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ISSN 1463–9076 CODEN PPCPFQ 26(7) 5723–6460 (2024)



Cover

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Inside cover

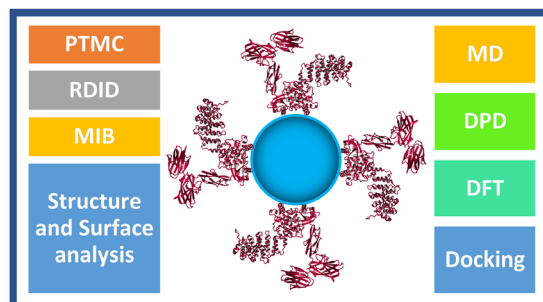
See Sukanta Das and Vaibhav S. Prabhudesai, pp. 5793–5801. Image reproduced by permission of Vaibhav S. Prabhudesai from *Phys. Chem. Chem. Phys.*, 2024, 26, 5793.

REVIEW

5744

In silico approaches to investigate enzyme immobilization: a comprehensive systematic review

Farzaneh Barati, Fakhrisadat Hosseini,* Rayeveh Vafae, Zahra Sabouri, Parinaz Ghadam, Seyed Shahriar Arab, Najmeh Shadfar and Firoozeh Piroozmand

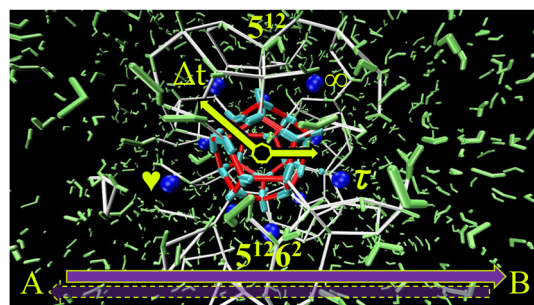


PERSPECTIVE

5762

Comparing brute force to transition path sampling for gas hydrate nucleation with a flat interface: comments on time reversal symmetry

Matthew R. Walsh



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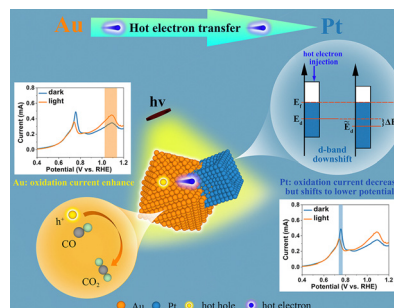
Fundamental questions
Elemental answers

COMMUNICATIONS

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Probing local charge transfer processes of Pt–Au heterodimers in plasmon-enhanced electrochemistry by CO stripping techniques

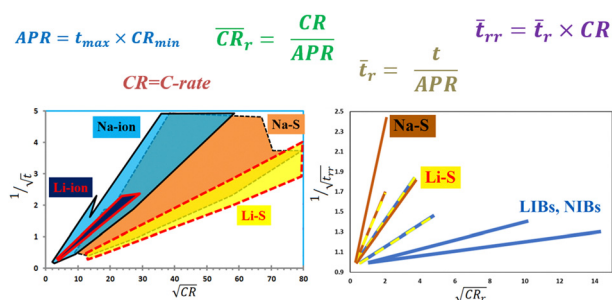
Chenxi Guo, Shiyu Xia, Yu Tian, Fenghua Li, Guobao Xu, Fengxia Wu* and Wenxin Niu*



5778

Normalization of charge/discharge time vs. current rate diagrams for rechargeable batteries

Elham Shahpouri, Naghmeh Abavi-Torghabeh, Mohammad Mahdi Kalantarian* and Piercarlo Mustarelli*

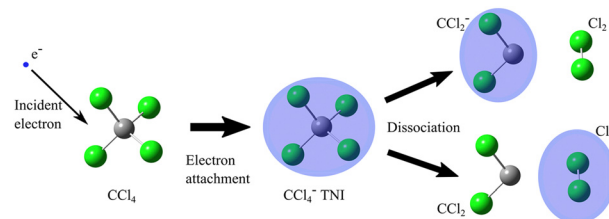


RESEARCH PAPERS

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Dissociative electron attachment to carbon tetrachloride probed by velocity map imaging

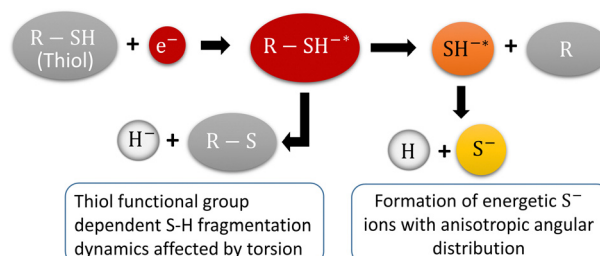
Anirban Paul, Dhananjay Nandi, Daniel S. Slaughter, Juraj Fedor and Pamir Nag*



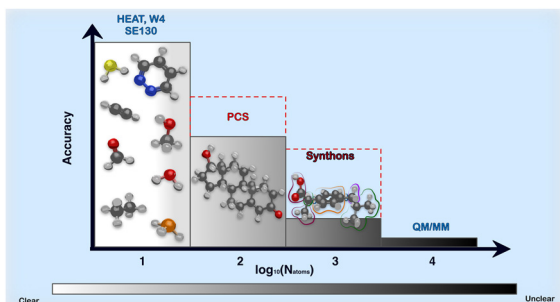
5793

Dynamics of dissociative electron attachment to aliphatic thiols

Sukanta Das and Vaibhav S. Prabhudesai*



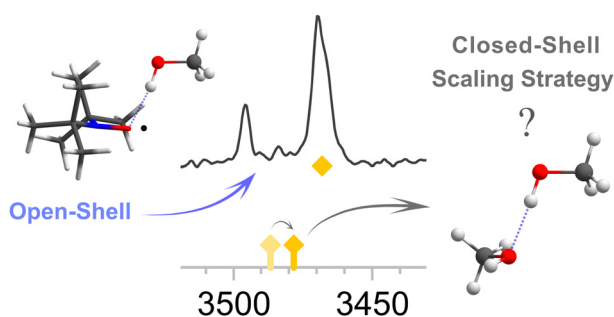
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Quantum chemistry meets high-resolution spectroscopy for characterizing the molecular bricks of life in the gas-phase

