

IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 26(38) 24719–25252 (2024)



Cover

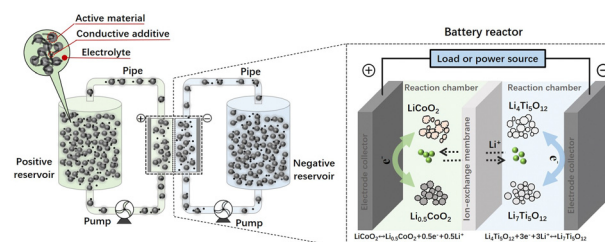
See Ding-Zheng Lin et al., pp. 24791–24798.
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REVIEW

24735

Latest progress and challenges associated with lithium-ion semi-solid flow batteries: a critical review

Man He, Xuelong Zhou and Jiapeng Liu*

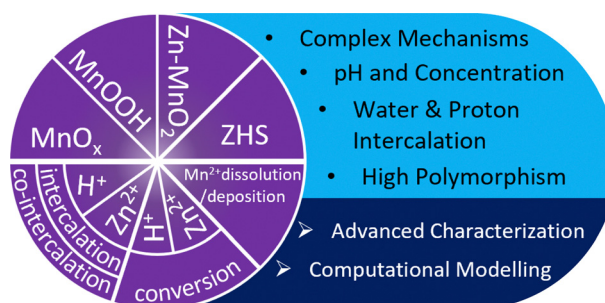


PERSPECTIVE

24753

Progress and perspectives on the reaction mechanisms in mild-acidic aqueous zinc–manganese oxide batteries

Matthew Bergschneider, Fantai Kong, Taesoon Hwang, Youhwan Jo, Denyce Alvarez and Kyeongjae Cho*



Environmental Science: Atmospheres

GOLD
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Fundamental questions
Elemental answers

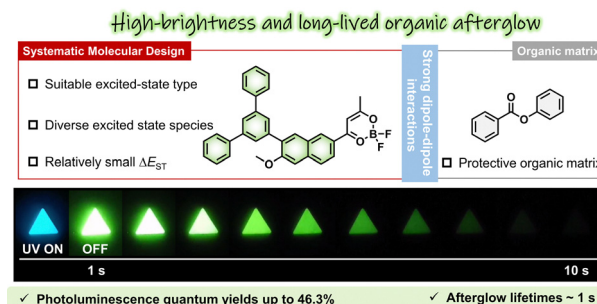


COMMUNICATIONS

24774

Engineering high-brightness and long-lived organic room-temperature phosphorescence via systematic molecular design

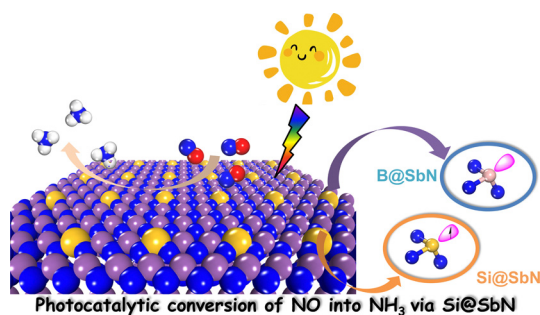
Guangming Wang, Yuanyuan Chen, Xuefeng Chen, Jinqi Zha,* Xiaoya Guo* and Kaka Zhang*



