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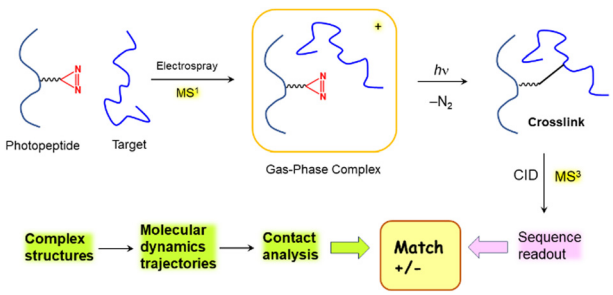
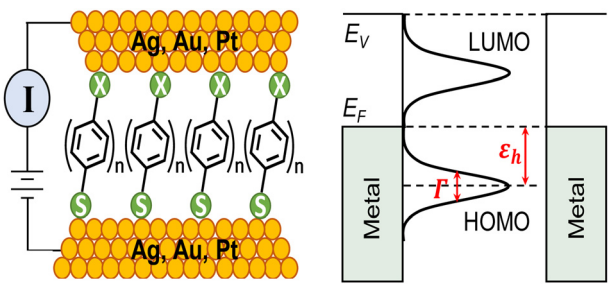
Inside cover
See Hamilton Varela *et al.*, pp. 32345–32355. Image reproduced by permission of Hamilton Varela from *Phys. Chem. Chem. Phys.*, 2023, **25**, 32345.

PERSPECTIVES





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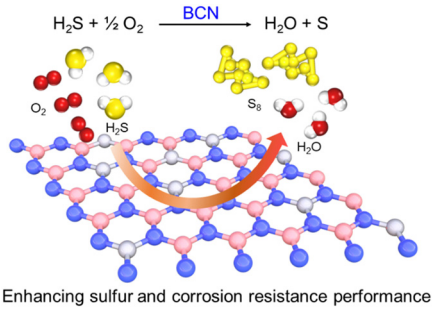

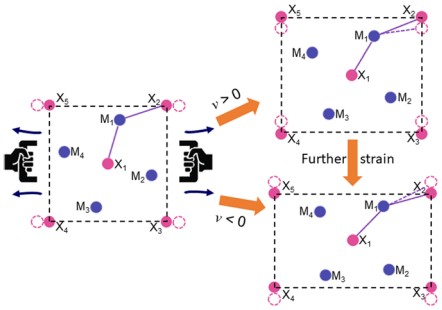

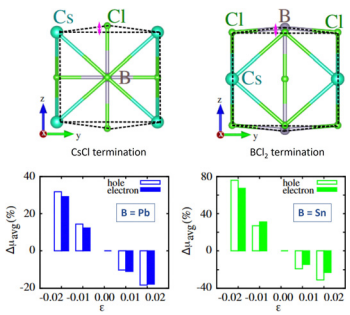

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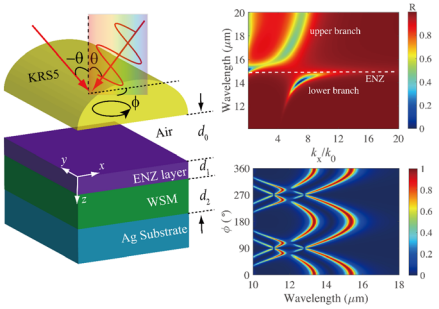

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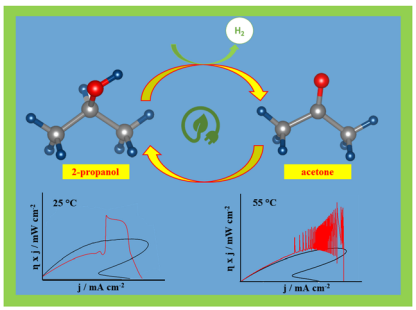

The oscillatory electro-oxidation of 2-propanol on platinum: the effect of temperature and addition of methanol

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

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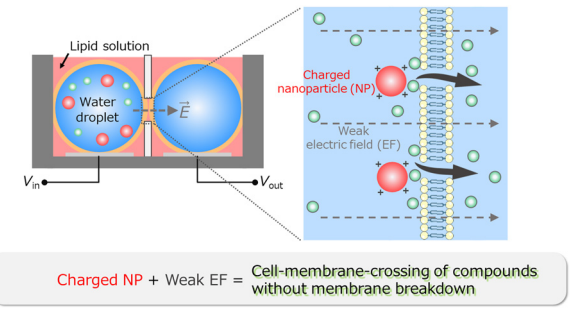