Vincenzo Barone

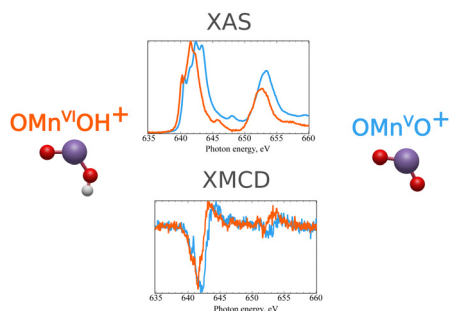
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Benchmarking the anisotropy of nitroxyl radical solvation with IR spectroscopy

Elisa M. Brás, Charlotte Zimmermann, Rui Fausto and Martin A. Suhm*

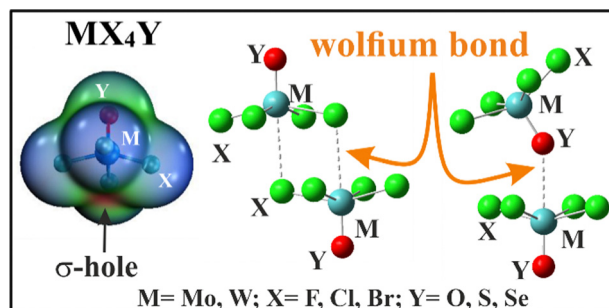
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Direct spectroscopic evidence for the high-spin state of dioxidomanganese(v)

Olesya S. Abyasova, Vicente Zamudio-Bayer, Max Flach, Mayara da Silva Santos, J. Tobias Lau and Konstantin Hirsch*

5836



Wolfium bonds in homodimers of MX_4Y ($M = Mo, W$; $X = F, Cl, Br$; $Y = O, S, Se$)

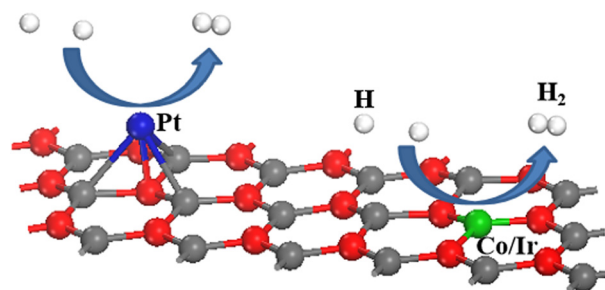
Mariusz Michalczyk,* Wiktor Zierkiewicz and Steve Scheiner



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ZnO monolayer-supported single atom catalysts for efficient electrocatalytic hydrogen evolution reaction

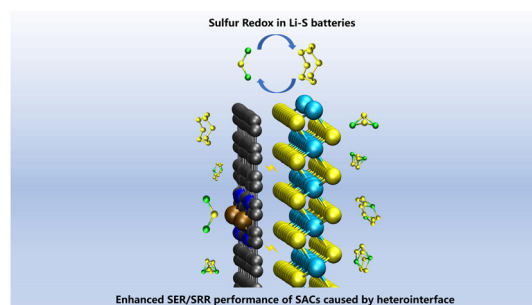
Rongzhi Wang and Jin-Cheng Zheng*



5858

The heterointerface effect to boost the catalytic performance of single atom catalysts for sulfur conversion in lithium–sulfur batteries

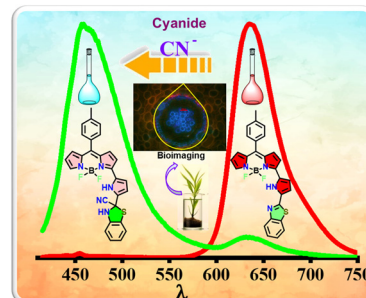
Haikuan Liang, Zhihao Zeng, Zhengping Qiao,* Yan Li* and Chengxin Wang



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An α -benzothiazolyl 3-pyrrolyl BODIPY probe for ratiometric selective sensing of cyanide ions and bioimaging studies

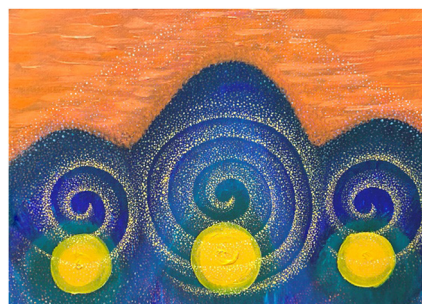
Kanhu Charan Behera, Roshnara Mohanty and Mangalampalli Ravikanth*



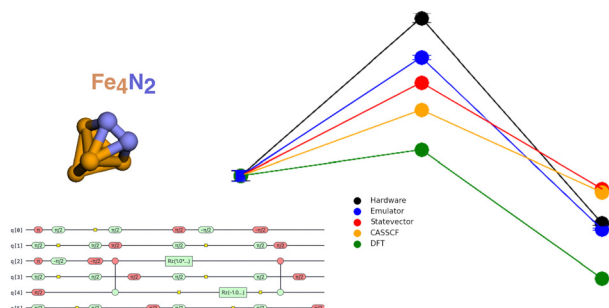
5879

A density-matrix adaptation of the Hückel method to weak covalent networks

Laura Van Dorn and Andrei Sanov*



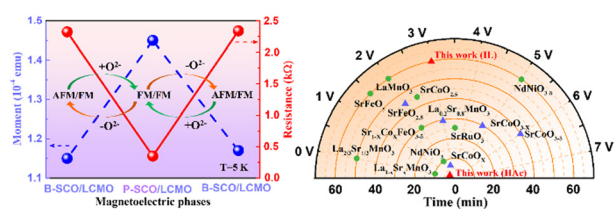
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Quantum hardware calculations of the activation and dissociation of nitrogen on iron clusters and surfaces

Georgia Christopoulou,* Cono Di Paola, Floris Eelke Elzinga, Aurelie Jallat, David Muñoz Ramo and Michal Krompiec