24779

Si@SbN: a promising solar photocatalyst for the reduction of NO

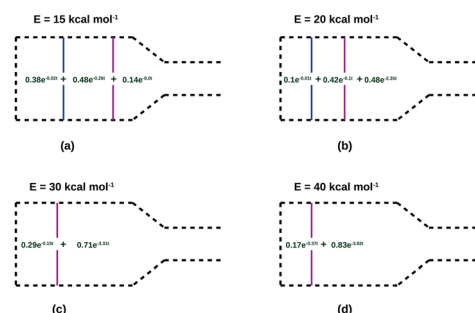
Lei Yang, Jiake Fan and Weihua Zhu*



24785

Role of non-statistical effects in deciding the fate of HO_3^* in the atmosphere

Philips Kumar Rai and Pradeep Kumar*

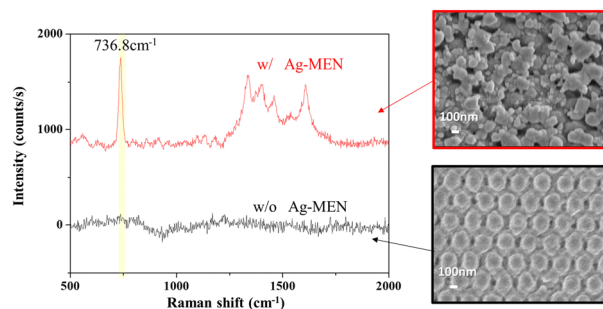


RESEARCH PAPERS

24791

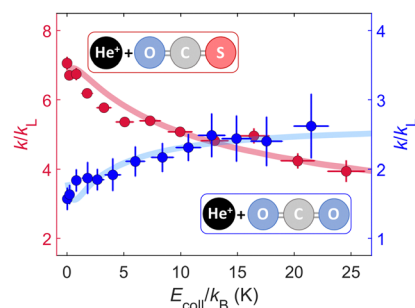
Silver microplasma-engineered nanoassemblies on periodic nanostructures for SERS applications

Zhuo-Fu Wang, Kai-Chun Tsai, Wei-Hung Chiang and Ding-Zheng Lin*



RESEARCH PAPERS

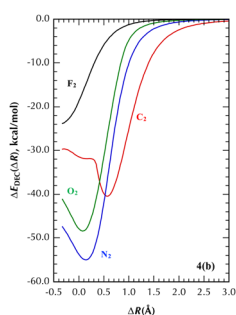
24799



Cold reactions of He⁺ with OCS and CO₂: competitive kinetics and the effects of the molecular multipole moments

Fernanda B. V. Martins, Valentina Zhelyazkova and Frédéric Merkt*

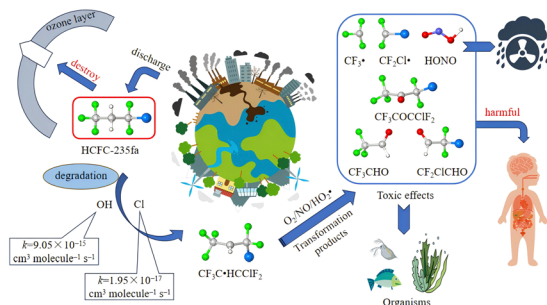
24809



Dynamical electron correlation and the chemical bond. III. Covalent bonds in the A₂ molecules (A = C–F)

Thom H. Dunning, Jr.* and Lu T. Xu

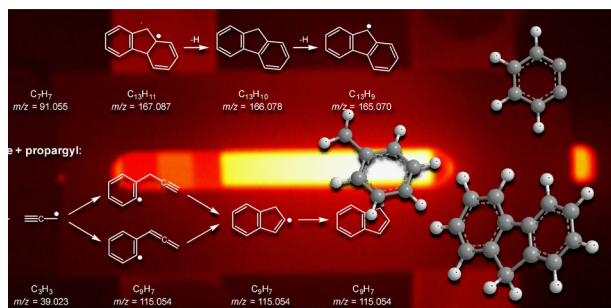
24821



Theoretical study on the mechanisms, kinetics and risk assessment of OH radicals and Cl atom initiated transformation of HCFC-235fa in the atmosphere

Tai-Xing Chi, Xin-Xin Li, Shuang Ni, Feng-Yang Bai,* Xiu-Mei Pan* and Zhen Zhao

24833



Experimental observation of molecular-weight growth by the reactions of o-benzyne with benzyl radicals

David E. Couch, Myrsini M. San Marchi and Nils Hansen*

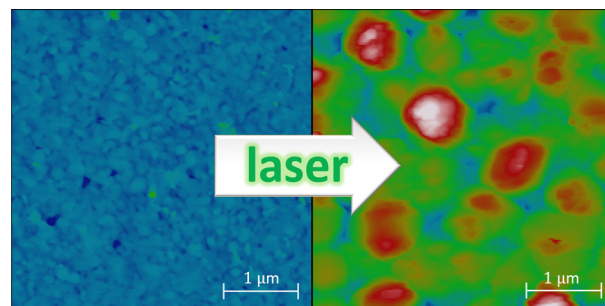


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24841

Laser-induced tuning of crystallization in tetracene thin films

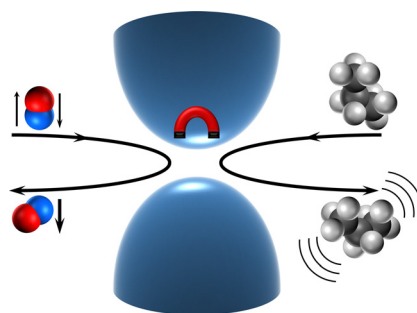
Andika Asyuda, Johannes Müller,
 Mohammad Fardin Gholami, Anton Zykov,
 Linus Pithan, Christoph T. Koch, Jürgen P. Rabe,
 Andreas Opitz* and Stefan Kowarik*