Enhancement of cell membrane permeability by using charged nanoparticles and a weak external electric field

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

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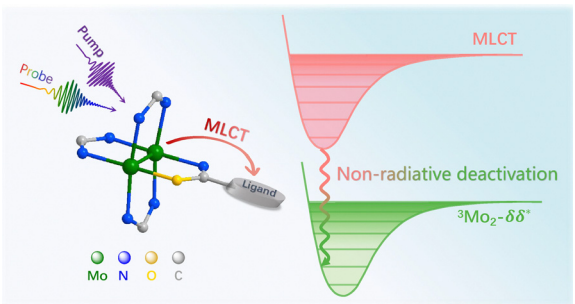

Influence of ligand variation on the deactivation process of metal-to-ligand charge transfer excited states in quadruply bonded dimolybdenum complexes

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

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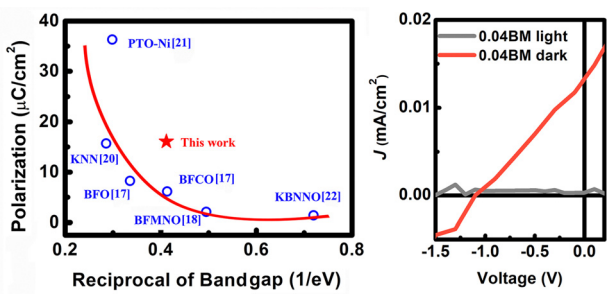

Simultaneous improvement of polarization and bandgap by finite solid solution engineering

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

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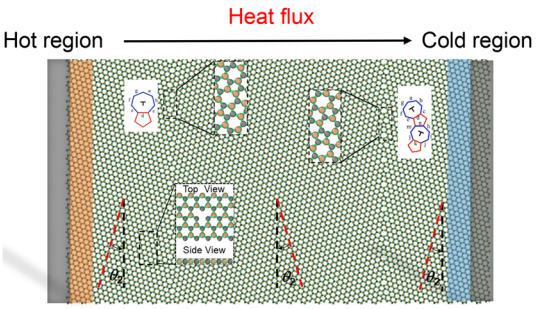
Impacts of defects on the mechanical and thermal properties of SiC and GeC monolayers

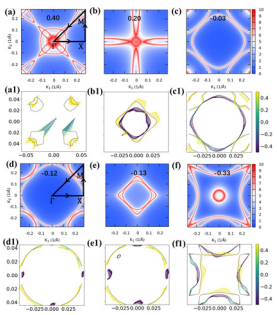
Kai Ren, Lei Huang, Huabing Shu, Guoqiang Zhang, Weihua Mu,* Huanping Zhang, Huasong Qin* and Gang Zhang*



32387

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

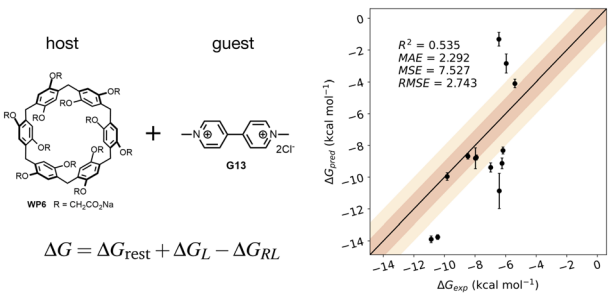
Wuyue Xu, Zhengxin Yan,* Kezhao Xiong, Juntao Kong, Wei Song, Dongxin Li, Qian Cheng, Zehua Zhao and Xingkun Liang



32393

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

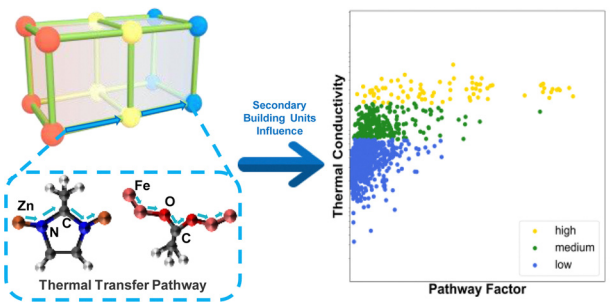
Matthew F. D. Hurley, Robert M. Raddi, Jason G. Pattis and Vincent A. Voelz*



