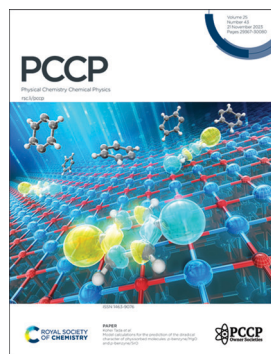


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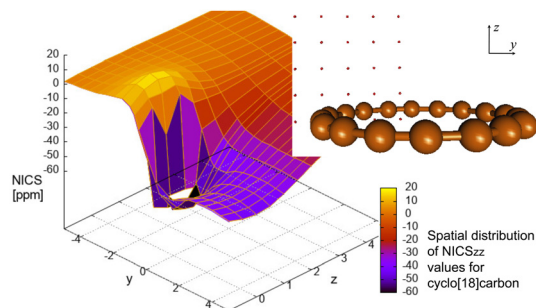
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Cyclo[*n*]carbons and catenanes from different perspectives: disentangling the molecular thread

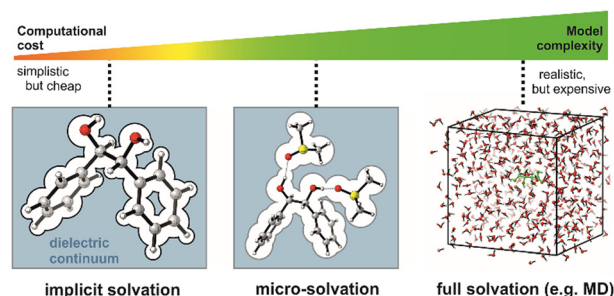
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MatAR: dynamic augmented reality platform for accessible molecular visualization

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Satayanaraya Bonakala, Johanne Medina,
Lamis Ayeche, Joelle Fadlallah and Fedwa El Mellouhi*

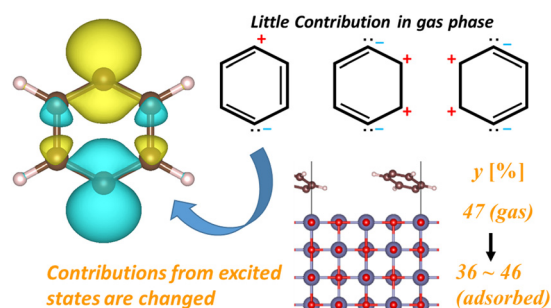


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Model calculations for the prediction of the diradical character of physisorbed molecules: *p*-benzyne/MgO and *p*-benzyne/SrO

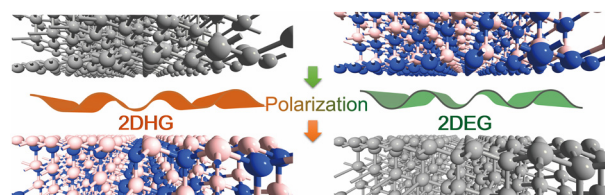
Kohei Tada,* Takashi Kawakami and Yoyo Hinuma



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Two-dimensional ambipolar carriers of giant density at the diamond/cubic-BN(111) interfaces: toward complementary logic and quantum applications

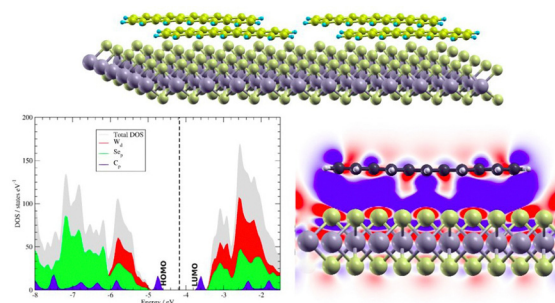
Jiadoo Zhu, Kai Su, Zeyang Ren, Yao Li, Jinfeng Zhang,*
Jincheng Zhang,* Lixin Guo and Yue Hao*



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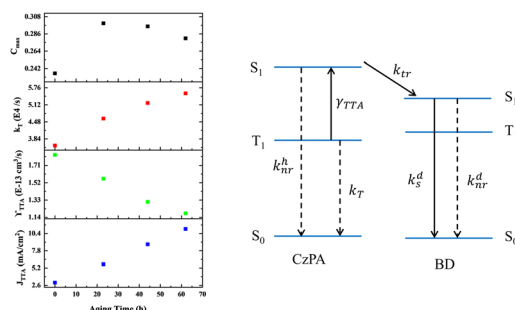
Interaction between pentacene molecules and monolayer transition metal dichalcogenides

E. Black, P. Kratzer and J. M. Morbec*



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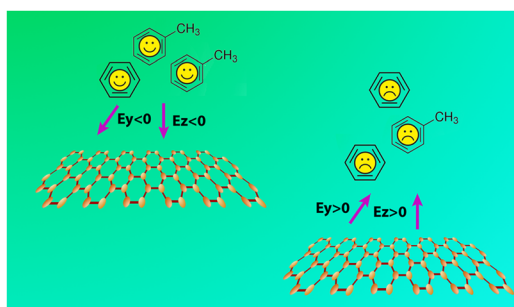
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Yibing Wu, Shu Xiao, Kaiwen Guo, Xianfeng Qiao, Dezhi Yang, Yanfeng Dai, Qian Sun, Jiangshan Chen and Dongge Ma*