24849

Infrared-driven dynamics and scattering mechanisms of NO radicals with propane and butane: impacts of pseudo Jahn–Teller effects

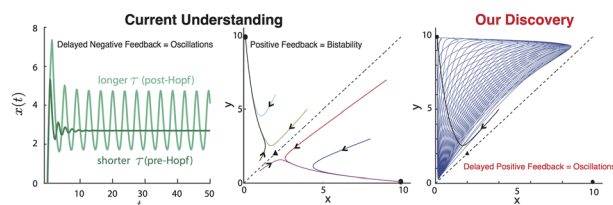
P. Garrett Burroughs, W. Churchill Wilkinson,
 Ellora Majumdar, Jacob D. Bole, Reeva Subedi,
 Joshua T. Kerrigan and Nathanael M. Kidwell*



24861

Oscillations in delayed positive feedback systems

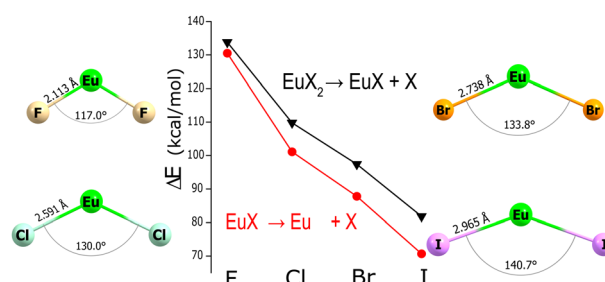
Christopher J. Ryzowicz, Richard Bertram and
 Bhargav R. Karamched*



24870

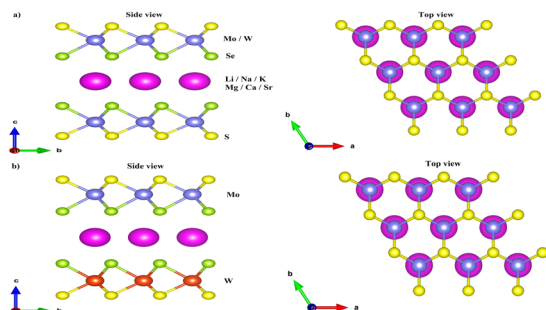
Composite *ab initio* vibrational spectroscopy and thermochemistry of low-valency lanthanide compounds: europium dihalides EuX₂ (X = F, Cl, Br, I)

Alexander N. Smirnov and Victor G. Solomonik*



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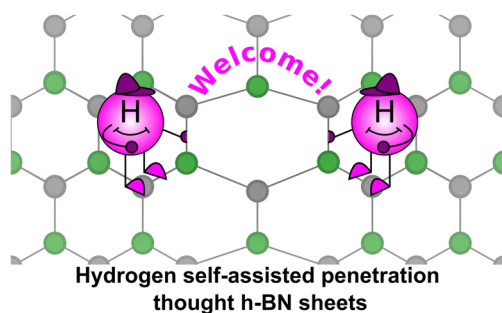
24881



Emergence of superconductivity by intercalation of alkali metals and alkaline earth metals in Janus transition-metal dichalcogenide heterostructures

Soukaina Er-Rahmany,* Mohammed Loulidi,*
Abdallah El Kenz, Abdelilah Benyoussef,
Mohamed Balli and Mohamed Azzouz

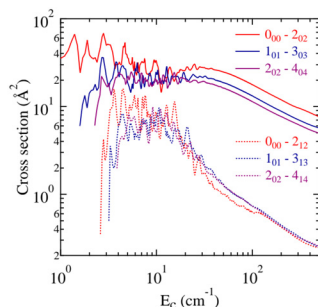
24894



Exploring h-BN as a hydrogen conductor and depository

Ekaterina V. Sukhanova,* Anton M. Manakhov,
Andrey Kovalskii, Abdulaziz S. Al-Qasim and
Zakhar I. Popov*

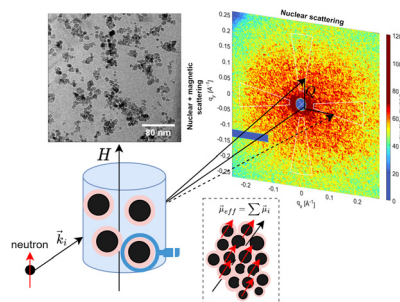
24901



Collisional excitation of propargylimine by helium: new *ab initio* 3D-potential energy surfaces and scattering calculations

