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Cover

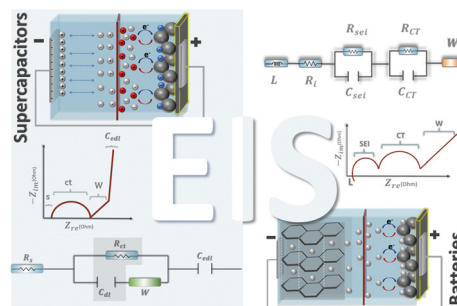
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TUTORIAL REVIEW

25748

Electrochemical impedance spectroscopy: from breakthroughs to functional utility in supercapacitors and batteries – a comprehensive assessment

Larissa A. Santa-Cruz, Fabiele C. Tavares, Lara F. Loguercio, Calink I. L. dos Santos, Rhauane A. Galvão, Otávio A. L. Alves, Maria Z. Oliveira, Roberto M. Torresi and Giovanna Machado*

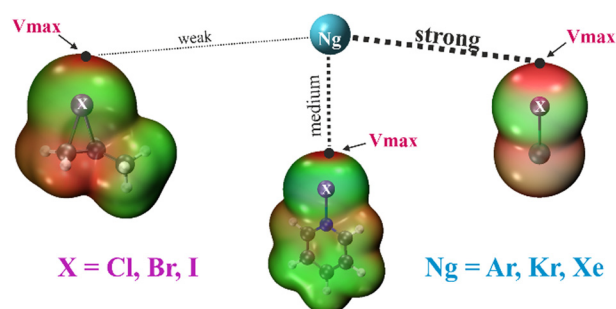


COMMUNICATIONS

25762

From weak to strong interactions between halogen and noble gas atoms in halonium complexes

Wiktor Zierkiewicz*, Steve Scheiner and Mariusz Michalczyk*



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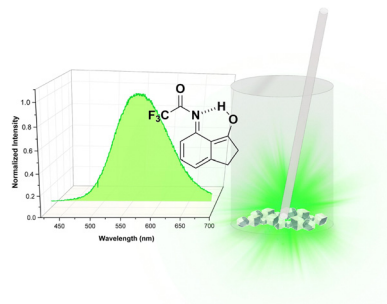


COMMUNICATIONS

25767

The indanone N–H type excited-state intra-molecular proton transfer (ESIPT); the observation of a mechanically induced ESIPT reaction

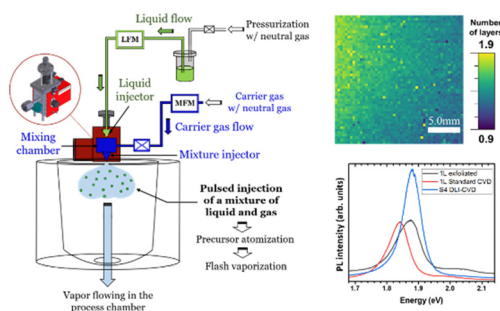
Jhu-Jyun You, Yan-Ding Lin, Chao-Hsien Hsu, Jiun-Wei Hu, Ying-Yi Tsai, Hao-Ting Qu, Kew-Yu Chen* and Pi-Tai Chou*



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Direct liquid injection pulsed-pressure MOCVD of large area MoS₂ on Si/SiO₂

Vincent Astié,* Felipe Wasem Klein, Houssin Makhlouf, Matthieu Paillet, Jean-Roch Huntzinger, Jean-Louis Sauvajol, Ahmed-Azmi Zahab, Sandrine Juillaguet, Sylvie Contreras, Damien Voiry, Périne Landois and Jean-Manuel Decams



RESEARCH PAPERS

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Automated exploration of the conformational degrees of freedom along reaction profiles - driving a FASTCAR

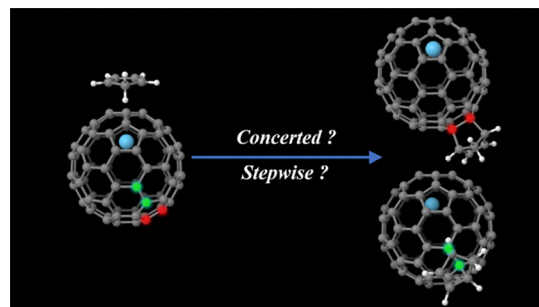
Oscar Gayraud,* Bastien Courbière and Frédéric Guégan*



