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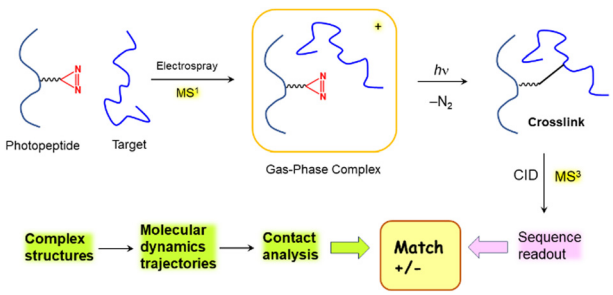

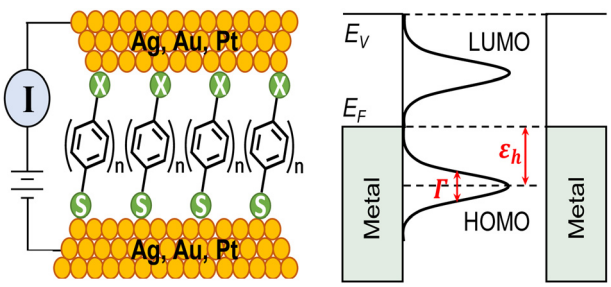

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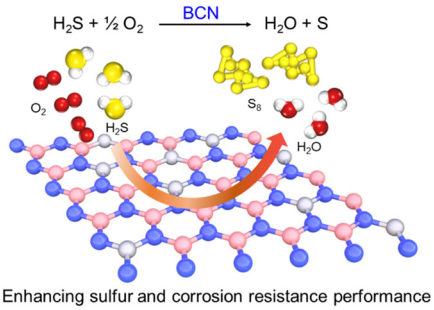

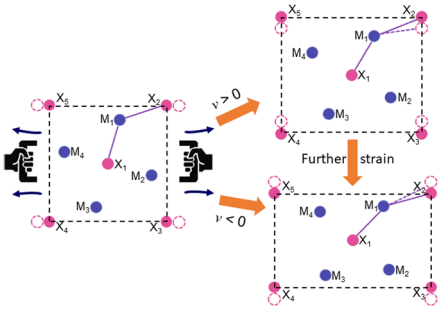

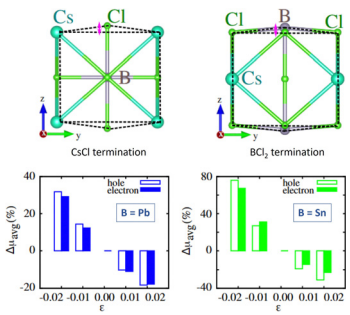

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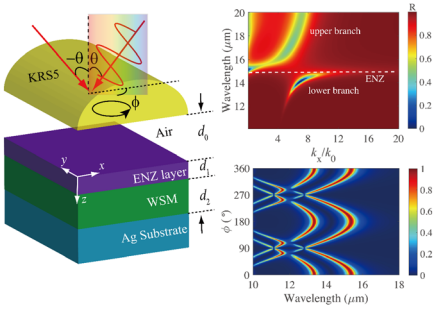

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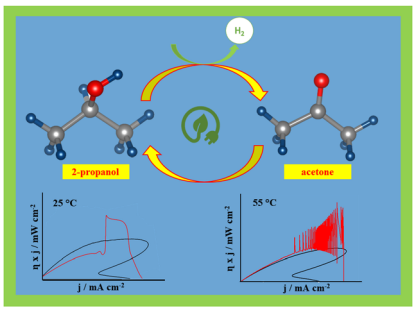

The oscillatory electro-oxidation of 2-propanol on platinum: the effect of temperature and addition of methanol