Yosra Tebai, Malek Ben Khalifa, Fehmi Khadri* and
Kamel Hammami

24912



Impact of coating type on structure and magnetic properties of biocompatible iron oxide nanoparticles: insights into cluster organization and oxidation stability

Amal Nasser,* Asma Qdemat, Harald Unterweger,
Rainer Tietze, Xiao Sun, Joachim Landers, Juri Kopp,
Baohu Wu, Marie-Sousai Appavou, Anastasiia Murmiliuk,
Elliot Paul Gilbert, Oleg Petravic* and Artem Feoktystov*

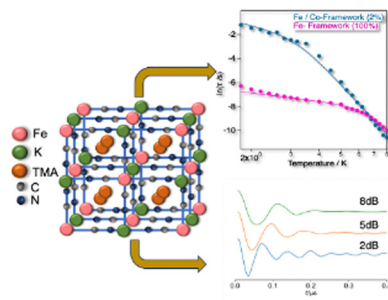


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24924

Spin coherence and magnetization dynamics of $\text{TMA}_2[\text{KCo}_{1-x}\text{Fe}_x(\text{CN})_6]$ toward coordination-framework spin qubits

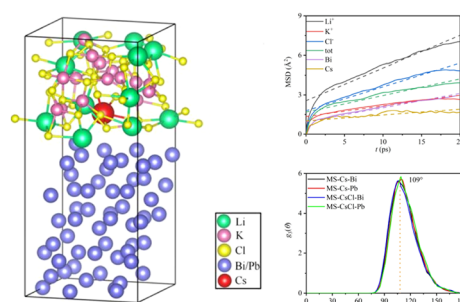
Shraddha Gupta,* Masanori Wakizaka,* Takeshi Yamane, Kazunobu Sato,* Ryuta Ishikawa, Nobuto Funakoshi and Masahiro Yamashita*



24931

First-principles molecular dynamics study on the behaviors of Cs in a mixed system of liquid metal and LiCl-KCl molten salt

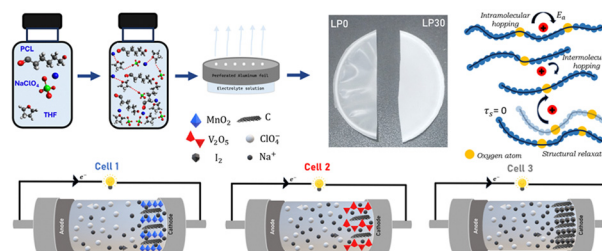
Wentao Zhou, Jia Song, Lve Lin, Xinyu Zhang, Shaoqiang Guo and Yafei Wang*



24941

Insight into ion dynamics in a NaClO_4 -doped polycaprolactone solid polymer electrolyte for solid state batteries

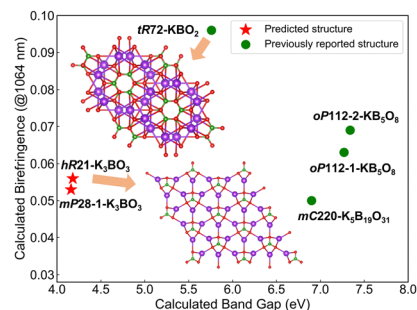
Supriya K. Shetty, Ismayil,* Pradeep Nayak, Y. N. Sudhakar, Kuldeep Mishra, Shahid Bashir and Ramesh Subramaniam



24954

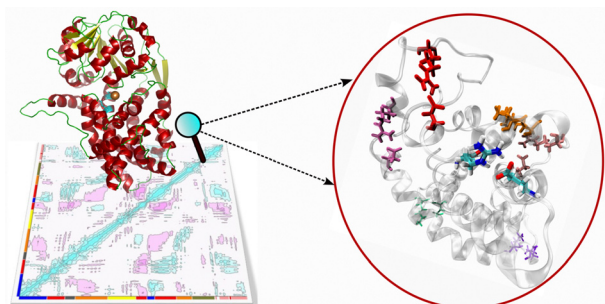
Prediction of ultraviolet optical materials in the $\text{K}_2\text{O-B}_2\text{O}_3$ system

Xiaoqing Guo, Yanting Wang and Haiyang Niu*



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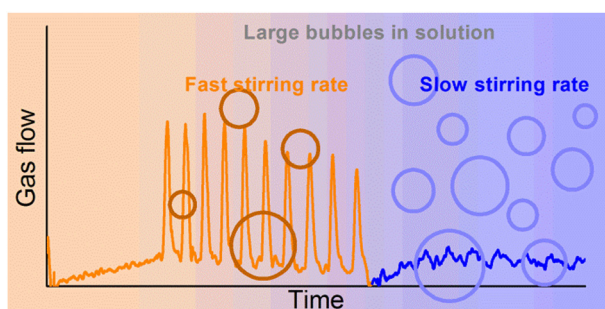
24963



