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Cover
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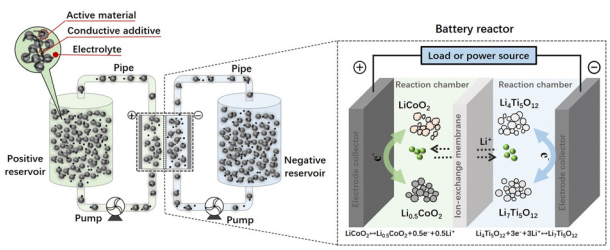
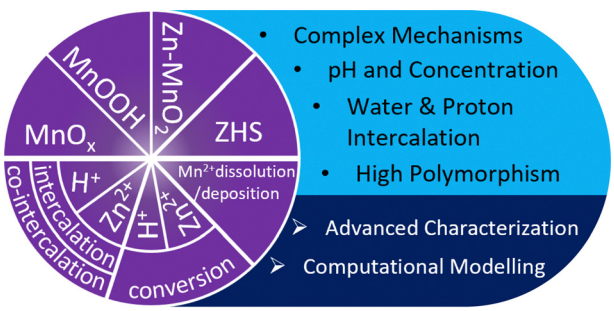
REVIEW



PERSPECTIVE



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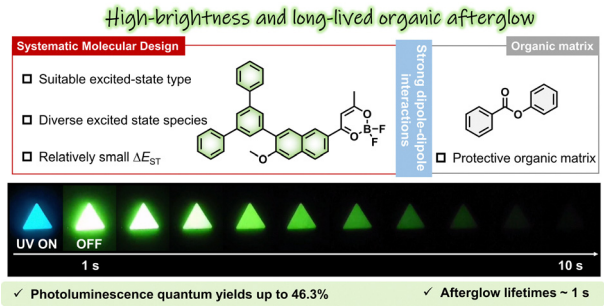

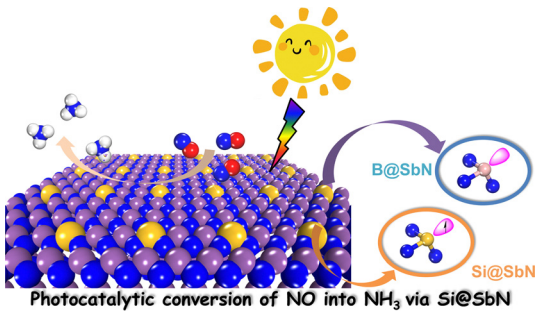

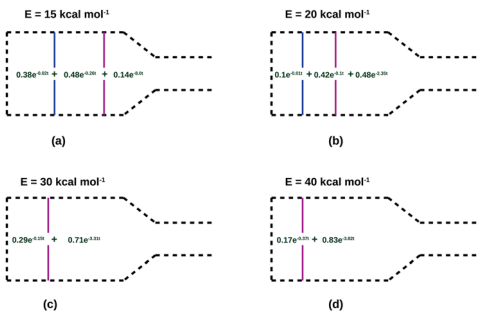

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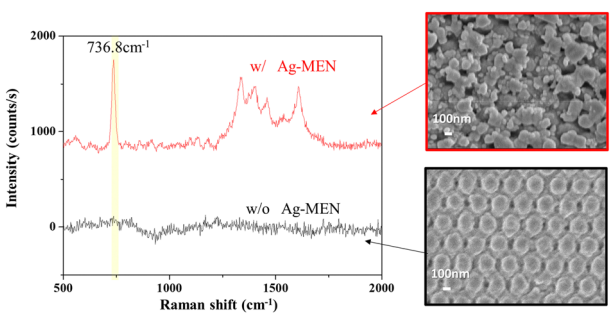

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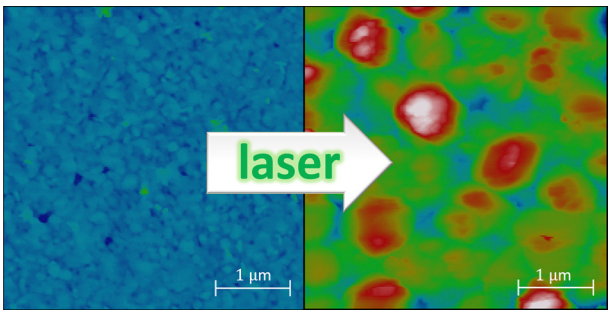