Gianluca Ragassi, André H. B. Dourado and Hamilton Varela*

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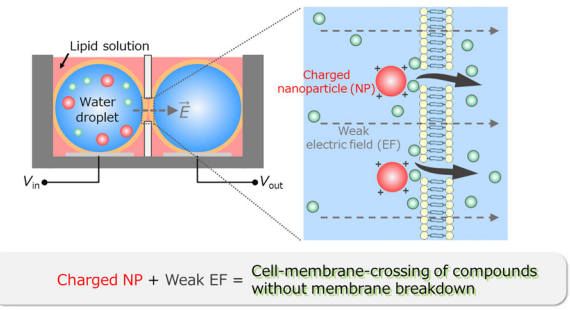

Enhancement of cell membrane permeability by using charged nanoparticles and a weak external electric field

Hideya Nakamura,* Takumi Okamura, Masaya Tajima, Ryuji Kawano, Misa Yamaji, Shuji Ohsaki and Satoru Watano

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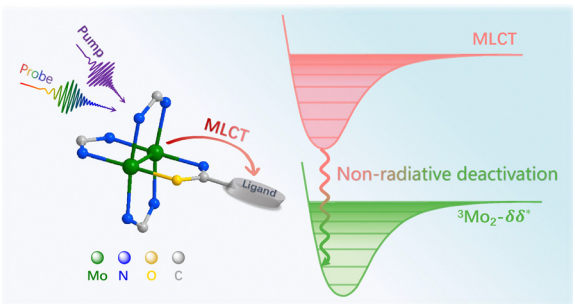

Influence of ligand variation on the deactivation process of metal-to-ligand charge transfer excited states in quadruply bonded dimolybdenum complexes

Yuqing Shi, Juanjuan Li, Can Cui, Guanzhi Wu* and Tao Cheng*

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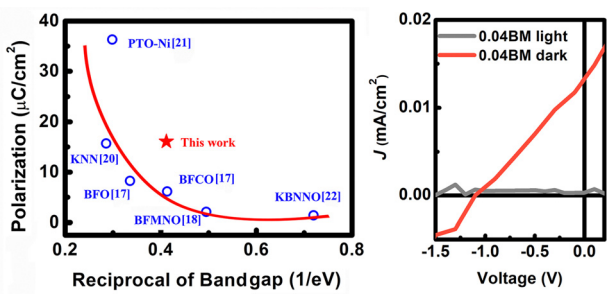

Simultaneous improvement of polarization and bandgap by finite solid solution engineering

Fei Guo,* Rui Liu, Siyuan Guo, Yaping Liu, Lei Gao and Shifeng Zhao*

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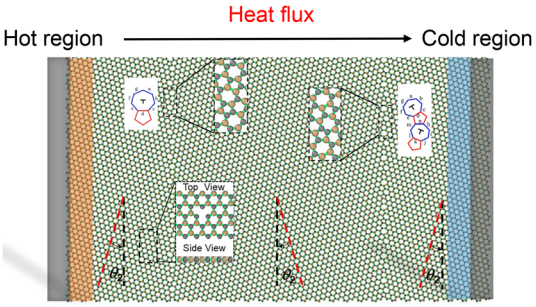
Impacts of defects on the mechanical and thermal properties of SiC and GeC monolayers

Kai Ren, Lei Huang, Huabing Shu, Guoqiang Zhang, Weihua Mu,* Huanping Zhang, Huasong Qin* and Gang Zhang*



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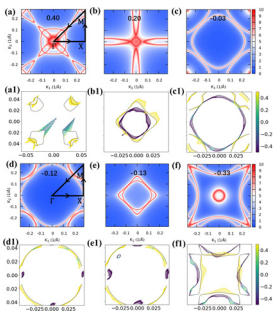
Ab initio study of the topological itinerant transport properties observed between excited edge states in a 2D compound with the $Mn_{15}B_{16}Ni$ composition