Salt-bridge mediated conformational dynamics in the figure-of-eight knotted ketol acid reductoisomerase (KARI)

Sanjib Thakuria and Sandip Paul*

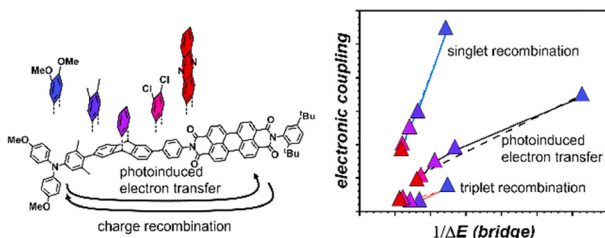
24975



Experimental support for the model of Bray–Liebhafsky oscillatory reaction based on the heterogeneous effects

Itana Nuša Bubanja, Annette Fiona Taylor and Dragomir Stanisavljev*

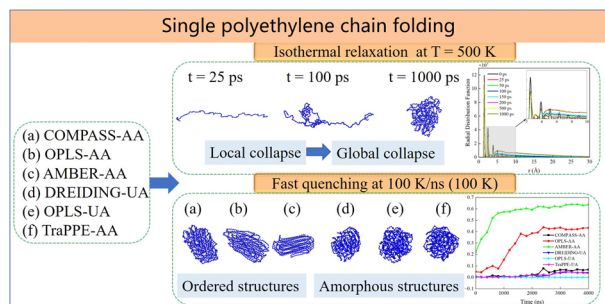
24983



Control of electronic and exchange coupling by bridge substituents in donor acceptor triads with triptycene bridges

Christoph Lambert,* Chantal Roger, Alexander Schmiedel, Marco Holzapfel, Nikita Lukzen and Ulrich E. Steiner*

24995



Molecular dynamics simulations of single polyethylene chain folding during fast quenching using all-atom and united-atom models

Jingfu Shi, Jianqiu Zhou,* Lei Liu and Changqing Miao*

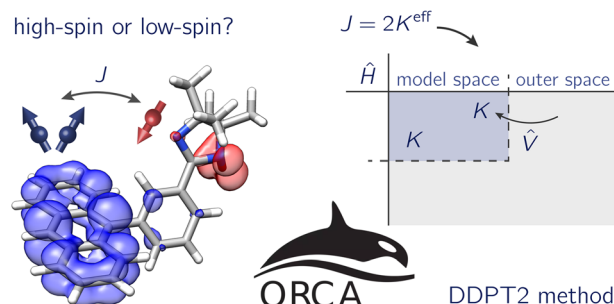


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25005

Elucidation of the exchange interaction in photoexcited three-spin systems – a second-order perturbational approach

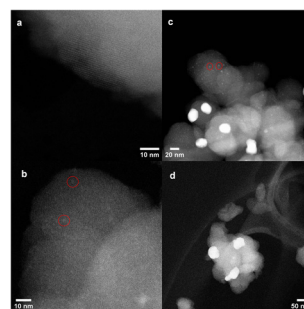
Michael Franz, Frank Neese* and Sabine Richert*



25021

Controlling nanocluster growth through nanoconfinement: the effect of the number and nature of metal–organic framework functionalities

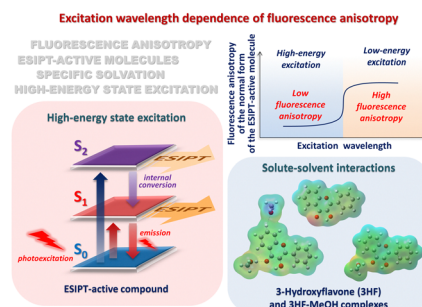
James King, Zhipeng Lin, Federica Zanca, Hui Luo, Linda Zhang, Patrick Cullen, Mohsen Danaie, Michael Hirscher, Simone Meloni, Alin M. Elena and Petra Á. Szilágyi*



25029

Excitation wavelength-dependent fluorescence anisotropy of 3-hydroxyflavone: revisiting the solvation processes and high-energy state excitation in ESIPT-active compounds