32407

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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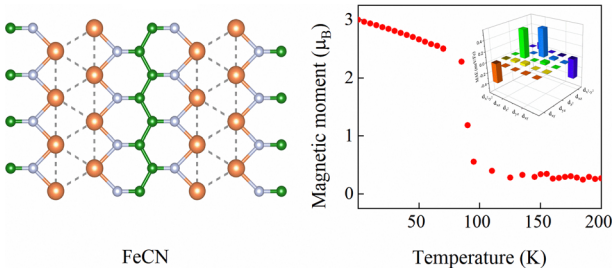

2D antiferromagnetic semiconducting FeCN with interesting properties

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

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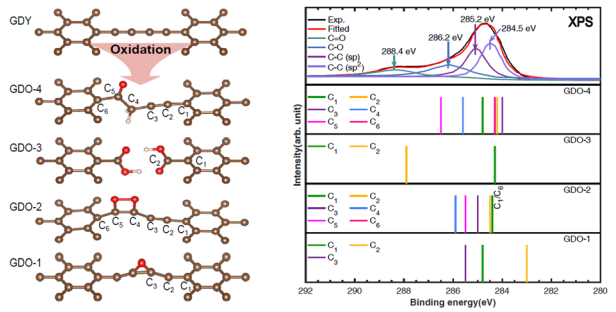

First-principles simulation of X-ray spectra of graphdiyne and graphdiyne oxides at the carbon K-edge

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

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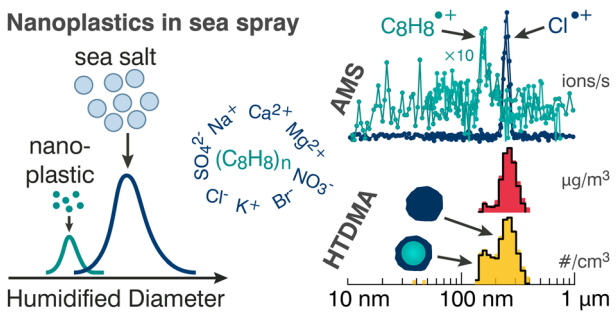

Morphology and hygroscopicity of nanoplastics in sea spray

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

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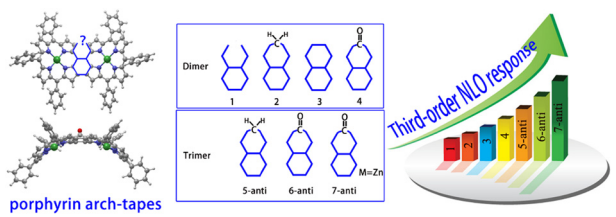

Theoretical study on porphyrin arch-tapes of carbonyl-inserted seven-membered rings with high nonlinear optical properties

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

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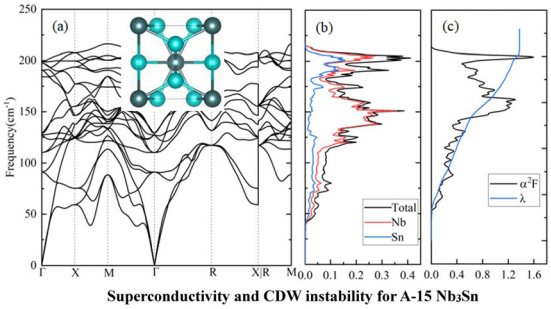
Coexistence of superconductivity and charge density wave instability in A15-Nb_3Sn

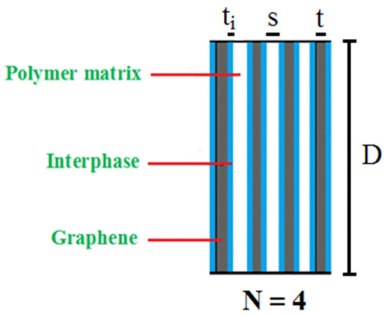
Li-Na Wu, Si-Tong Yang, Jin-Ke Shen, Jian-Sheng Zhang and Fei-Hu Liu*



32460

Percolation onset and conductivity of nanocomposites assuming an incomplete dispersion of graphene nanosheets in a polymer matrix