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



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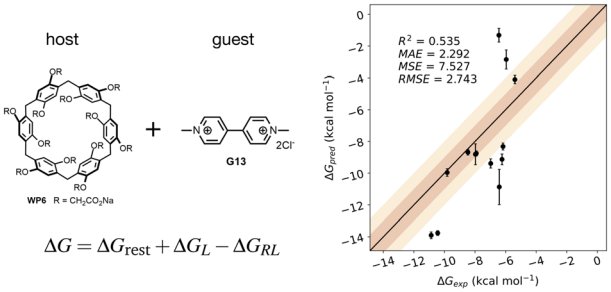
Expanded ensemble predictions of absolute binding free energies in the SAMPL9 host–guest challenge

Matthew F. D. Hurley, Robert M. Raddi, Jason G. Pattis and Vincent A. Voelz*



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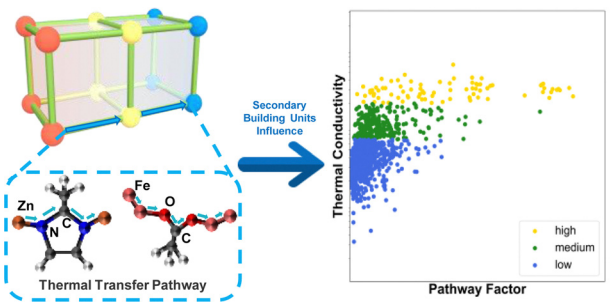
Understanding the influence of secondary building units on the thermal conductivity of metal–organic frameworks *via* high-throughput computational screening

Yuanchuang Lin, Ruihuan Cheng, Tiangui Liang, Weixiong Wu, Song Li* and Wei Li*



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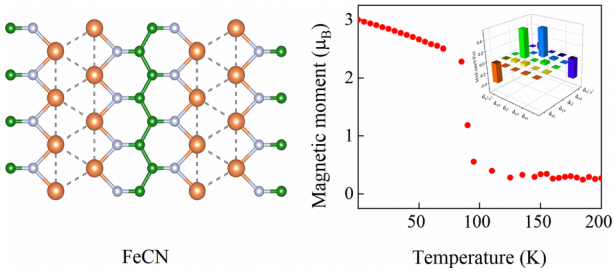

2D antiferromagnetic semiconducting FeCN with interesting properties

Zhicui Wang, Huan Lou, Xu Yan, Yong Liu* and Guochun Yang*

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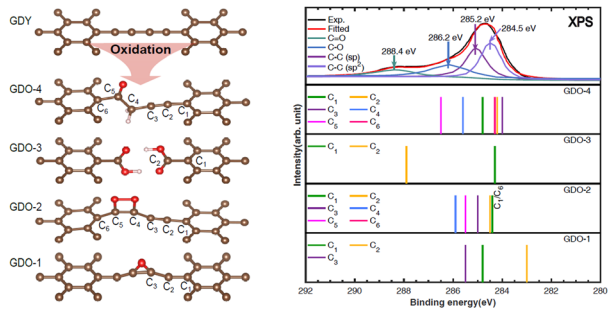

First-principles simulation of X-ray spectra of graphdiyne and graphdiyne oxides at the carbon K-edge

Jing Ming, Jun-Rong Zhang, Xiu-Neng Song, Xin Li, Weijie Hua* and Yong Ma*

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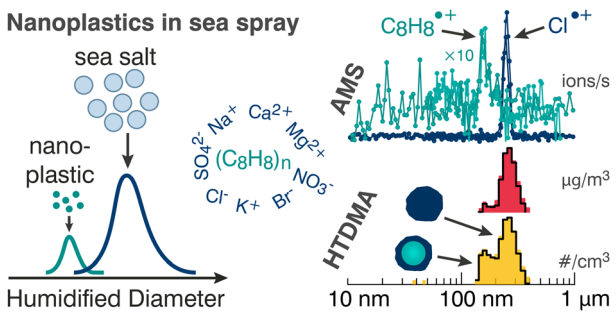

Morphology and hygroscopicity of nanoplastics in sea spray

Sarah Suda Petters,* Eva Rosendal Kjærgaard, Freja Hasager, Andreas Massling, Marianne Glasius and Merete Bilde*