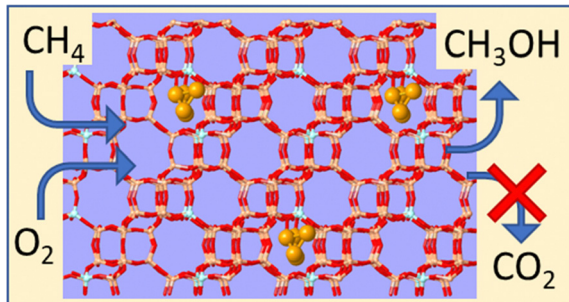
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Highly efficient and fast modulation of magnetic coupling interaction in the SrCoO_{2.5}/La_{0.7}Ca_{0.3}MnO₃ heterostructure

Huihui Ji, Siqi Wang, Guowei Zhou,* Xuanchi Zhou, Jiarui Dou, Penghua Kang, Jingsheng Chen* and Xiaohong Xu*

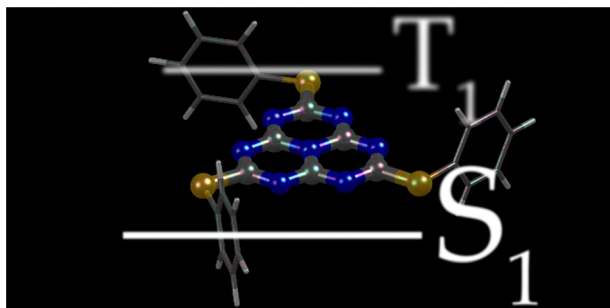
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An alternative catalytic cycle for selective methane oxidation to methanol with Cu clusters in zeolites

Mario Gallego, Avelino Corma and Mercedes Boronat*

5922



Experimental and computational studies of the optical properties of 2,5,8-tris(phenylthiolato)-heptazine with an inverted singlet–triplet gap

Daniel Blasco,* Rinat T. Nasibullin, Rashid R. Valiev, Miguel Monge, José M. López-de-Luzuriaga and Dage Sundholm*

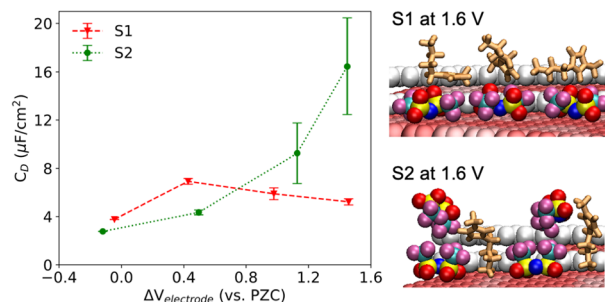


RESEARCH PAPERS

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Influence of surface nanostructure-induced innermost ion structuring on capacitance of carbon/ionic liquid double layers

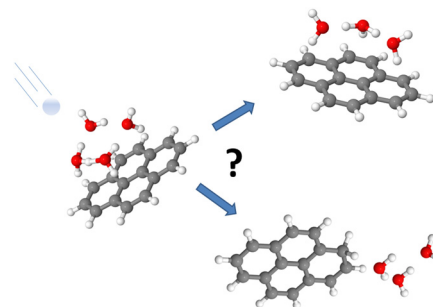
Yi-Jung Tu* and Sheng-Ting Peng



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Diversity of protonated mixed pyrene–water clusters investigated by collision induced dissociation

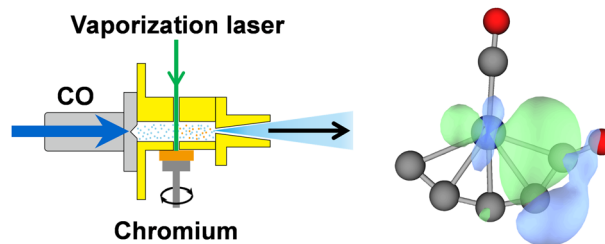
Arya M. Nair, Héloïse Leboucher, Lorris Toucouere, Sébastien Zamith,* Christine Joblin, Jean-Marc L'Hermite, Alexandre Marciniak and Aude Simon



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Spectroscopic characterization of carbon monoxide activation by neutral chromium carbides

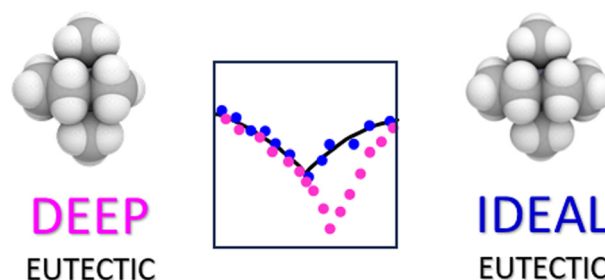
Tiantong Wang, Zhaoyan Zhang, Shuai Jiang, Wenhui Yan, Shangdong Li, Jianxing Zhuang, Hua Xie, Gang Li* and Ling Jiang*



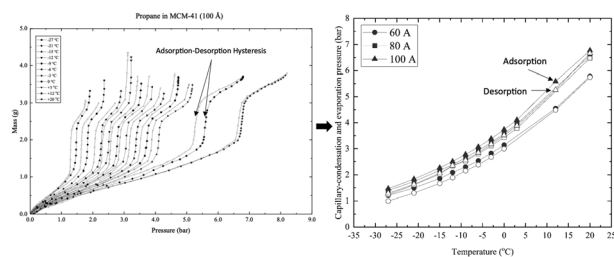
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Exploring asymmetry induced entropy in tetraalkylammonium–urea DES systems: what can be learned from inelastic neutron scattering?

Catarina F. Araújo, Paulo Ribeiro-Claro, Pedro D. Vaz, Svemir Rudić, Rafael A. F. Serrano, Liliana P. Silva, J. A. P. Coutinho and Mariela M. Nolasco*



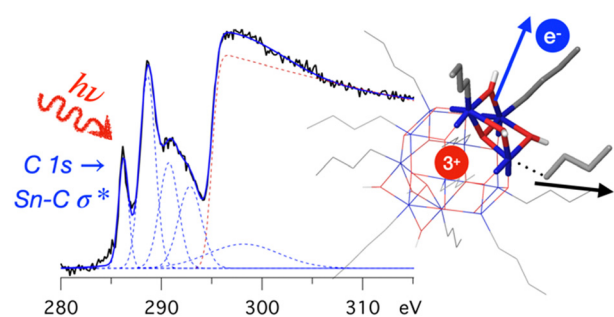
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The effect of confinement on the phase behavior of propane in nanoporous media: an experimental study probing capillary condensation, evaporation, and hysteresis at varying pore sizes and temperatures