25788

Computational insights into Diels–Alder reactions of paramagnetic endohedral metallofullerenes: M@C₈₂ (M = Sc, Y, La) and La@C₇₂

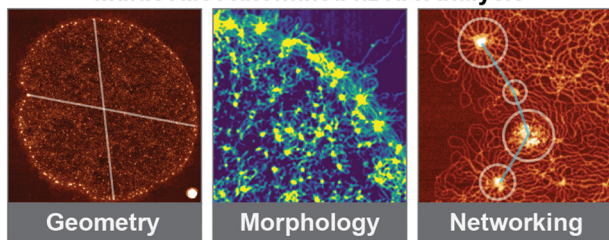
Linfeng Nie, Yuanyuan Sun* and Yang Wang*



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25798

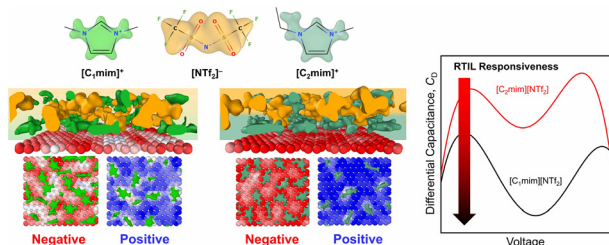
Multiscale Automated kDNA Analysis



Multiscale topological analysis of kinetoplast DNA via high-resolution AFM

Bradley Diggines, Sylvia Whittle, Indresh Yadav, Elizabeth P. Holmes, Daniel E. Rollins, Thomas E. Catley, Patrick S. Doyle* and Alice L. B. Pyne*

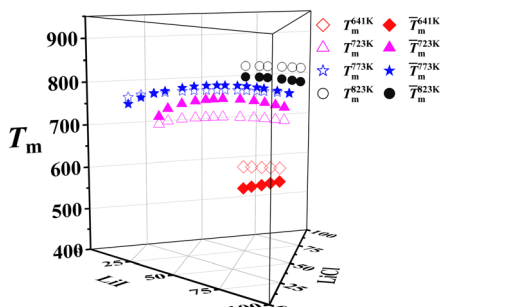
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Symmetric effect on electrical double-layer characteristics and molecular assembly interplay in imidazolium-based ionic liquid electrolytes in supercapacitor models

Michael Armstrong, Natthiti Chiangraeng, Monchai Jitvisate, Sakhorn Rimjaem, Kohji Tashiro and Piyarat Nimmanpipug*

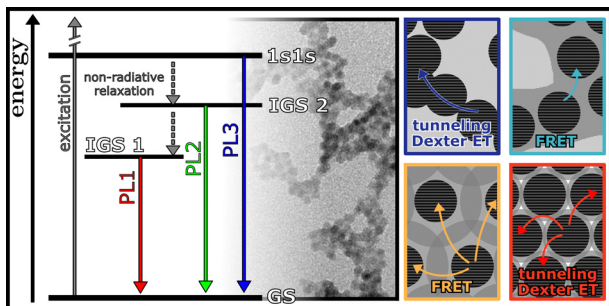
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The correlation of the liquidus curves and valence electron structures of a ternary lithium halide molten-salt electrolyte for liquid metal batteries

Boyang Li, Yongquan Guo,* Zhenyu Yang, Xinze Wang, Yichen Feng, Wei Tang, Siqi Peng and Tong Su

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Energy transfer in near-infrared photoluminescent PbS/CdS quantum dot-based three-dimensional networks and films