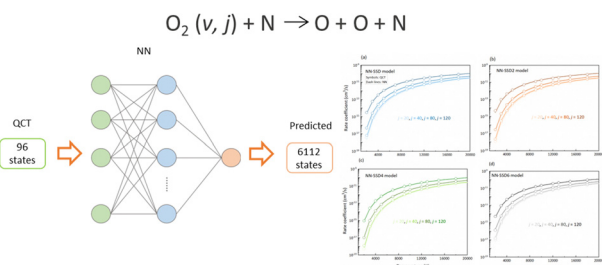
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Enhanced sensing performance of armchair stanene nanoribbons for lung cancer early detection using an electric field

Maedeh Mashhadbani and Edris Faizabadi*

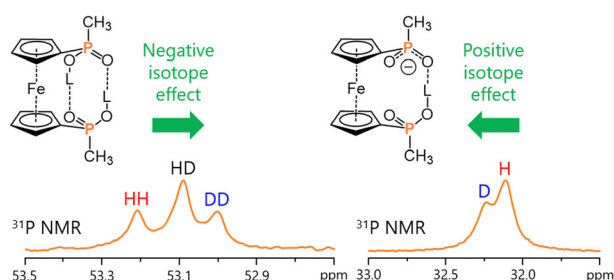
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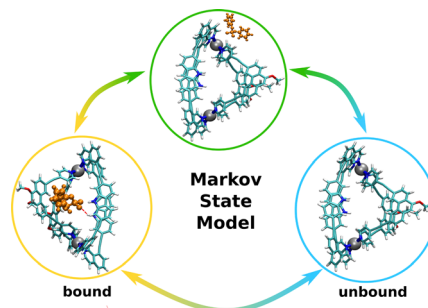


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Dynamics of organophosphate guest encapsulation in heteroleptic coordination cages

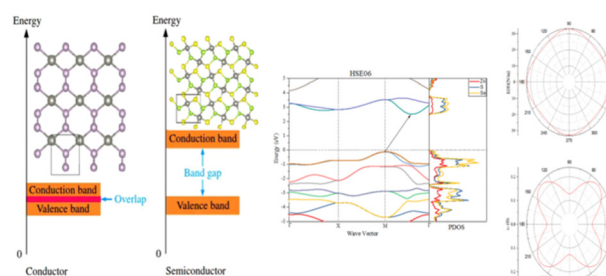
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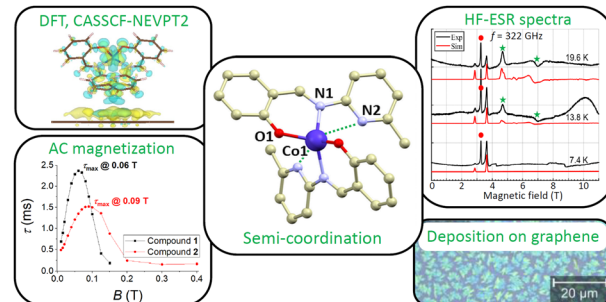
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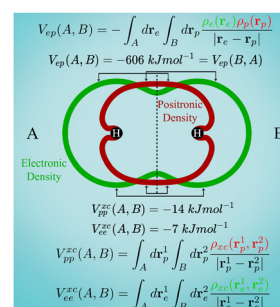
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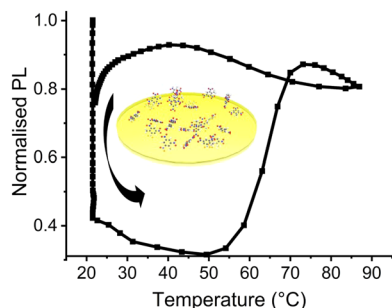
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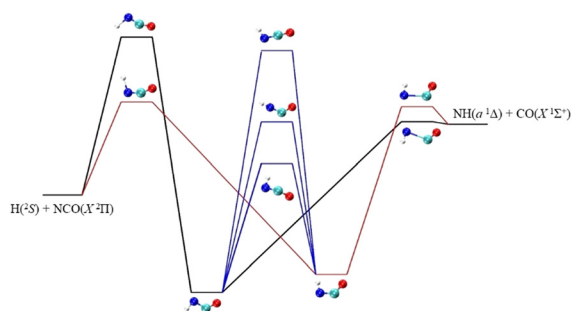
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Thermal control of organic semiconductors for trace detection of explosives

Edward B. Ogugu, Ross N. Gillanders, Salam Mohammed and Graham A. Turnbull*

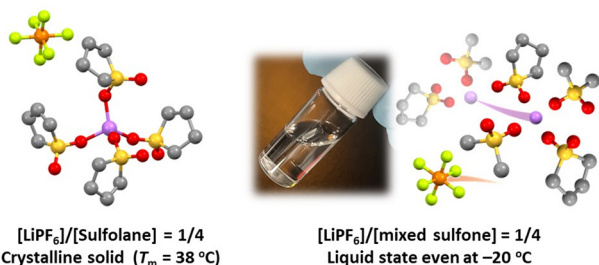
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Full-dimensional potential energy surface for the photodissociation of HNCO via its S_1 band