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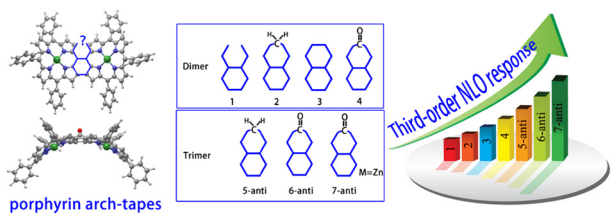

Theoretical study on porphyrin arch-tapes of carbonyl-inserted seven-membered rings with high nonlinear optical properties

Jin-Ting Ye,* Li-Hui Wang and Jia-Qi Yu*

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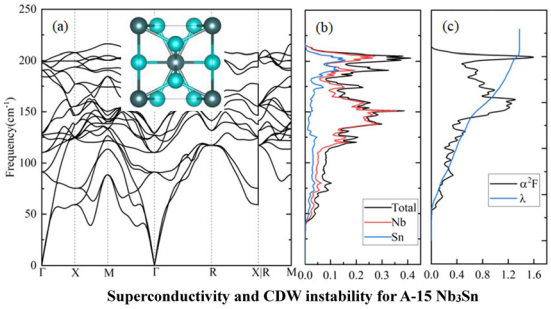

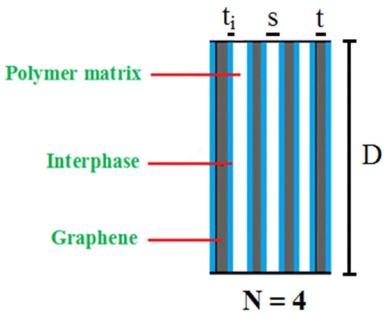

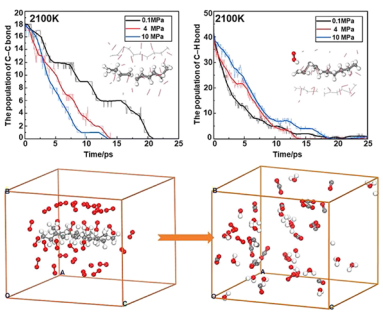

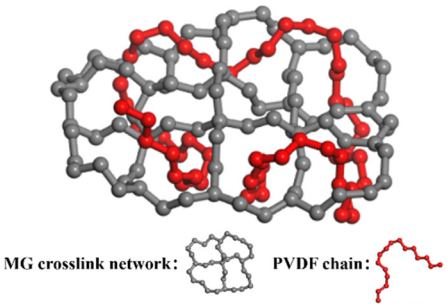

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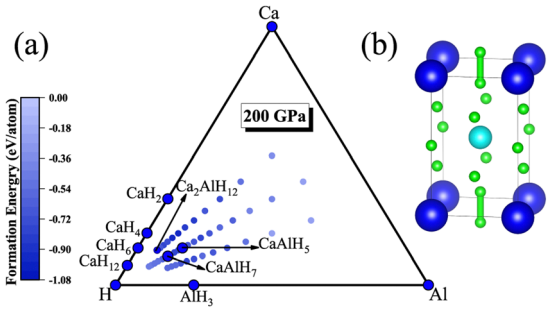
Phase diagrams and superconductivity of ternary Ca–Al–H compounds under high pressure

Ming Xu, Defang Duan, Mingyang Du, Wendi Zhao, Decheng An, Hao Song* and Tian Cui*



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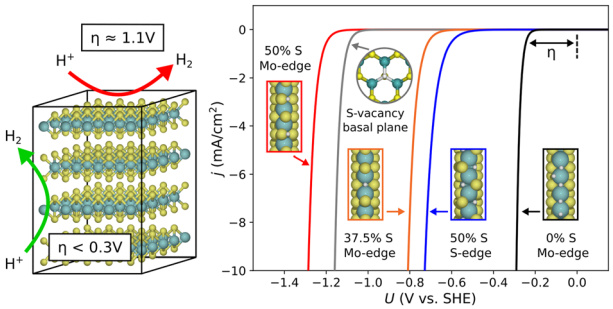
Sulfur-deficient edges as active sites for hydrogen evolution on MoS_2