Rami M. Alloush, Keerti Vardhan Sharma* and Mohammad Piri

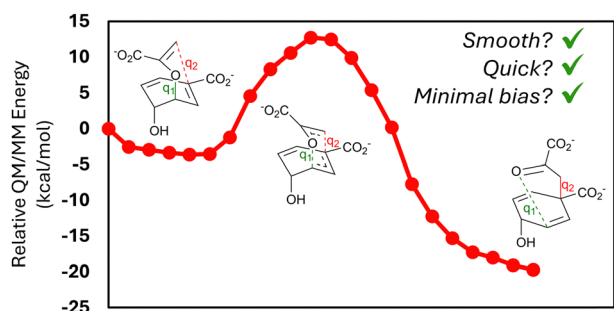
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Soft X-ray absorption and fragmentation of tin-oxo cage photoresists

Jarich Haitjema, Sonia Castellanos, Olivier Lugier, Ivan Bernal, Rebecka Lindblad, Martin Timm, Christine Bülow, Vicente Zamudio-Bayer, J. Tobias Lau, Bernd von Issendorff, Ronnie Hoekstra, Katharina Witte, Benjamin Watts, Thomas Schlathöler* and Albert M. Brouwer*

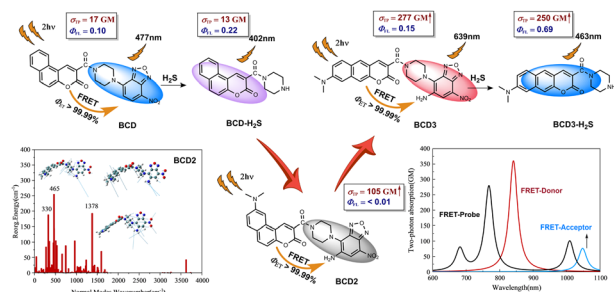
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Exploration of biochemical reactivity with a QM/MM growing string method

Neil R. McFarlane and Jeremy N. Harvey*

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Excellent ratiometric two-photon fluorescent probes for hydrogen sulfide detection based on the fluorescence resonance energy transfer mechanism

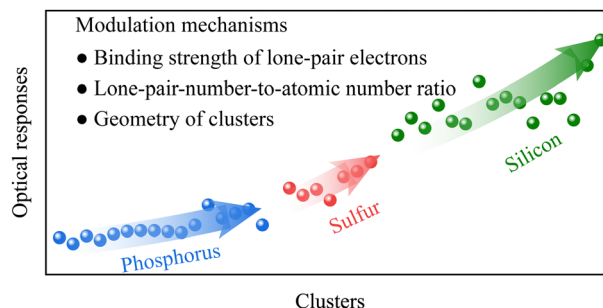
Xue-Xue Ma, Ming-Hui Geng, Xia-Yu Cheng, Tong-Shu Zhang, Zong-Liang Li and Ke Zhao*



6022

Size-dependent linear and nonlinear optical responses of silicon clusters

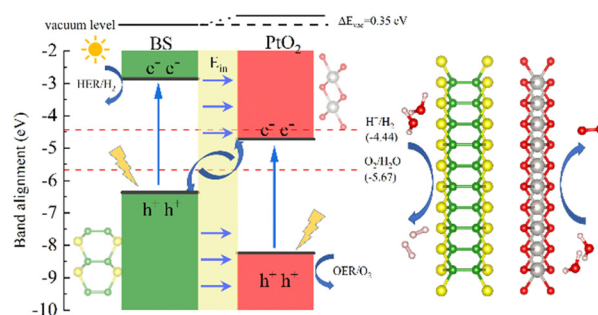
Quanjie Zhong



6029

A direct Z-scheme BS/PtO₂ van der Waals heterojunction for enhanced visible-light photocatalytic water splitting: a first-principles study

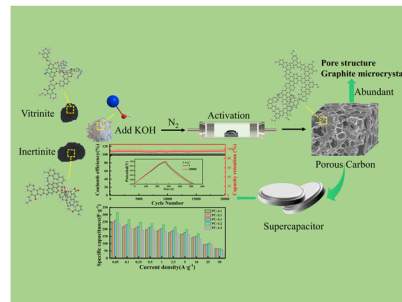
Bowe Zhou, ZiTao Zhu, Zhengdong Sun, Meng Zhang* and Xiao Wang



6037

Enhanced supercapacitor performance of porous carbon through tuning maceral composition proportion of coal

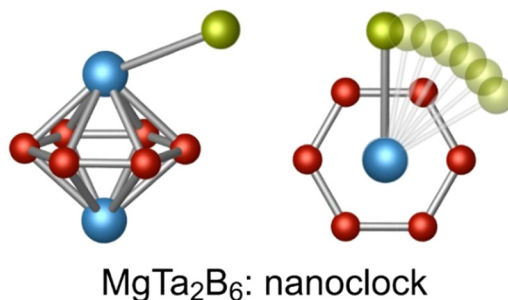
Ruirui Zhao, Jian Hao,* Xiao Yang, Ruyi Zhang, Caixia Chi, Hui Zhang and Qingjie Guo



6049

Boron-based ternary MgTa₂B₆ cluster: a turning nanoclock with dynamic structural fluxionality

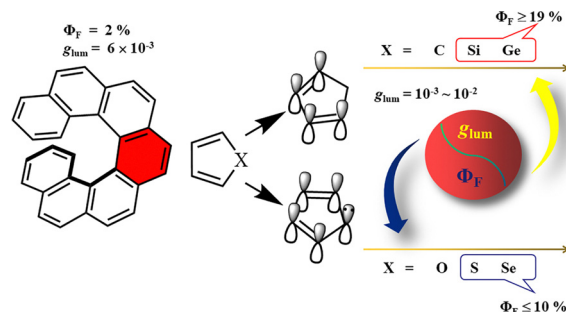
Fang-Lin Liu, Jin-Chang Guo and Hua-Jin Zhai*



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The influence of heteroatoms on the circularly polarized luminescence performance of [7]helicene derivatives: aromatic vs. non-aromatic five-membered rings