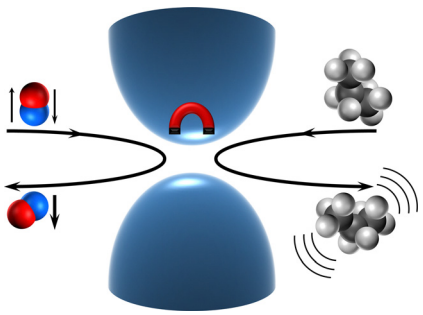

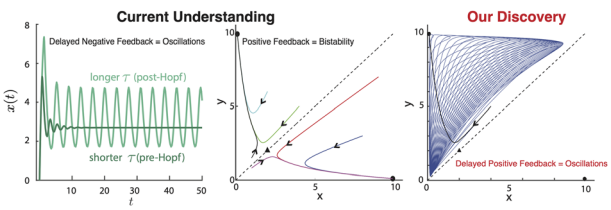

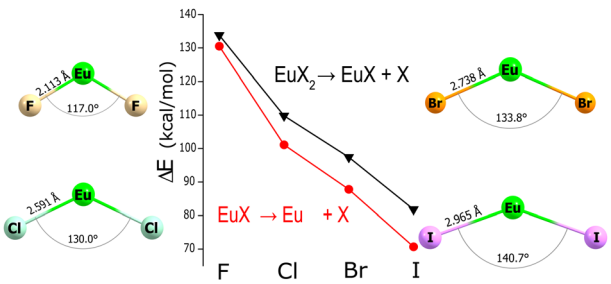

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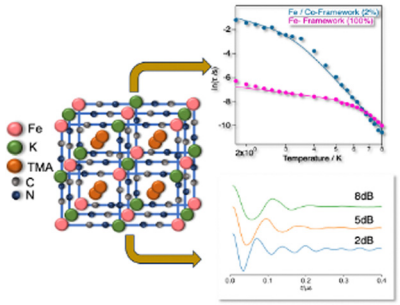

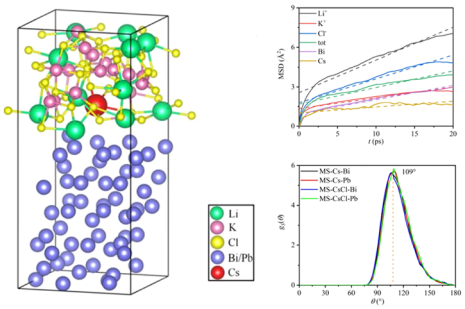

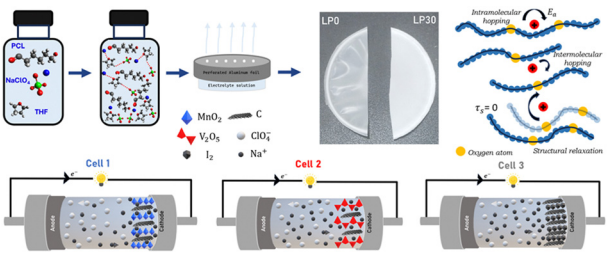

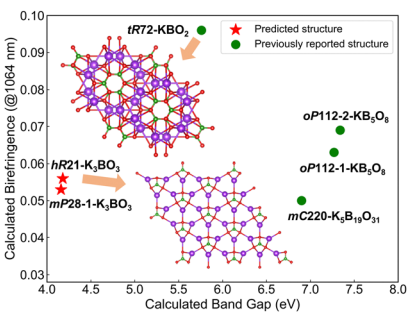

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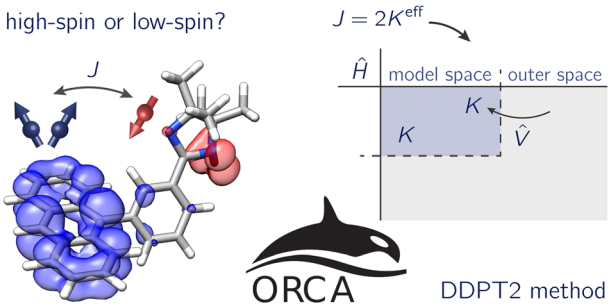