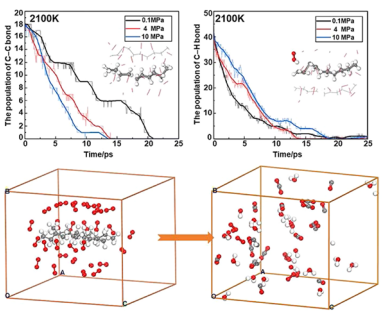
Yasser Zare,* Muhammad Tajammal Munir and Kyong Yop Rhee*



32471

Oxidation kinetic mechanism of *n*-decane under high temperature and pressure: a first-principles molecular dynamics study

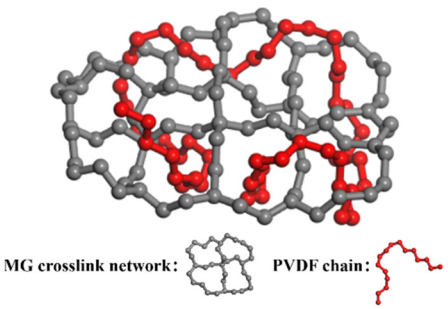
Teng Zhang, Wenbo Xia, Wei Fan,* Lang Chen* and Jun Chen*



32482

Crosslinking modification and hydrogen bonding synergy to achieve high breakdown strength and energy density of PMMA-*co*-GMA/PVDF dielectric composite films

Shuo Zheng, Xuanchen Zhao, Junhao Xie and Shulin Sun*



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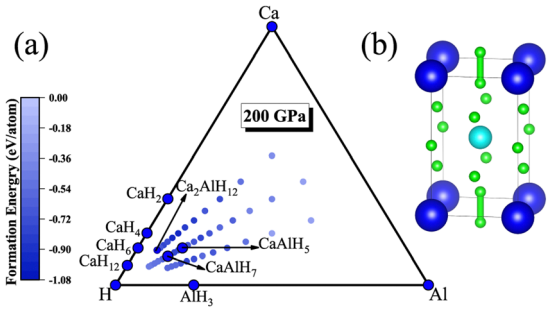
Phase diagrams and superconductivity of ternary Ca–Al–H compounds under high pressure

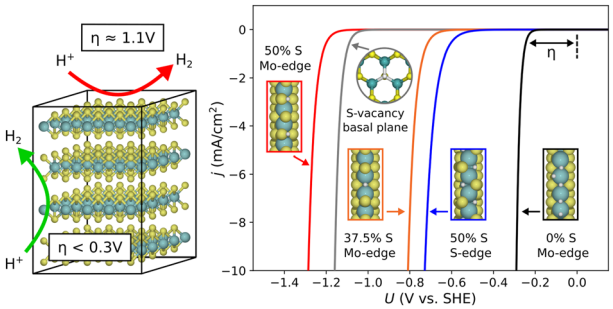
Ming Xu, Defang Duan, Mingyang Du, Wendi Zhao, Decheng An, Hao Song* and Tian Cui*



32541

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

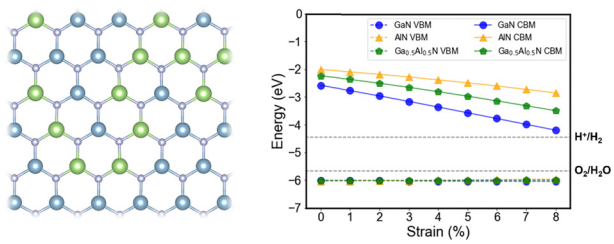
Sander Ø. Hanslin, Hannes Jónsson and Jaakko Akola*



32549

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

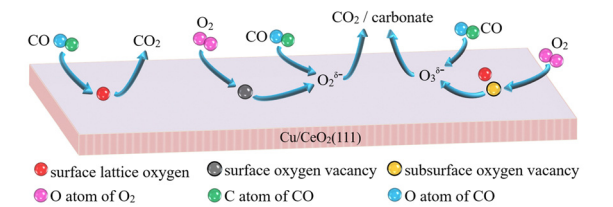
Yiqing Chen, Ying Zhao, Pengfei Ou* and Jun Song*



32557

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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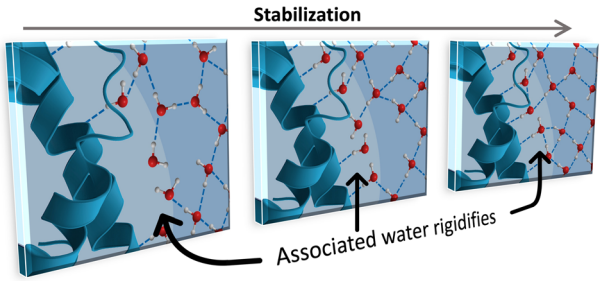