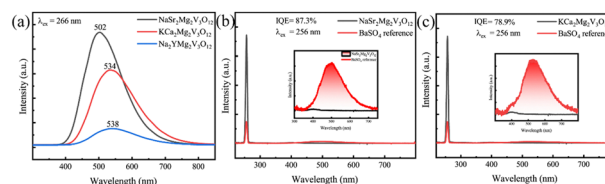
Dzmitryi Ushakou* and Marek Józefowicz*



25048

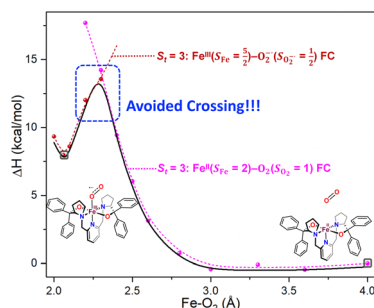
Structure and luminescence characteristics of self-activated vanadate garnet phosphors

Jing Xie, Yue Zhong, Tao Su, Wenming Wang, Yan Pan, Xiantao Wei* and Yong Li*



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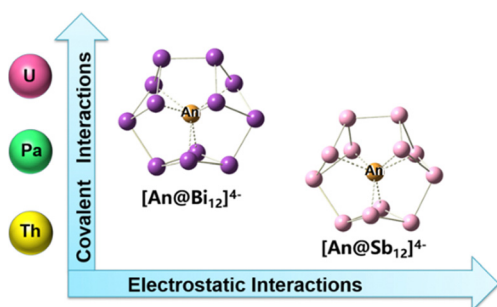
25057



Insights into dioxygen binding on metal centers: an *ab initio* multireference electronic structure analysis

Peng Zhang, Way-Zen Lee and Shengfa Ye*

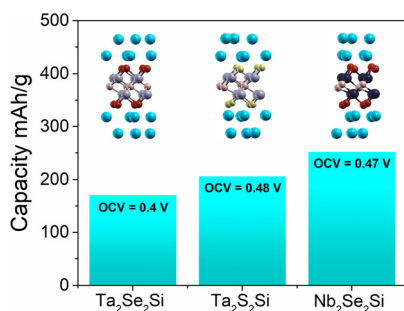
25069



Actinide endohedral inter-metalloid clusters of the group 15 elements

Nai-Xin Zhang, Cong-Zhi Wang,* Jian-Hui Lan, Qun-Yan Wu and Wei-Qun Shi*

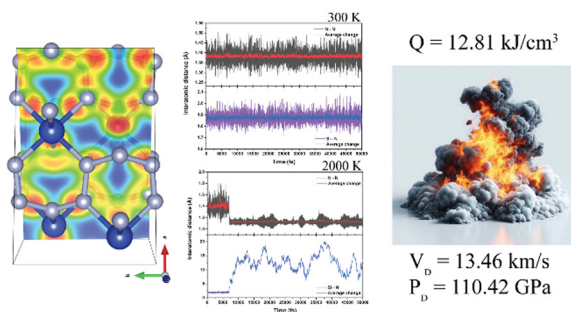
25076



Transition metal Si-chalcogenides: a new two-dimensional anode material for Na-ion batteries

K. H. Yeoh,* Y. H. R. Chang,* K.-H. Chew, D. S. Ong, C. F. Dee, B. T. Goh, E. Y. Chang and H. W. Yu

25089



Exploration of Si–N compounds as high energy density materials

Paras Patel, Saurav Patel, Madhavi H. Dalsaniya, Dominik Kurzydłowski, Krzysztof J. Kurzydłowski and Prafulla K. Jha*

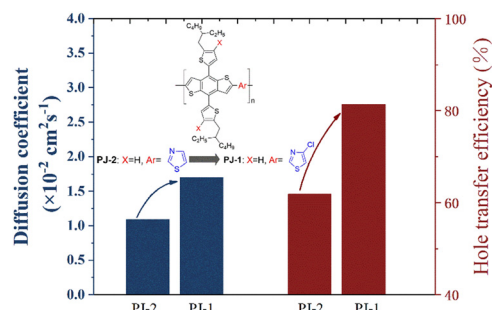


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25098

The exciton dynamics and charge transfer in polymers with the effects of chlorine substituents

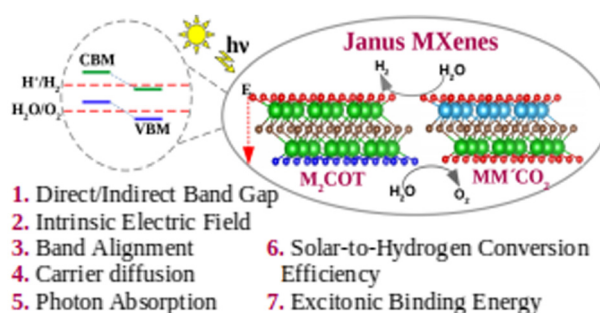
Xu Han, Guangliu Ran, Hao Lu and Shumei Sun*