Sander Ø. Hanslin, Hannes Jónsson and Jaakko Akola*



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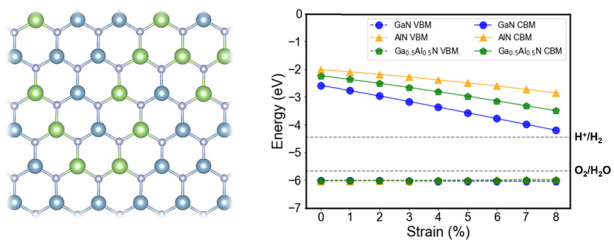
Two-dimensional III-nitride alloys: electronic and chemical properties of monolayer $Ga_{(1-x)}Al_xN$

Yiqing Chen, Ying Zhao, Pengfei Ou* and Jun Song*



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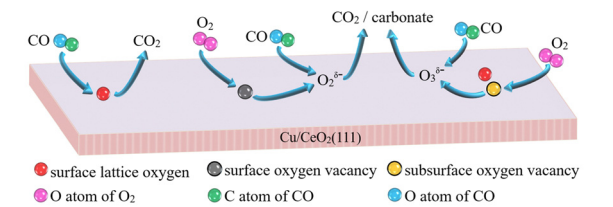
Formation of superoxide and ozone-like species on Cu doped CeO_2(111) and their CO oxidation reactivity: a DFT study

Hao Wang, Yuan Li, Jiao Han, Caishun Zhang, Honghao Wang, Daosheng Liu, Xiaoning Hou, Lei Zhang* and Zhixian Gao*



CO oxidation on $O_2^{\delta-}$ and $O_3^{\delta-}$ was more energetically favorable than directly on lattice oxygen.

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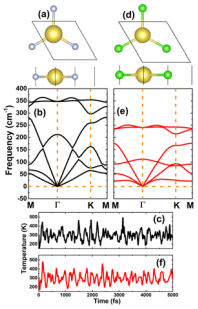

Doping-mediated electronic and magnetic properties of graphene-like ionic NaX (X = F and Cl) monolayers

Bich Ngoc Nguyen Thi, Chu Viet Ha, Nghiem Thi Ha Lien, J. Guerrero-Sanchez and D. M. Hoat*

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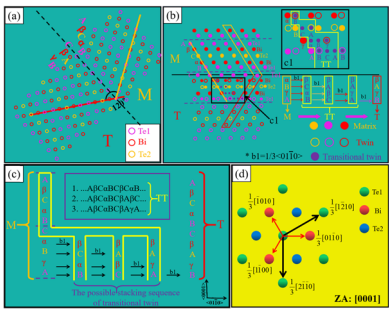
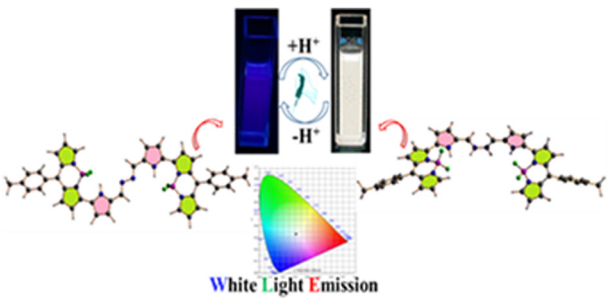


Transitional structure of {0001} twin in a deformed p-type $(Bi,Sb)_2Te_3$ alloy: a direct experimental basis for understanding the twinning mechanism

Jie Ren, Wenbin Guo, Fuzhou Han,* Qichen Wang, Yi Cao, Songbin Li, Geping Li,* Muhammad Ali, Jianan Hu, Fusen Yuan and Yingdong Zhang