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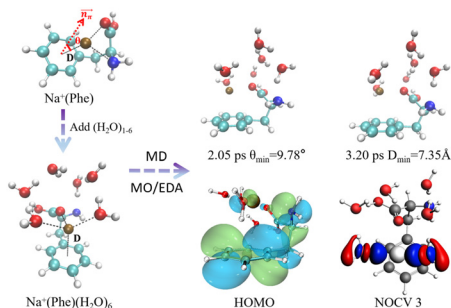
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High-concentration LiPF₆/sulfone electrolytes: structure, transport properties, and battery application

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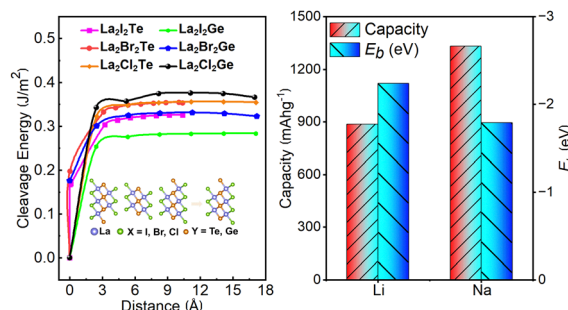


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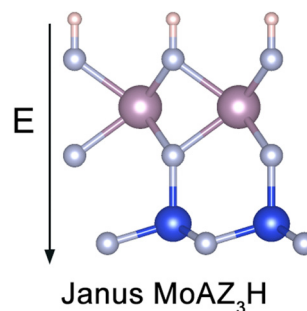
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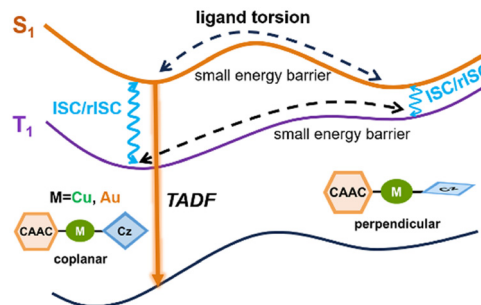
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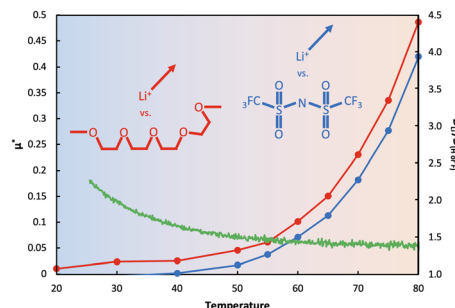
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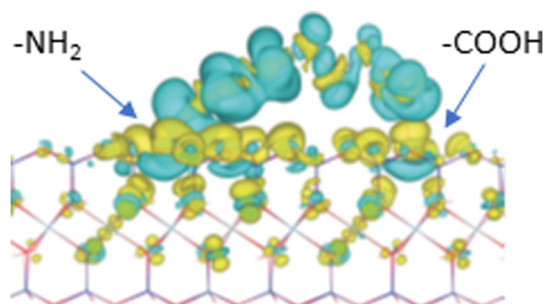
Accelerated lithium-ion diffusion via a ligand 'hopping' mechanism in lithium enriched solvate ionic liquids

Timothy Harte, Bhagya Dharmasiri,* Garima S. Dobhal, Tiffany R. Walsh* and Luke C. Henderson*



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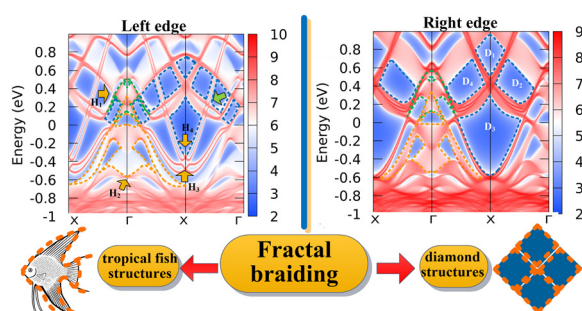
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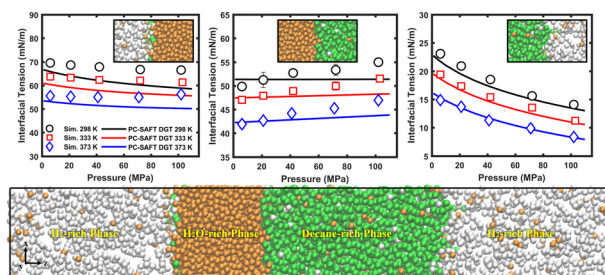
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Evolution of local edge state braiding and spin topological transport characterization of Te-doped monolayer 1T'-MoS₂

Qian Cheng, Zhengxin Yan,* Wei Song, Juntao Kong, Dongxin Li, Wuyue Xu, You Xie, Xingkun Liang and Zehua Zhao

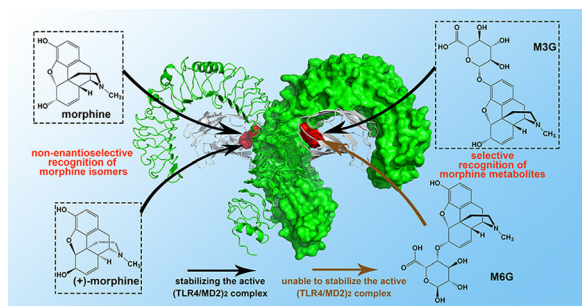
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Yafan Yang,* Jingyu Wan,* Jingfa Li, Guangsi Zhao and Xiangyu Shang*