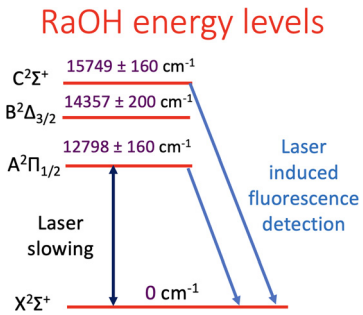

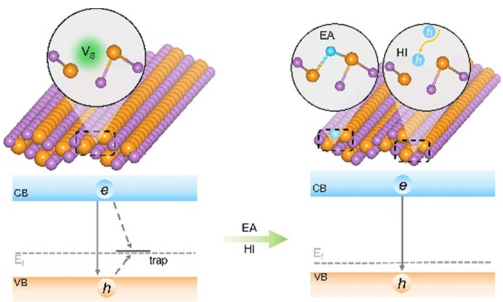

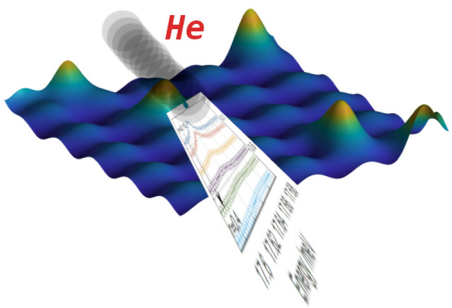

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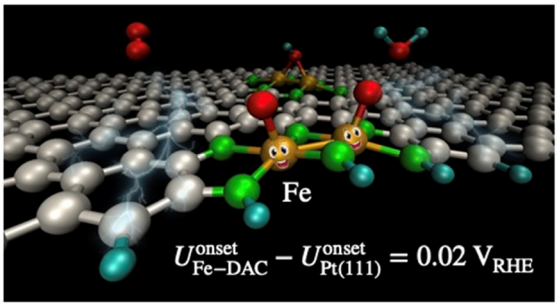
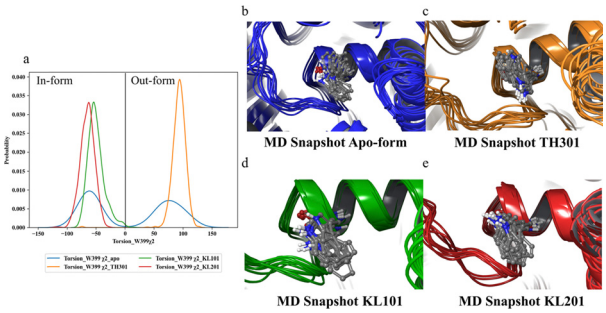


Graphene-edge-supported iron dual-atom for oxygen reduction electrocatalysts

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*

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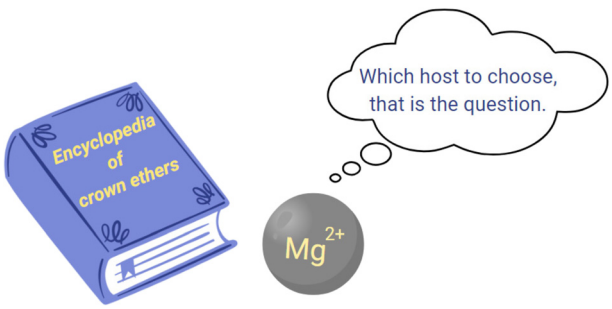

Density functional theory study of crown ether–magnesium complexes: from a solvated ion to an ion trap

Katarina Ćeranić, Branislav Milovanović and Milena Petković*

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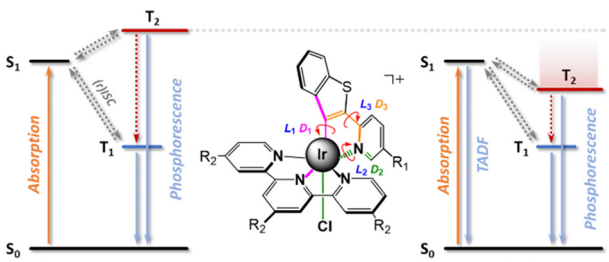

Computational study of the photophysical properties and electronic structure of iridium(III) photosensitizer complexes with electron-withdrawing groups