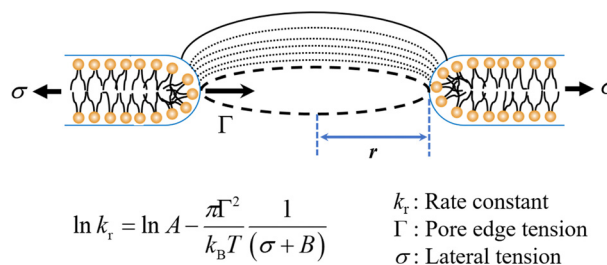
Yan Liu, Zhiying Ma,* Hang Su, Ran Wei, Zhitao Shen* and Hua Wang



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Determination of pore edge tension from the kinetics of rupture of giant unilamellar vesicles using the Arrhenius equation: effects of sugar concentration, surface charge and cholesterol

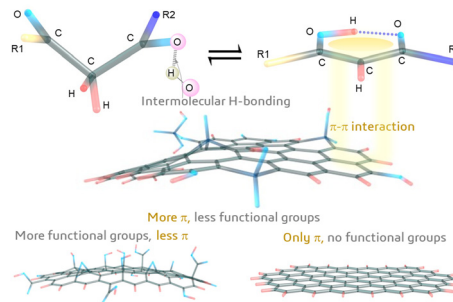
Mohammad Abu Sayem Karal,* Md. Masum Billah and Md. Kabir Ahamed



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Keto-enol tautomerism of β -diketo molecules in the presence of graphitic materials through π - π stacking

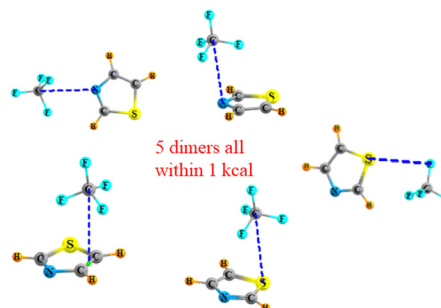
Sayantana Maity, Jaipriya Khatri, Vijay Kumar* and Basab Bijayi Dhar*



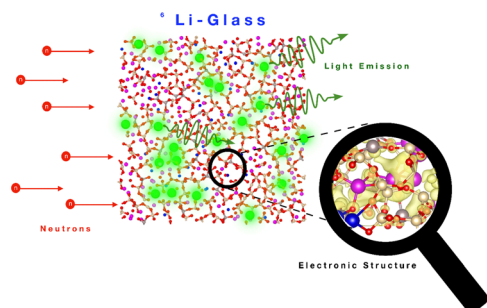
6127

Types of noncovalent bonds within complexes of thiazole with CF_4 and SiF_4

Steve Scheiner* and Akhtam Amonov



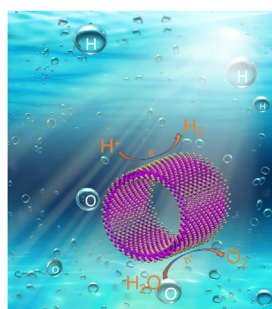
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First-principles study of lithium aluminosilicate glass scintillators

E. M. Ghardi,* A. Scrimshire, R. Smith, P. A. Bingham, S. C. Middleburgh, W. E. Lee and M. J. D. Rushton*

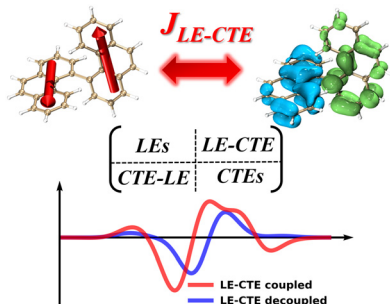
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Application of GaS nanotubes as efficient catalysts in photocatalytic hydrolysis: a first principles study

Huanyu Zhao, Yingtao Zhu,* Chao Wang, Yujiao Zhang and Long Zhang

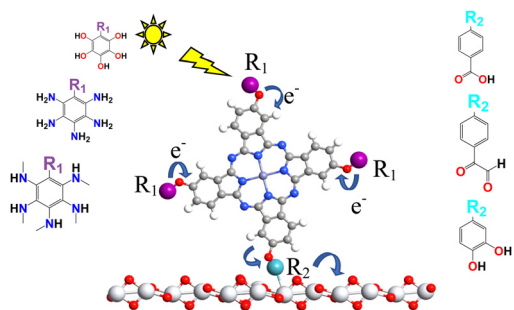
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Identification of the interchromophore interaction in the electronic absorption and circular dichroism spectra of bis-phenanthrenes

Yuchuan Xu, Xunkun Huang, Yu-Chen Wang, Yi Zhao and WanZhen Liang*

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Toward the search for new photosensitizers for DSSCs: theoretical study of both substituted Zn(II) and Si(IV) phthalocyanines

Michael Zambrano-Angulo and Gloria Cárdenas-Jirón*

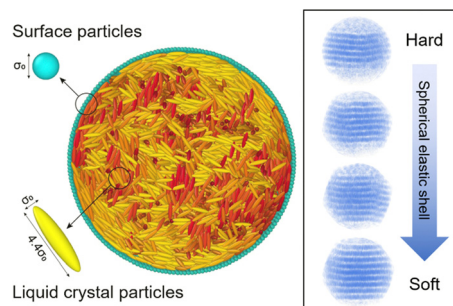


RESEARCH PAPERS

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Exploring the interplay of liquid crystal orientation and spherical elastic shell deformation in spatial confinement

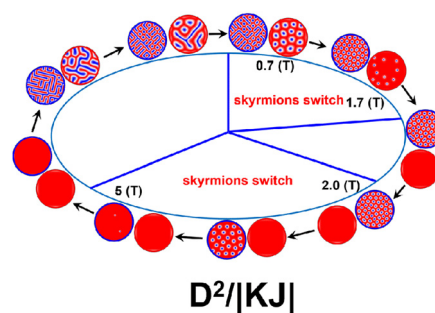
You-Lu Liu, You-Liang Zhu, Yan-Chun Li* and Zhong-Yuan Lu*



6189

Magnetic skyrmions and their manipulations in a 2D multiferroic $\text{CuCrP}_2\text{Te}_6$ monolayer