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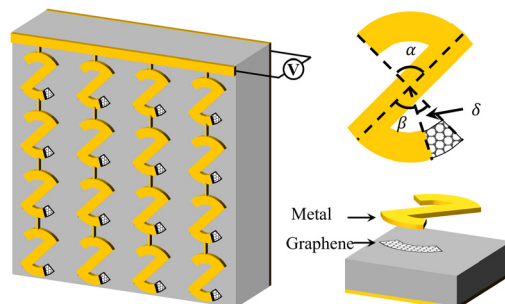


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Active control of circular dichroism in a graphene–metal hybridized metamaterial driven by symmetry-protected bound states in the continuum

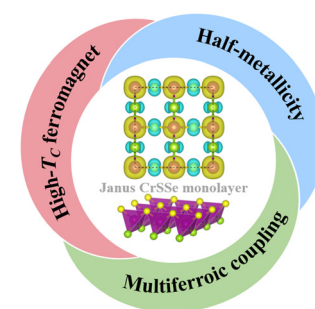
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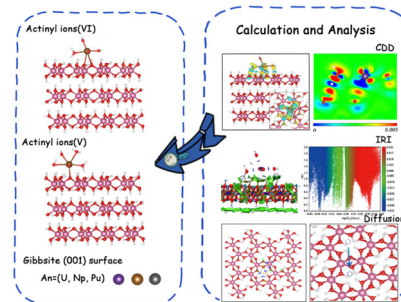
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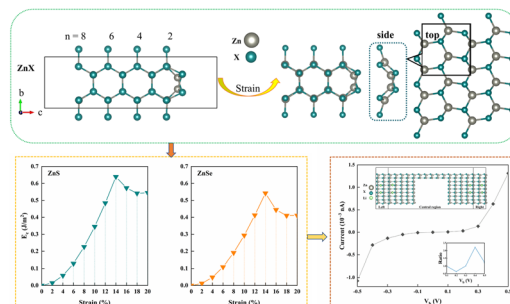
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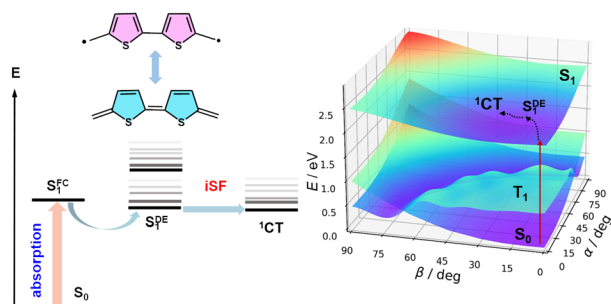
Exfoliable and self-healable two-dimensional materials from wurtzite zinc chalcogenides as building blocks of nanodevices

Jin Li,* Xinbo Chen, Maoyun Di and Lei Qin



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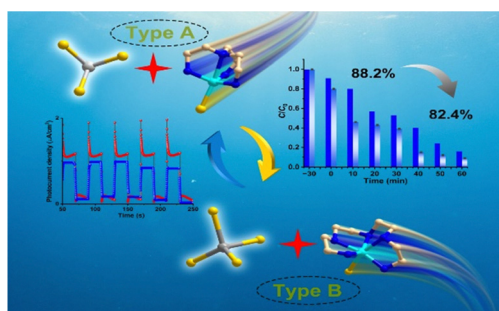
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Excitation localization/delocalization induced intramolecular singlet fission in cyclopentadithiophene-based quinoidal derivatives

Jin Wen,* Jie Zhou, Xuesi Li, Meng Lv, Jun Huang, Zheng Li, Boyuan Zhang, Ming Wang, Jinquan Chen and Meifang Zhu

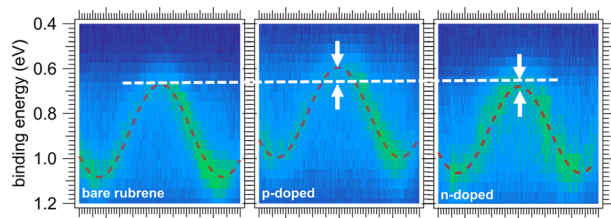
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Syntheses, crystal structure, and photoelectric properties of two Zn-based chalcogenidoantimonates Zn-Sb-Q (Q = S, Se)

Lirong Zhang, Huiling Zhao, Xin Liu,* Gele Teri and Menghe Baiyin*

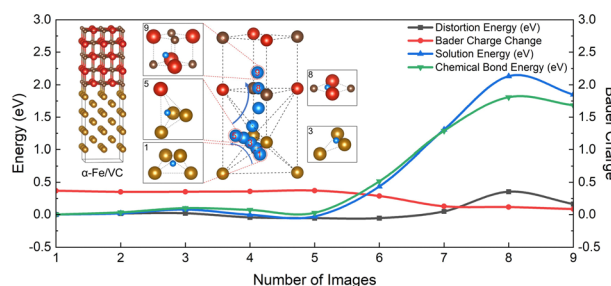
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Surface doping of rubrene single crystals by molecular electron donors and acceptors

Christos Gatsios, Andreas Opitz,* Dominique Lungwitz, Ahmed E. Mansour, Thorsten Schultz, Dongguen Shin, Sebastian Hammer, Jens Pflaum, Yadong Zhang, Stephen Barlow, Seth R. Marder and Norbert Koch*