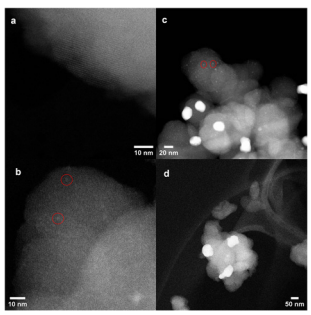

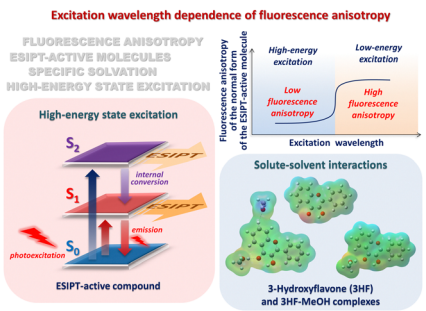

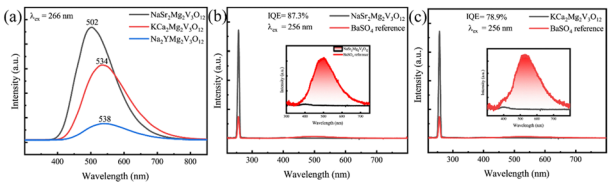

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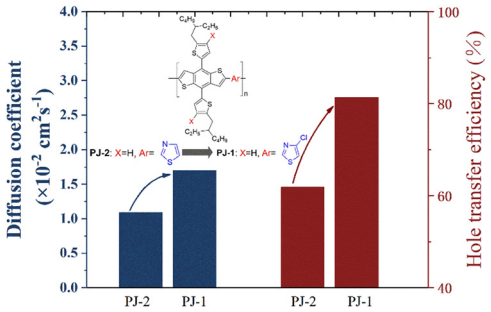
25098

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

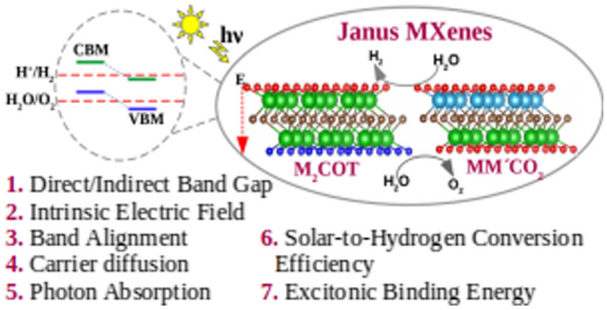
Xu Han, Guangliu Ran, Hao Lu and Shumei Sun*



25105

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

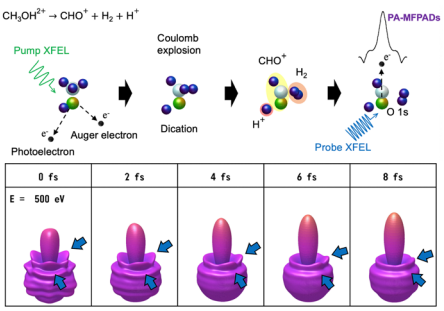
Swati Shaw* and Subhradip Ghosh*



25118

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

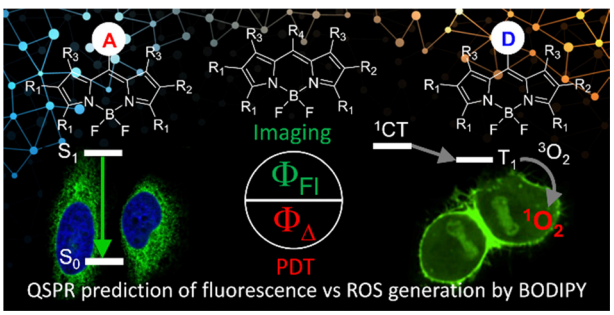
Kazuki Yoshikawa, Manabu Kanno,* Hao Xue, Naoki Kishimoto,* Soki Goto, Fukiko Ota, Yoshiaki Tamura, Florian Trinter,* Kilian Fehre, Leon Kaiser, Jonathan Stindl, Dimitrios Tsitsonis, Markus Schöffler, Reinhard Dörner, Rebecca Boll, Benjamin Erk, Tommaso Mazza, Terence Mullins, Daniel E. Rivas, Philipp 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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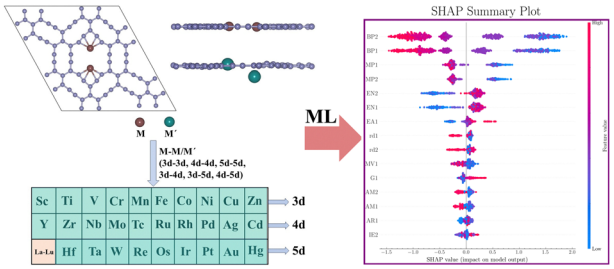

DFT and machine learning guided investigation into the design of new dual-atom catalysts based on α-2 graphyne