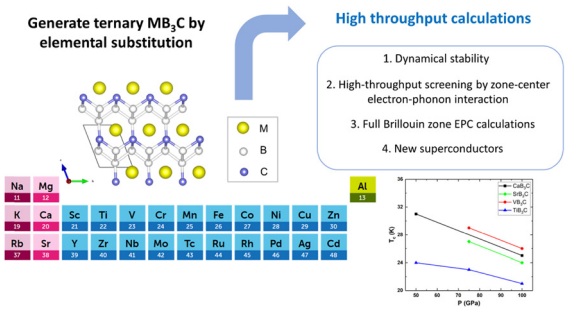
32584



A white light emitting single halochromic hydrazine bridged bis(3-pyrrolyl BODIPY) fluorophore

Kanhu Charan Behera and Mangalampalli Ravikanth*

32594



Prediction of superconductivity in metallic boron–carbon compounds from 0 to 100 GPa by high-throughput screening

Feng Zheng, Yang Sun,* Renhai Wang, Yimei Fang, Feng Zhang, Shunqing Wu,* Qiubao Lin,* Cai-Zhuang Wang, Vladimir Antropov and Kai-Ming Ho

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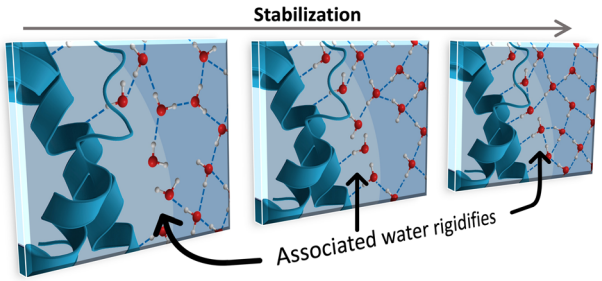
32602

Osmolyte induced protein stabilization: modulation of associated water dynamics might be a key factor

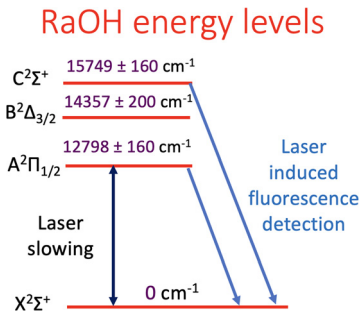
Kuldeep Singh Negi, Nilimesh Das, Tanmoy Khan and Pratik Sen*



32613

Relativistic coupled-cluster calculations of RaOH pertinent to spectroscopic detection and laser cooling

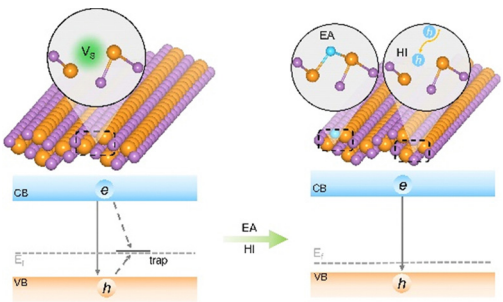
Chaoqun Zhang, Phelan Yu, Chandler J. Conn, Nicholas R. Hutzler* and Lan Cheng*



32622

Blocking recombination centers by controlling the charge density of a sulfur vacancy in antimony trisulfide

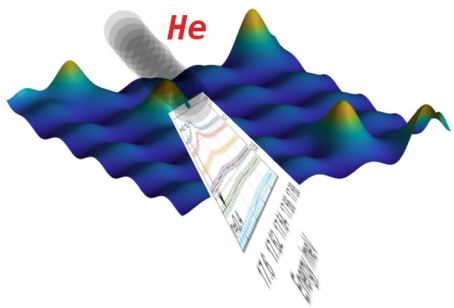
Xiao Han, Qi Zhao, Xiaodan Yan, Ting Meng* and Jinlu He*



32632

Blue shifts in helium-surface bound-state resonances and quantum effects in cosine-law scattering