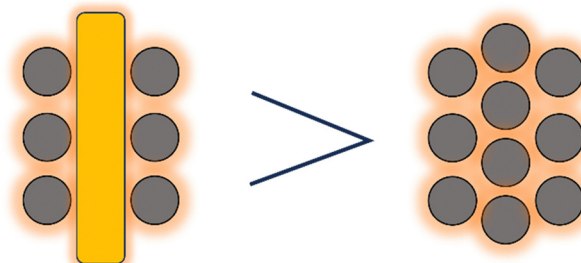
Minghao Liu, Tsz Lok Wan, Kaiying Dou, Lei Zhang, Wei Sun, Jiawei Jiang, Yandong Ma, Yuantong Gu* and Liangzhi Kou*



6196

Dipole–multipole plasmonic coupling between gold nanorods and titanium nitride nanoparticles for enhanced photothermal conversion

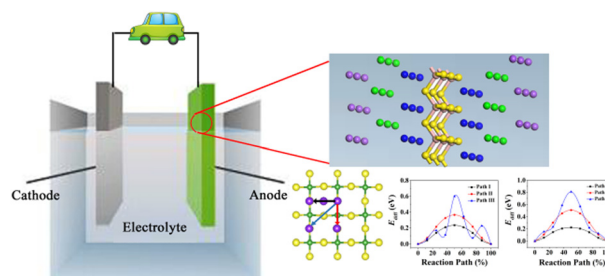
Min Xi,* Chenyang Xu, Li Zhong,* Cui Liu, Nian Li, Shudong Zhang* and Zhenyang Wang



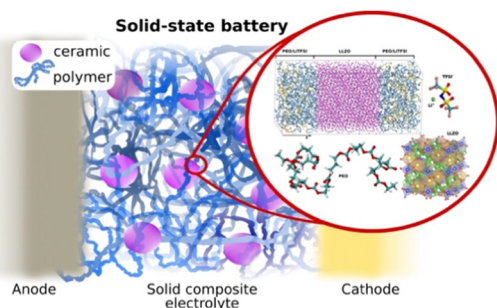
6208

A metallic two-dimensional b-BS_2 monolayer as a superior Na/K-ion battery anode

Zhifang Yang, Wenliang Li* and Jingping Zhang*



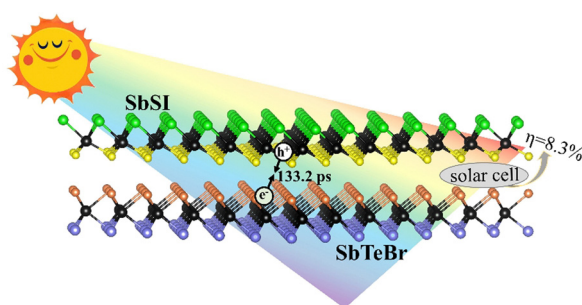
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The sensitive aspects of modelling polymer–ceramic composite solid-state electrolytes using molecular dynamics simulations

Melania Kozdra, Daniel Brandell, C. Moyses Araujo and Amber Mace*

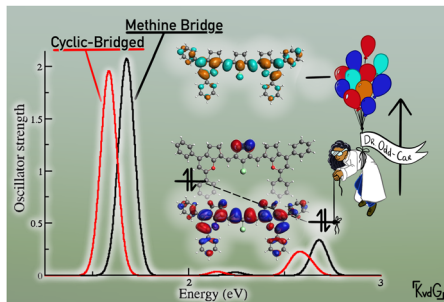
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Two-dimensional Janus SbTeBr/SbSI heterostructures as multifunctional optoelectronic systems with efficient carrier separation

Hong-yao Liu, Huan Yang* and Yujun Zheng*

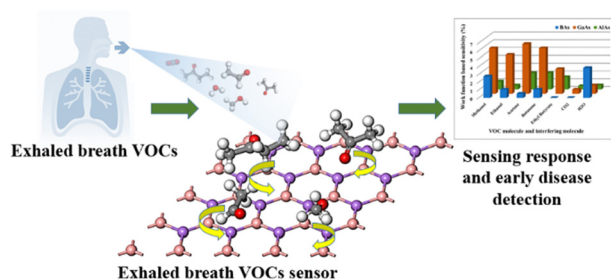
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Cyclopentene ring effects in cyanine dyes: a handle to fine-tune photophysical properties

Natália P. Neme, Thomas L. C. Jansen and Remco W. A. Havenith*

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Interaction of the III-As monolayer with SARS-CoV-2 biomarkers: implications for biosensor development

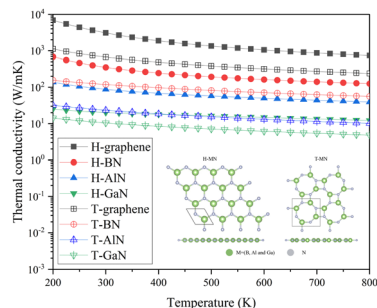
Sudipta Saha, Deb Indronil Sajib and Md. Kawsar Alam*



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Effect of atomic substitution and structure on thermal conductivity in monolayers H-MN and T-MN (M = B, Al, Ga)

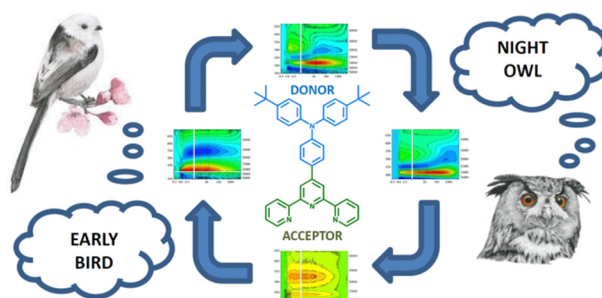
Yulin Zhang, Siyu Gan, Jialu Li, Yi Tian, Xihao Chen, Gehong Su,* Yu Hu* and Ning Wang*



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Early bird or night owl? Controlling the ultrafast photodynamics of triphenylamine substituted 2,2':6',2''-terpyridine

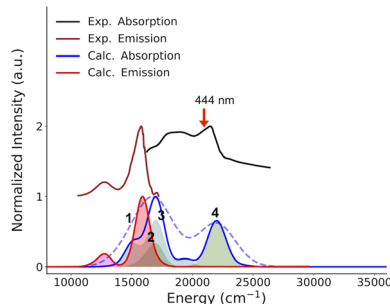
Anna Maria Maroñ,* Oliviero Cannelli,* Etienne Christophe Socie, Piotr Lodowski, Malte Oppermann, Barbara Machura and Majed Chergui