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Understanding the migration mechanism of hydrogen atom from the α -Fe matrix into nano-precipitates via DFT calculations

Yuan Ma, Shaojie Zhou, Yang He,* Yanjing Su, Lijie Qiao and Lei Gao*

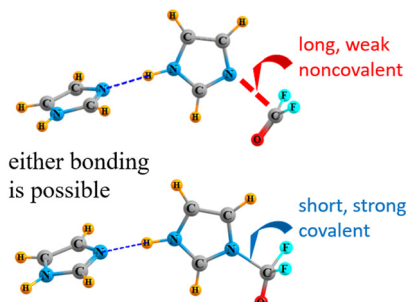


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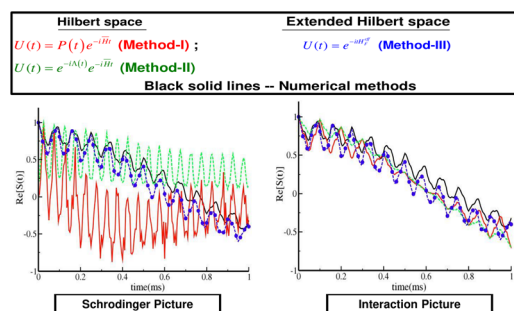
Xin Wang, Qingzhong Li* and Steve Scheiner*



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A perspective on the relative merits/demerits of time-propagators based on Floquet theorem

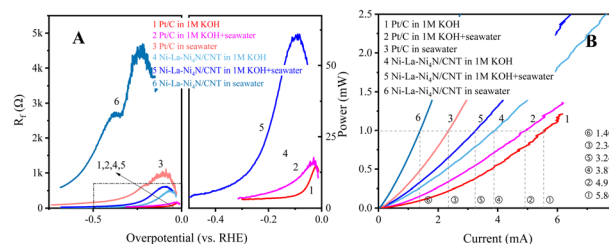
Shreyan Ganguly and Ramesh Ramachandran*



29774

Investigation of seawater electrolyte on hydrogen evolution reaction from the perspective of kinetics and energy consumption using an Ni-based electrocatalyst supported on carbon nanotubes

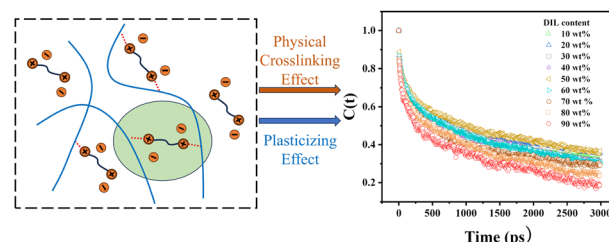
Lin Zhu, Siyue Zhang, Zheng Ai, Yan Zhang, Baoli Wang, Ruyi Zou and Wei Sun*



29783

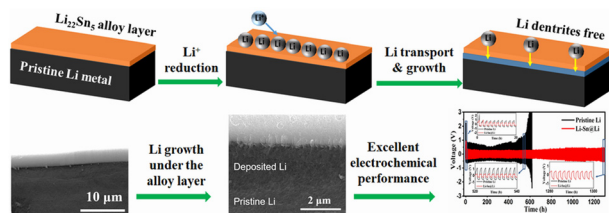
Structural, energetic and dynamic investigation of poly(ethylene oxide) in imidazolium-based ionic liquids with different cationic structures

Yongjie Dan, Huan Luo, Pengjian Gong, Dadong Yan, Yanhua Niu* and Guangxian Li*



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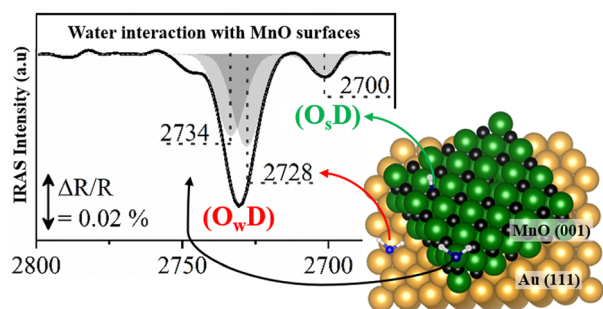
29797



Spatially isolating Li^+ reduction from Li deposition via a $\text{Li}_{22}\text{Sn}_5$ alloy protective layer for advanced Li metal anodes

Jia Xie, Jing Xue,* Hongyi Wang and Jingze Li*

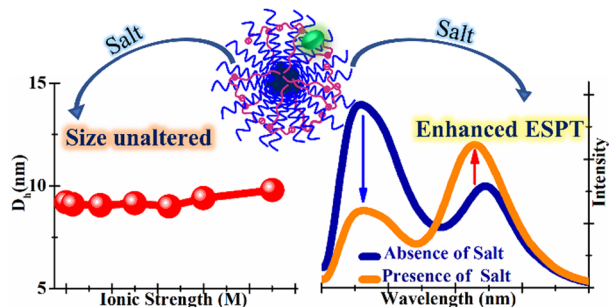
29808



Interaction of water and carbon monoxide with $\text{MnO}(001)$ thin films on $\text{Au}(111)$

Jade Barreto, Niklas Nilus, Heloise Tissot, Shamil Shaikhutdinov, Hans Joachim Freund and Fernando Stavale*