Luke Staszewski and Nadav Avidor*



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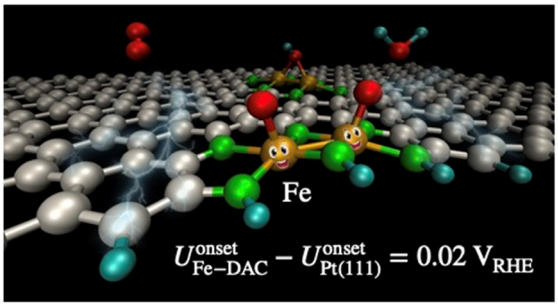
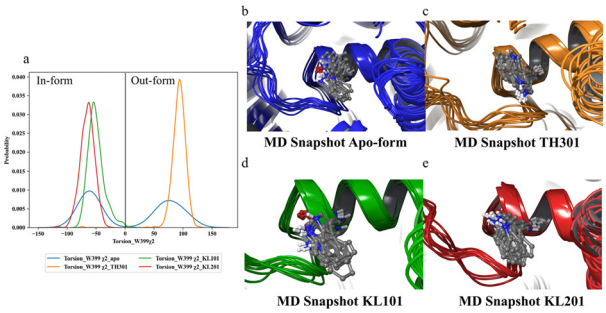
32637



Graphene-edge-supported iron dual-atom for oxygen reduction electrocatalysts

Joel F. Sumbowo, Farhan A. Ihsan, Fadjar Fathurrahman, Nadya Amalia, Fiki T. Akbar, Hadi T. Yudistira, Nadhratun N. Mobarak, Hermawan K. Dipojono, Sasfan A. Wella* and Adhitya G. Saputro*

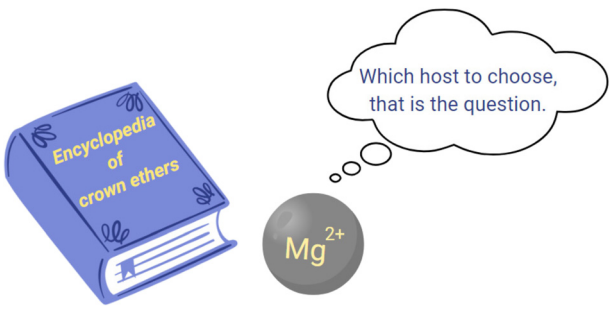
32648



Elucidating TH301's influence on the torsion angle of CRY1 W399 using replica exchange with solute tempering (REST) molecular dynamics (MD) simulations

Yeongrae Cho, Kexin Li, Jin Hyup Lee, Seung Pil Pack and Art E. Cho*

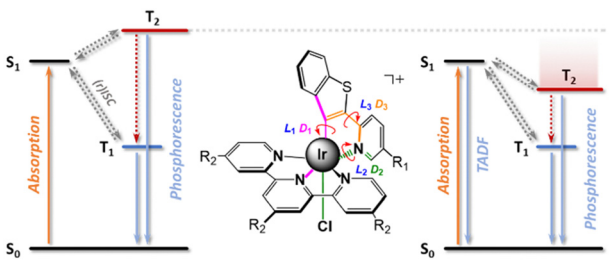
32656



Density functional theory study of crown ether–magnesium complexes: from a solvated ion to an ion trap

Katarina Ćeranić, Branislav Milovanović and Milena Petković*

32666



Computational study of the photophysical properties and electronic structure of iridium(III) photosensitizer complexes with electron-withdrawing groups

Yunlong Shang, Zhoujie Zhang, Mengping Huang, Na Shu, Hanyu Luo, Qiyan Cao, Bingbing Fan, Yu Han, Min Fang,* Yong Wu* and Jiawei Xu*

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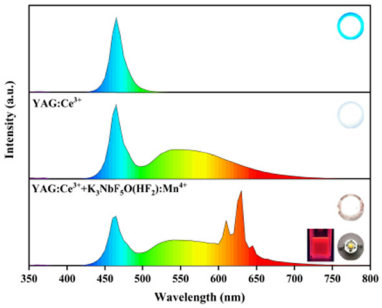