25105

Performance parameters of infra-red and visible-active MXene photocatalysts for water splitting

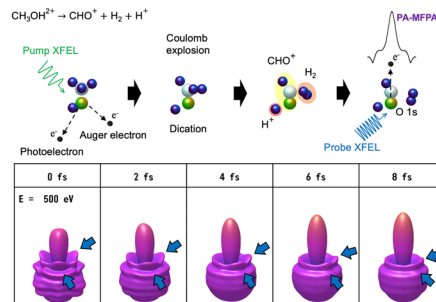
Swati Shaw* and Subhradip Ghosh*



25118

Time-resolved photoelectron diffraction imaging of methanol photodissociation involving molecular hydrogen ejection

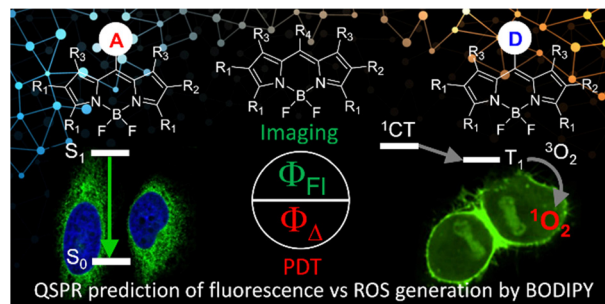
Kazuki Yoshikawa, Manabu Kanno,* Hao Xue, Naoki Kishimoto,* Soki Goto, Fukiko Ota, Yoshiaki Tamura, Florian Trinter,* Kilian Fehre, Leon Kaiser, Jonathan Stindl, Dimitrios Tsitsonis, Markus Schöffler, Reinhard Dörner, Rebecca Boll, Benjamin Erk, Tommaso Mazza, Terence Mullins, Daniel E. Rivas, Philipp Schmidt, Sergey Usenko, Michael Meyer, Enliang Wang, Daniel Rolles, Artem Rudenko, Edwin Kukk, Till Jahnke, Sergio Díaz-Tendero,* Fernando Martín, Keisuke Hatada* and Kiyoshi Ueda*



25131

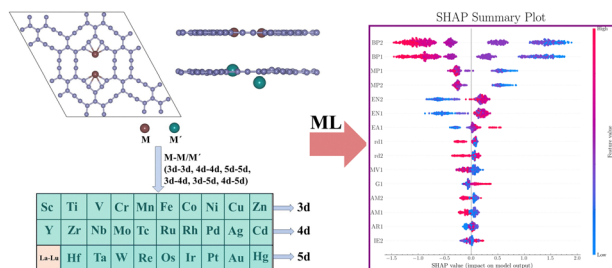
Predicting fluorescence to singlet oxygen generation quantum yield ratio for BODIPY dyes using QSPR and machine learning

Platon P. Chebotaev, Andrey A. Buglak,* Aimee Sheehan and Mikhail A. Filatov*



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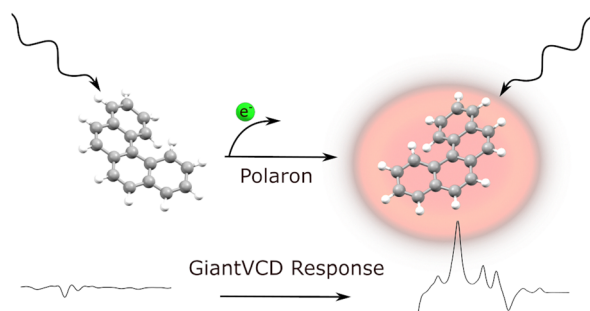
25143



DFT and machine learning guided investigation into the design of new dual-atom catalysts based on α -2 graphyne

Chandra Chowdhury,* Esackraj Karthikraja and Venkatesan Subramanian

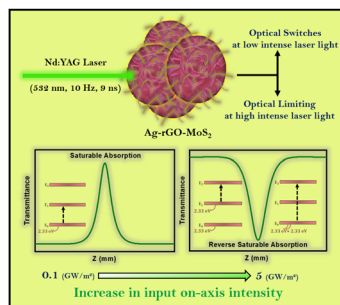
25156



Introducing the new concept of a chiral-polaron giant-IRAV signature, optical-active giant-response in vibrational circular dichroism