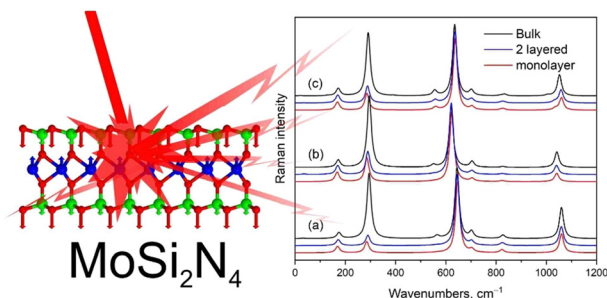
29816



Effect of salt addition on a triblock copolymer-zwitterionic surfactant assembly: insight from excited-state proton transfer

Tapas Pal and Kalyanasis Sahu*

29831



Phonon dynamics in MoSi_2N_4 : insights from DFT calculations

A. S. Oreshonkov,* E. V. Sukhanova and Z. I. Popov



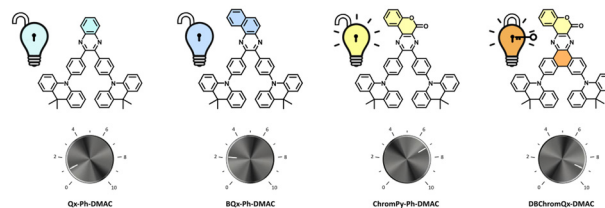
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29842

Intramolecular locking and coumarin insertion: a stepwise approach for TADF design

S. Paredis, T. Cardeynaels, S. Brebels, J. Deckers, S. Kuila, A. Lathouwers, M. Van Landeghem, K. Vandewal, A. Danos,* A. P. Monkman, B. Champagne and W. Maes*

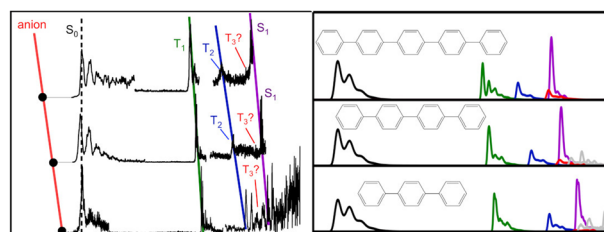
Stepwise TADF switch



29850

Electron affinities and lowest triplet and singlet state properties of *para*-oligophenylenes ($n = 3-5$): theory and experiment

Timo Schulz, Paul Konieczny, Dennis R. Dombrowski, Simon Metz, Christel M. Marian* and Rainer Weinkauf*



29867

From bonds to interactions: comprehensive molecular characterization via polarizable bond-dipole approach

Jia-Yi Zhu, Qi Liu, Xiao-Nan Jiang, Xiao-Han Zheng, Lei Wang, Qiang Hao* and Chang-Sheng Wang*

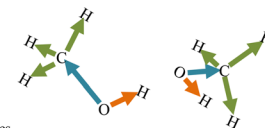
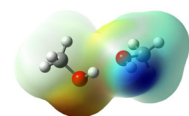
$$U = U_{bond} + U_{angle} + U_{ba} + U_{dih} + U_{ele}^{perm} + U_{ele}^{pol} + U_{vdW} + U_{orb}$$

$$U_{ele}^{perm} = \sum \frac{\mu_i \mu_j}{R_{ij}^3} f(\theta, \theta', \zeta)$$

$$U_{ele}^{pol} = \sum \frac{\mu_i \delta \mu_j + \delta \mu_i \mu_j + \delta \mu_i \delta \mu_j}{R_{ij}^3} f(\theta, \theta', \zeta)$$

$$U_{ele} = U_{ele}^{perm} + U_{ele}^{pol} = \sum \frac{(\mu_i + \delta \mu_i)(\mu_j + \delta \mu_j)}{R_{ij}^3} f(\theta, \theta', \zeta)$$

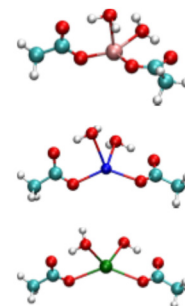
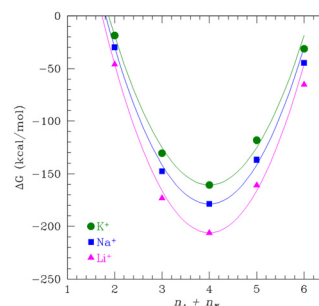
R_{ij} is the distance between the center of two bond dipoles



29881

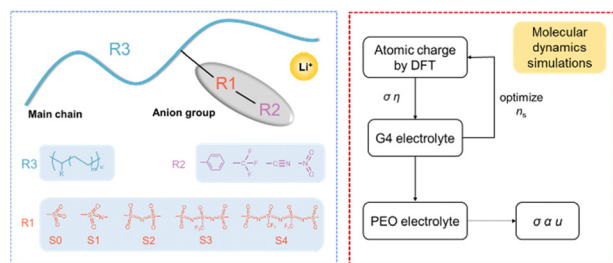
Binding of carboxylate and water to monovalent cations