Chandra Chowdhury,* Esackraj Karthikraja and Venkatesan Subramanian

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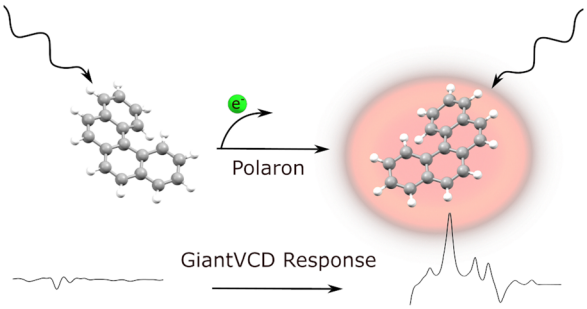

Introducing the new concept of a chiral-polaron giant-IRAV signature, optical-active giant-response in vibrational circular dichroism

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

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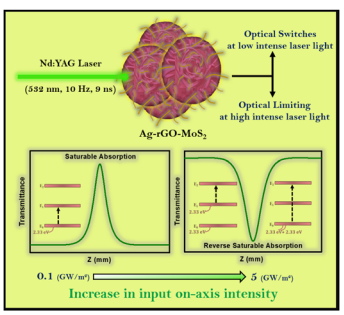

Insights into nonlinear absorption transitions in a silver-incorporated reduced graphene oxide–molybdenum disulfide (Ag–rGO–MoS_2) hybrid

M. Abith and T. C. Sabari Girisun*

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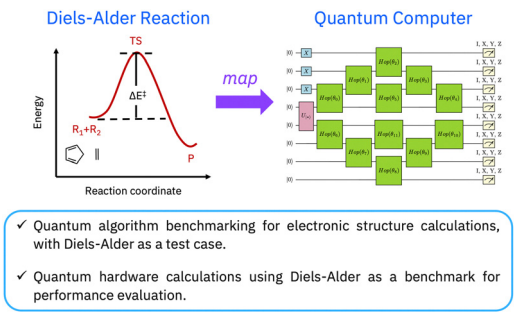

Simulation of a Diels–Alder reaction on a quantum computer

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

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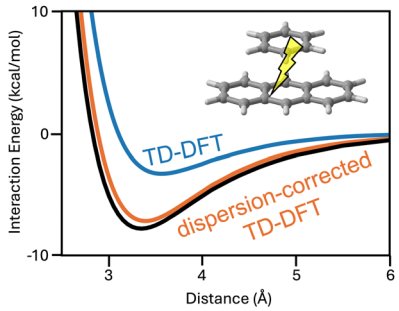
Exploring non-covalent interactions in excited states: beyond aromatic excimer models

Ariel C. Jones and Lars Goerigk*



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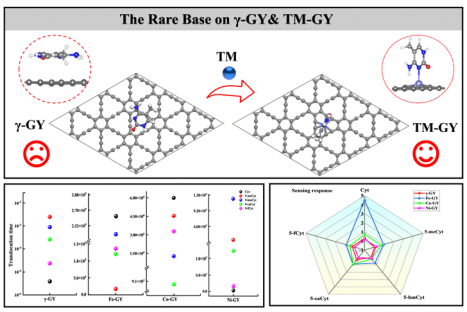
Adsorption of rare bases on transition metal doped γ-graphyne nanosheets: a DFT study

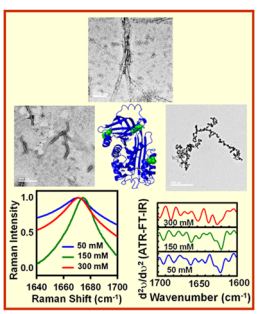
Xia Zeng, Ruiying Zhang, Ruirui Li, Ruimei Li,* Hong Cui, Caibin Zhao, Shengrui Zhang and Lingxia Jin*



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

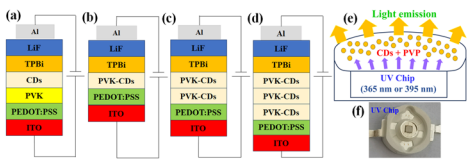
Jielong Li, Rongbin Deng, Muci Li, Jingwei Wu, Bingyu Wang, Liming Liu,* Zichuan Yi, Honghang Wang and Xiaowen Zhang*

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]×2/TPBi/LiF/Al.

Device B3: ITO/PEDOT:PSS/[PVK-CDs]×3/TPBi/LiF/Al.



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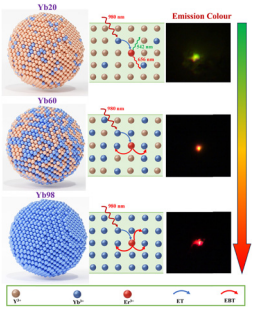

Effect of Yb^{3+} concentration on the upconversion emission properties of sub 10 nm RbY_2F_7:Yb, Er nanoparticles

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