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A theoretical spectroscopy study of the photoluminescence properties of narrow band Eu²⁺-doped phosphors containing multiple candidate doping centers. Prediction of an unprecedented narrow band red phosphor

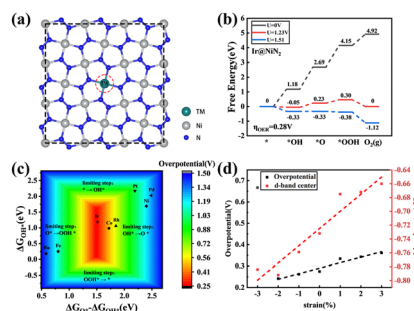
Rami Shafei, Philipp Jean Strobel, Peter J. Schmidt, Dimitrios Maganas,* Wolfgang Schnick* and Frank Neese*



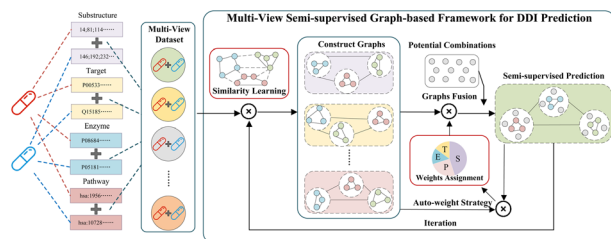
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Enhanced OER catalytic activity of single metal atoms supported by the pentagonal NiN₂ monolayer: insight from density functional theory calculations

Dong-Yin Sun, Long-Hui Li, Guo-Tao Yuan, Yu-Lou Ouyang, Rui Tan, Wen-Jin Yin, Xiao-Lin Wei and Zhen-Kun Tang*



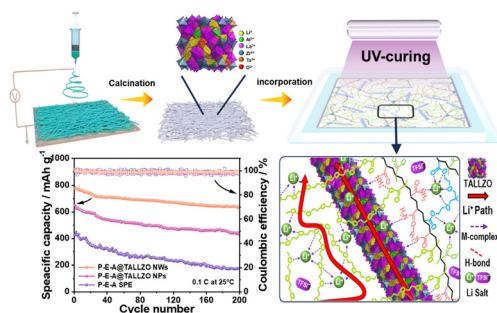
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A low-cost machine learning framework for predicting drug–drug interactions based on fusion of multiple features and a parameter self-tuning strategy

Zexiao Liang, Canxin Lin, Guoliang Tan, Jianzhong Li,* Yan He and Shuting Cai

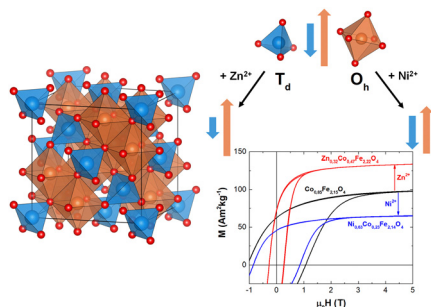
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Improving the ionic conductivity of polymer electrolytes induced by ceramic nanowire fillers with abundant lithium vacancies

Jianlong Ding, Wenqiang Wang,* Yifan Zhang, Hongchun Mu, Xiaomin Cai, Zhengyu Chang and Gengchao Wang*

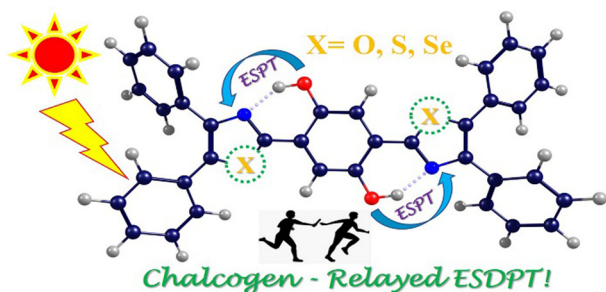
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Chemical engineering of cationic distribution in spinel ferrite nanoparticles: the effect on the magnetic properties

Miran Baričić,* Pierfrancesco Maltoni,* Gianni Barucca, Nader Yaacoub, Alexander Omelyanchik, Fabio Canepa, Roland Mathieu and Davide Peddis*

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Regulated stepwise ESDPT mechanism associated with chalcogen substitutions in BDIBD derivatives

Chang Liu, Jinfeng Zhao,* Jiahe Chen, Mingwei Wang, Mengmeng Hou and Liang Yang

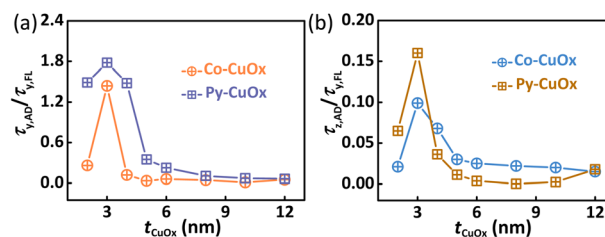


RESEARCH PAPERS

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Observation of the out-of-plane orbital antidamping-like torque

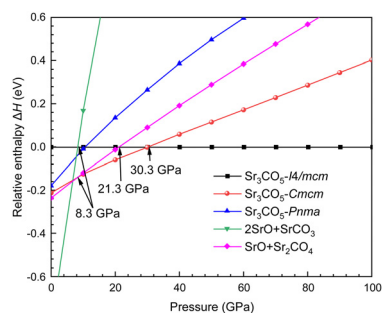
Zeyang Gong, Fu Liu, Xinhong Guo and Changjun Jiang*



6351

Study of high-pressure thermophysical properties of orthocarbonate Sr_3CO_5 using deep learning molecular dynamics simulations

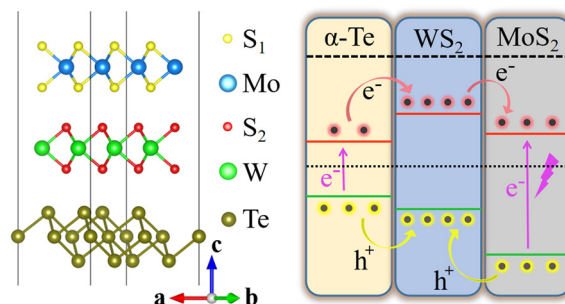
Xin-Xuan Wang, Ting Song,* Zhen-Shuai Lei, Xiao-Wei Sun, Jun-Hong Tian and Zi-Jiang Liu