Mark J Stevens* and Susan L. B. Rempe*



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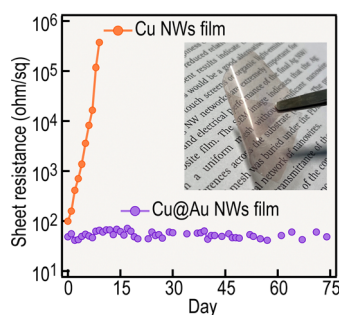
29894



Toward a molecular understanding of the conductivity of lithium-ion conducting polyanion polymer electrolytes by molecular dynamics simulation

Haiming Hua, Boyang Huang, Xueying Yang, Jun Cheng,* Peng Zhang* and Jinbao Zhao*

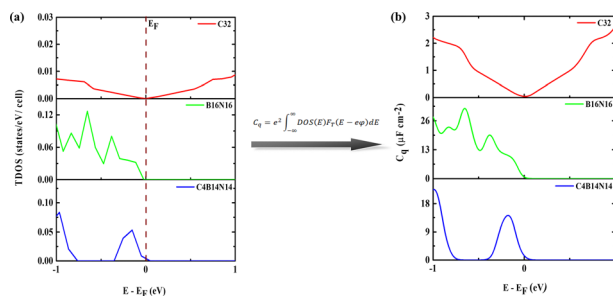
29905



Direct coating of gold nanolayers to enhance the oxidation resistance of copper nanowire flexible transparent conductive films

Quan Xiong, Xingzhong Zhu,* Juan Xu, Weiqiang Yuan, Jizhe Zhang and Caixia Kan*

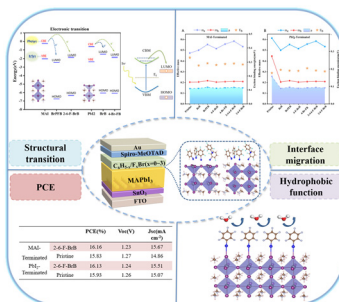
29914



Density functional theory studies on graphene/h-boron nitride hybrid nanosheets for supercapacitor electrode applications

Naveena Paramasivam, Anandan Sambandam and Baskaran Natesan*

29924



Exploring the effect of C₆H_{5-x}/F_xBr (x = 0–3) passivating agent on surface properties at different termination ends: first principles

Changcheng Chen,* Yan Cai, Yirui Zhang, Ziyi Zhang, Songya Wang, Shuli Gao, Wen Chen, Shuangna Guo, Elyas Abduryim, Chao Dong, Xiaoning Guan,* Ying Liu and Pengfei Lu*

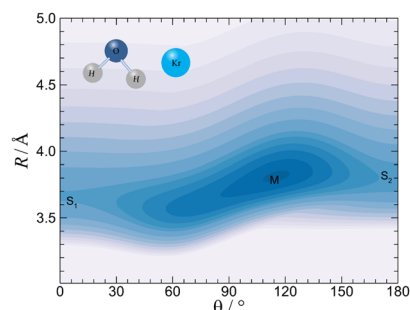


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29940

An intramolecular vibrationally excited intermolecular potential energy surface and predicted 2OH overtone spectroscopy of H₂O–Kr

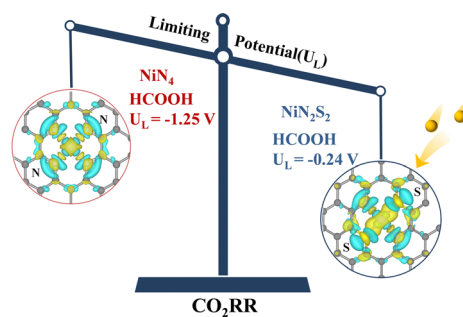
Xiao-Long Zhang, Shu-Bin Yang, Dan Hou* and Hui Li*



29951

N,S coordination in Ni single-atom catalyst promoting CO₂RR towards HCOOH

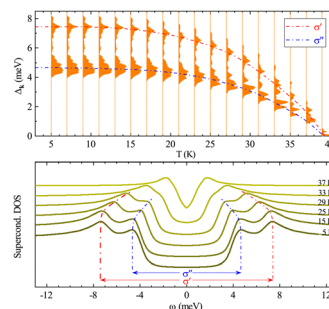
Zengxuan Chen, Shoufu Cao, Jiao Li, Chunyu Yang, Shuxian Wei, Siyuan Liu, Zhaojie Wang* and Xiaoqing Lu*



29960

Two-gap-like anisotropic superconductivity in a bulk boron kagome lattice

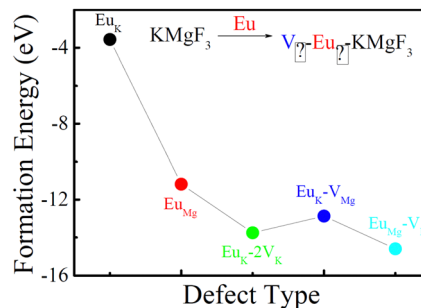
Shuming Zeng, Geng Li* and Yinchang Zhao*



29968

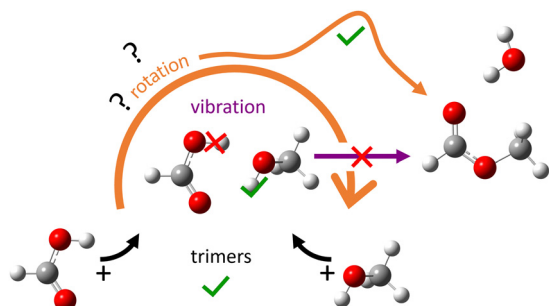
Probing site-selective doping and charge compensating defects in KMgF₃: insights from a hybrid DFT study