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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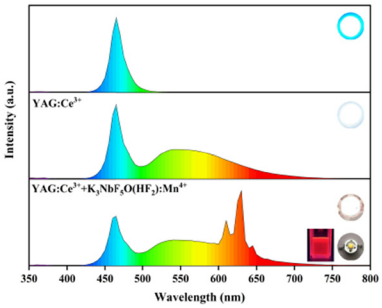
A highly efficient Mn^{4+} activated Nb-based oxyfluoride red fluorescent material with excellent water stability: preparation and performance analysis

Ruiyang Wang, Hui Zhou, Wenjie Shi, Xiaofang Yu,* Xiaoyun Mi,* Xiuling Liu and Yanping Wang



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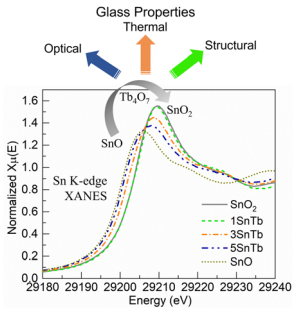
XANES analysis of phosphate glasses melted with Tb_4O_7 and SnO: evaluating the impact of valence states on structural, thermal, and luminescent properties

José A. Jiménez,* Dugan Hayes, Cali Antolini and Benjamin J. Reinhart



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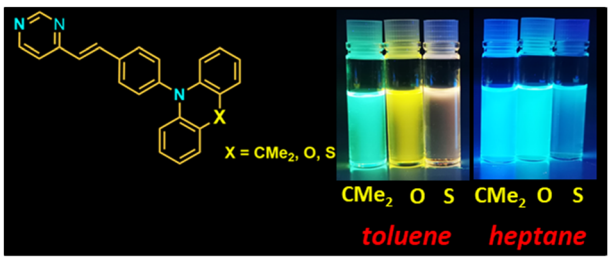
Styrylpyrimidine chromophores with bulky electron-donating substituents: experimental and theoretical investigation

Maxime Hodée, Julien Massue,* Sylvain Achelle,* Arnaud Fihey,* Denis Tondelier, Gilles Ulrich, Françoise Robin-le Guen and Claudine Katan



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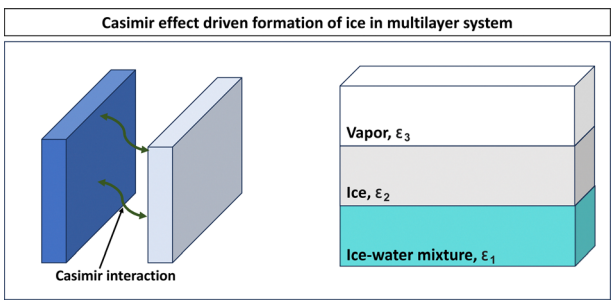
van der Waals induced ice growth on partially melted ice nuclei in mist and fog

M. Boström,* Y. Li,* I. Brevik, C. Persson, S. Carretero-Palacios and O. I. Malyi*



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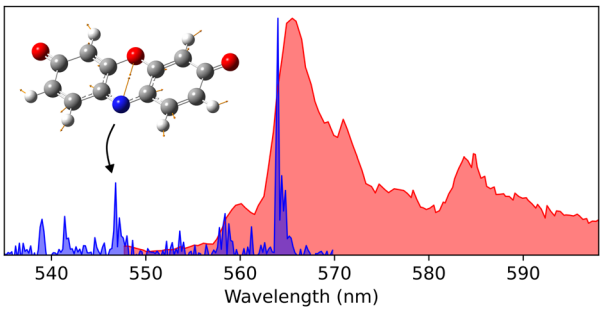
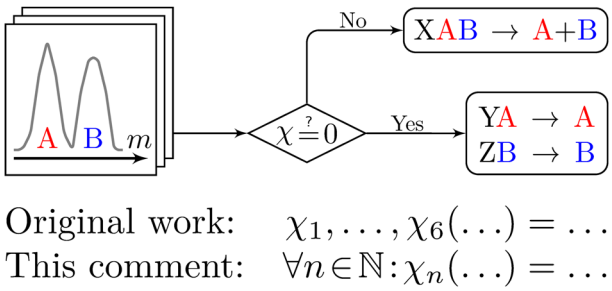


Cryogenic fluorescence spectroscopy of oxazine ions isolated *in vacuo*

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

COMMENT

32723



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

32726

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

Leszek J. Frasinski

32727

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*

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*