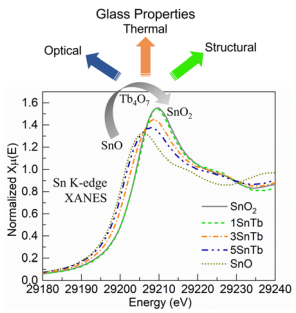

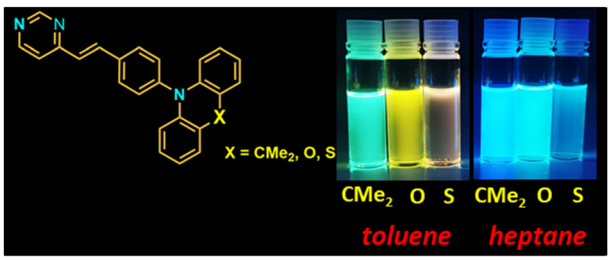

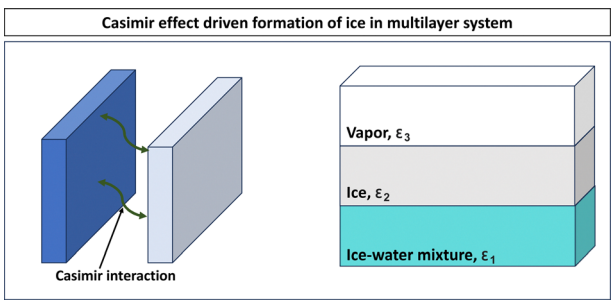

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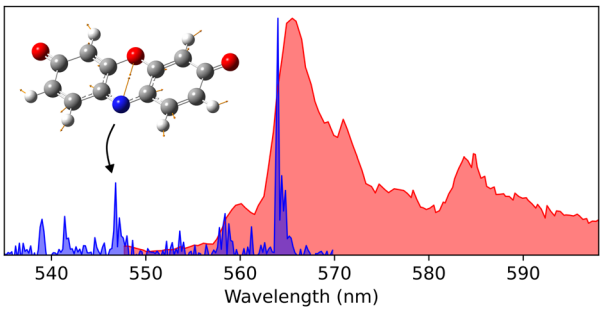
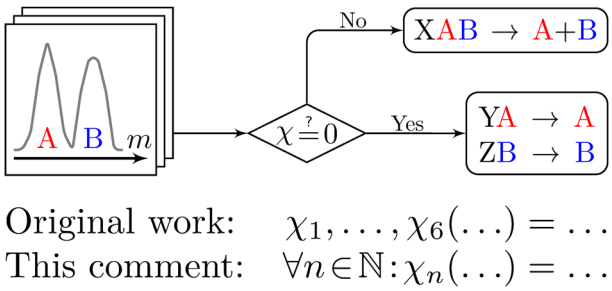


Cryogenic fluorescence spectroscopy of oxazine ions isolated *in vacuo*

Christina Kjær,* Emil Vogt, Jeppe Langeland, Nanna Falk Christensen, Thomas Toft Lindkvist, Henrik G. Kjaergaard and Steen Brøndsted Nielsen

COMMENT



Comment on "Cumulant mapping as the basis of multi-dimensional spectrometry" by Leszek J. Frasinski, *Phys. Chem. Chem. Phys.*, 2022, 24, 20776–20787

Åke Andersson

CORRECTIONS

Correction: Cumulant mapping as the basis of multi-dimensional spectrometry

Leszek J. Frasinski

Correction: Understanding the charge transfer dynamics of the Cu_2WS_4–CNT–FeOOH ternary composite for photo-electrochemical studies

Preeti Dagar, Nandan Ghorai, Manisha Bungla, Hirendra N. Ghosh* and Ashok K. Ganguli*

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CORRECTIONS

32728

Correction: UV and VUV-induced fragmentation of tin-oxo cage ions

Jarich Haitjema, Lianjia Wu, Alexandre Giuliani, Laurent Nahon, Sonia Castellanos and Albert M. Brouwer*

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