Pampa Modak, Brindaban Modak* and A. Arya*



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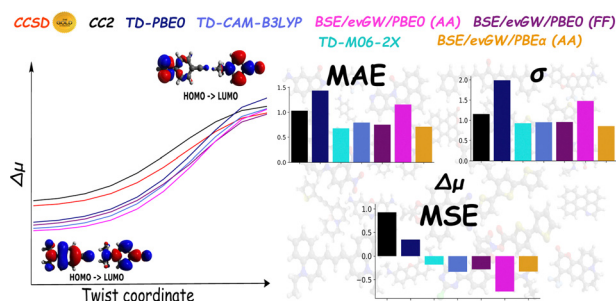
29982



Formic acid–methanol complexation vs. esterification: elusive pre-reactive species identified by vibrational spectroscopy

Sophie M. Schweer, Maxim Gawrilow, Arman Nejad and Martin A. Suhm*

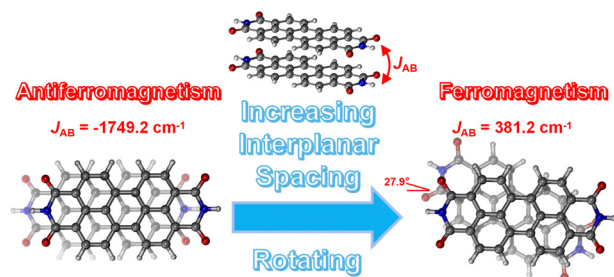
29993



Excess and excited-state dipole moments of real-life dyes: a comparison between wave-function, BSE/GW, and TD-DFT values

Iryna Knysh, Jose D. J. Villalobos-Castro, Ivan Duchemin, Xavier Blase* and Denis Jacquemin*

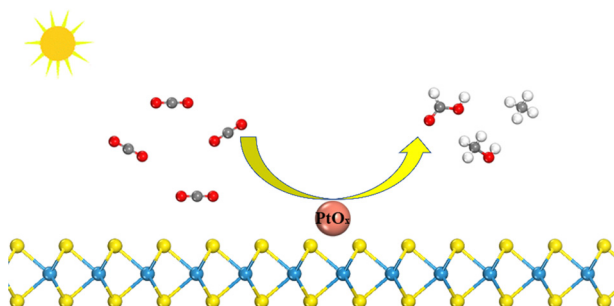
30005



A theoretical study on π -stacking and ferromagnetism of the perylene diimide radical anion dimer and tetramer

Hanlin Gan, Qinglin Jiang and Yuguang Ma*

30014



WS₂ supported PtO_x clusters for efficient photocatalytic CO₂ reduction: a DFT study

Linghao Zhu, Cong Qin, Yan Wang* and Jianliang Cao*

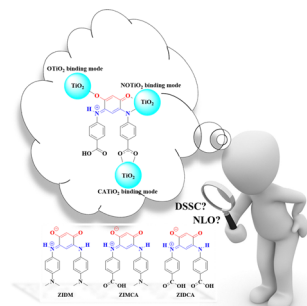


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30023

A promising small-sized near-infrared absorbing zwitterionic dye for DSSC and NLO applications: DFT and TD-DFT approaches

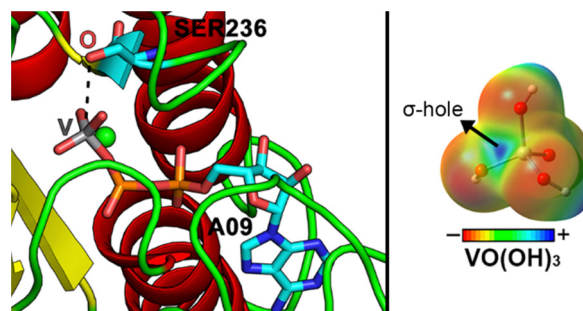
Suryapratap J. Sharma and Nagaiyan Sekar*



30040

Biological noncovalent N/O...V interactions: insights from theory and protein data bank analyses

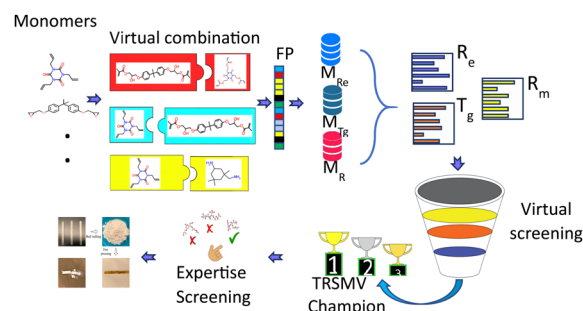
Sergi Burguera, Antonio Frontera and Antonio Bauzá*



30049

Overcoming the barrier: designing novel thermally robust shape memory vitrimers by establishing a new machine learning framework

Cheng Yan,* Xiaming Feng, John Konlan, Patrick Mensah and Guoqiang Li



30066

Emerging quasi-one-dimensional material NbS₄ with high carrier mobility and good visible-light adsorption performance for nanoscale applications

Ru Yu, Feng Xiao, Wen Lei, Wei Wang, Yiping Ma, Xujia Gong and Xing Ming*

