen,* Henry F. Schaefer,* Trevor A. Hamlin* and F. Matthias Bickelhaupt*

9074

Correction: Ionic migration induced loss analysis of perovskite solar cells: a poling study

Xue Zheng, Wenjie Ming, Pingping Liu, Jie Zhang, Hongfei Zhou, Ming Chen, Weimin Li, Boyuan Huang,* Huan Wang* and Chunlei Yang*

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