Fabio Biffoli, Marco Bonechi, Marco Pagliai, Massimo Innocenti, Roberto Giovanardi and Claudio Fontanesi*

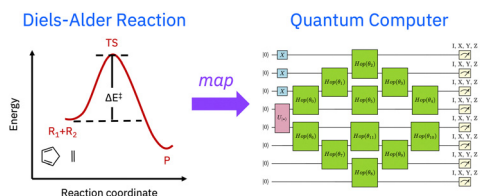
25169



Insights into nonlinear absorption transitions in a silver-incorporated reduced graphene oxide-molybdenum disulfide (Ag-rGO-MoS₂) hybrid

M. Abith and T. C. Sabari Girisun*

25181



Simulation of a Diels-Alder reaction on a quantum computer

Ieva Liepuoniute,* Mario Motta, Thaddeus Pellegrini, Julia E. Rice, Tanvi P. Gujarati, Sofia Gil and Gavin O. Jones*

- ✓ Quantum algorithm benchmarking for electronic structure calculations, with Diels-Alder as a test case.
- ✓ Quantum hardware calculations using Diels-Alder as a benchmark for performance evaluation.

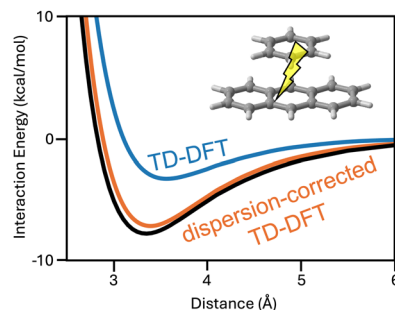


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25192

Exploring non-covalent interactions in excited states: beyond aromatic excimer models

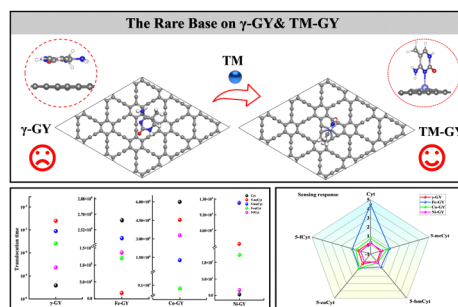
Ariel C. Jones and Lars Goerigk*



25208

Adsorption of rare bases on transition metal doped γ -graphyne nanosheets: a DFT study

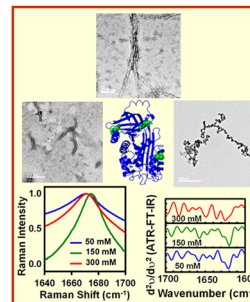
Xia Zeng, Ruiying Zhang, Ruirui Li, Ruimei Li,* Hong Cui, Caibin Zhao, Shengrui Zhang and Lingxia Jin*



25222

Intrinsic conformational preference in the monomeric protein governs amyloid polymorphism

Anjali Giri and Mily Bhattacharya*



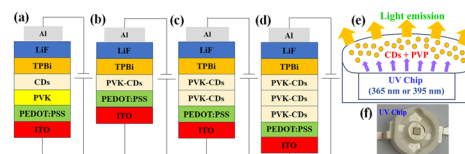
25232

Electroluminescent and photoluminescent light-emitting diodes from carbon dots and device architecture optimization

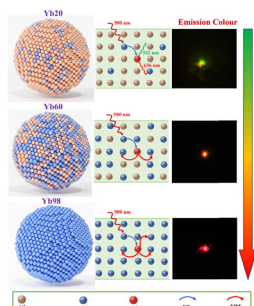
Jielong Li, Rongbin Deng, Muci Li, Jingwei Wu, Bingyu Wang, Liming Liu,* Zichuan Yi, Honghang Wang and Xiaowen Zhang*

Device A: ITO/PEDOT:PSS/PVK/CDs/TPBi (80 nm)/LiF (2 nm)/Al (120 nm).

Device B1: ITO/PEDOT:PSS/[PVK-CDs]/TPBi/LiF/Al.

Device B2: ITO/PEDOT:PSS/[PVK-CDs] $\times$ 2/TPBi/LiF/Al.Device B3: ITO/PEDOT:PSS/[PVK-CDs] $\times$ 3/TPBi/LiF/Al.

25240



Effect of Yb³⁺ concentration on the upconversion emission properties of sub 10 nm RbY₂F₇:Yb, Er nanoparticles

Ajith Kumar Lakshmanan, Snigdhadev Chakraborty, Basudev Roy and J. Senthilselvan*