6362

Tunability of electronic properties in the 2D MoS_2/α -tellurene/ WS_2 heterotrilaier via biaxial strain and electric field

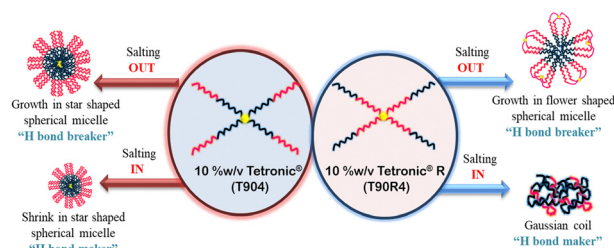
Wenli Zhang, Zhuang Ma, Jing Wang, Bin Shao* and Xu Zuo*



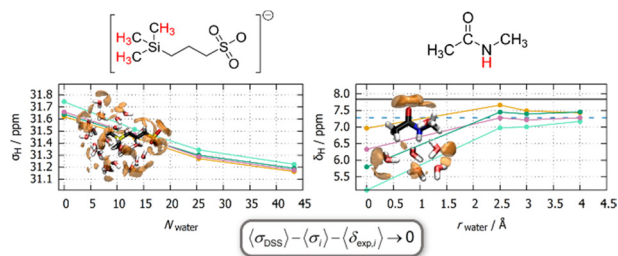
6372

Additive-anchored thermoresponsive nanoscale self-assembly generation in normal and reverse Tetronics®

Dhruvi Patel, Payal Vaswani, Debes Ray, Dhiraj Bhatia, Vinod K. Aswal, Ketan Kuperkar* and Pratap Bahadur



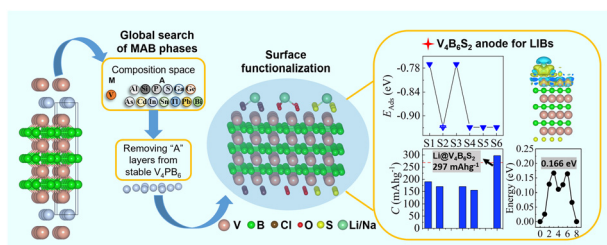
6386



The accuracy limit of chemical shift predictions for species in aqueous solution

Stefan Maste, Bikramjit Sharma, Tim Pongratz, Bastian Grabe, Wolf Hiller, Markus Beck Erlach, Werner Kremer, Hans Robert Kalbitzer, Dominik Marx* and Stefan M. Kast*

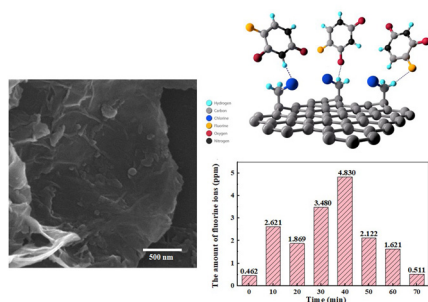
6396



Top-down design of high-performance V-based MBene anode for Li/Na-ion batteries

Shaohan Li, Weiwei Sun,* Tingwei Zhu, Siwei Wang, Jing Zhang,* Jin Yu,* Wei Zheng, Guobing Ying, Litao Sun and Huayun Geng

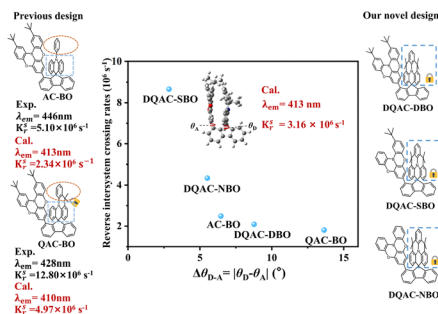
6410



A high loading nanocarrier for the 5-fluorouracil anticancer drug based on chloromethylated graphene

R. Safaiee,* H. Aminzadeh, A. R. Sardarian, Sh. Nasresfahani and M. H. Sheikhi

6420



Designing thermally activated delayed fluorescence emitters with through-space charge transfer: a theoretical study

Jinhui Song, Xin Lv, Junjing Gu, ChiYung Yam* and Lingyi Meng*

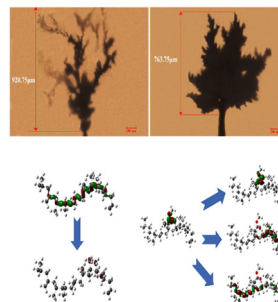


RESEARCH PAPERS

6429

Electrical tree properties of grafted polypropylene studied by electro-luminescence and free radical excitation analysis

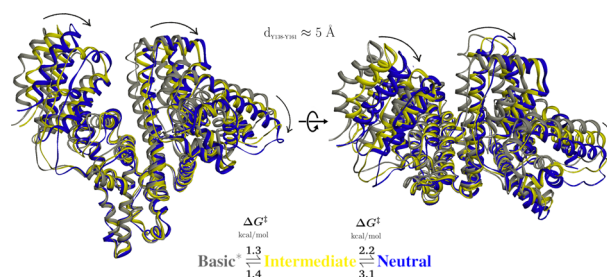
Yaru Zhang, Wenjia Zhang, Shixun Hu,* Juan Li, Mingti Wang, Qi Zhang, Hao Yuan, Changlong Yang, Qi Li* and Jinliang He*



6436

Structural and thermodynamic characterization of allosteric transitions in human serum albumin with metadynamics simulations

Thales Souza Freire,* Julio Zukerman-Schpector, Ran Friedman and Iñez Caracelli



6448

Elucidating the chemical dynamics of the elementary reactions of the 1-propynyl radical ($\text{CH}_3\text{CC}\cdot$; X^2A_1) with 2-methylpropene ($(\text{CH}_3)_2\text{CCH}_2$; X^1A_1)

Iakov A. Medvedkov, Anatoliy A. Nikolayev, Zhenghai Yang, Shane J. Goettl, Alexander M. Mebel* and Ralf I. Kaiser*