Denis Pluta, Rebecca T. Graf, Dirk Dorfs and Nadja C. Bigall*

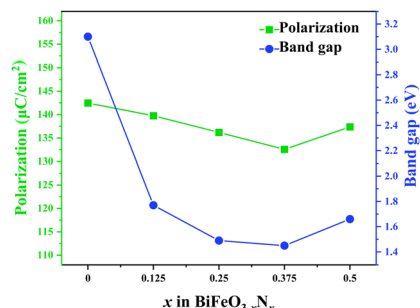


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Intermediate bands and p-orbital tuning of the band structure of BiFeO₃ for photovoltaic application

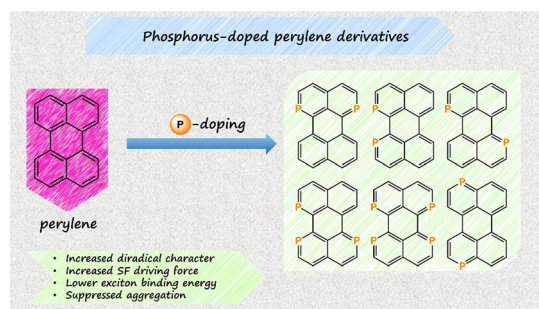
Xi Wang, Sa Zhang,* Liang Qiao, Li Ma and Haiyan Xiao



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Theoretical design of phosphorus-doped perylene derivatives as efficient singlet fission chromophores

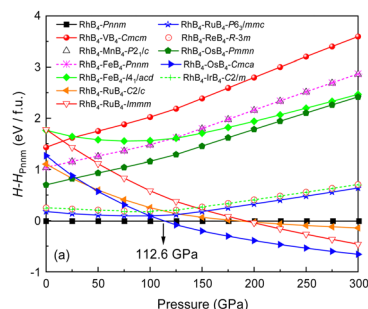
Tianyu Li, Lin Xue, Lishuang Ma, Xianyuan Wang, Xiaonan Fan, Boce Cui, Linglong Tang, Wen Yao, Teng Zhang, Li Shen* and Heyuan Liu*



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A new pressure-densified orthogonal hard superconducting phase of RhB₄

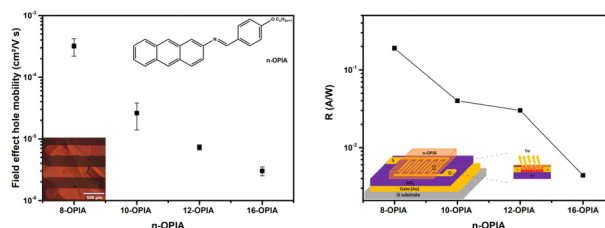
Ting Song,* Hai-Jun Peng, Meng-Ru Chen, Shuang-Gang Xu, Xi-Long Dou and Xiao-Wei Sun



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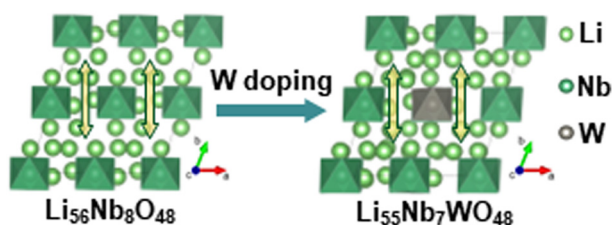
A new homologous series of semi-conducting liquid crystals based on phenyl-anthracene: synthesis and effect of the alkoxy terminal chain on charge transport and photoconductive properties

A. Moghnieh,* P.-E. Danjou, Y. Boussoualem, K. Ferchichi and A. Daoudi



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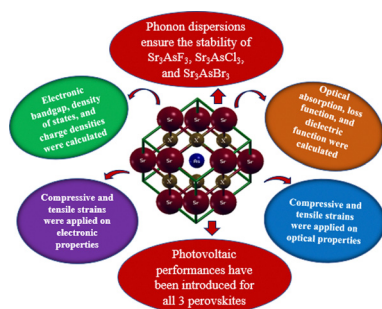
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Theoretical calculations of the performance of Li_7NbO_6 and its doped Phases as solid electrolytes

Shihao Feng, Zhixing Wang, Guoshang Zhang, Pengfei Yue, Wengao Pan, Qiongqiong Lu, Huajun Guo, Xinhai Li, Guochun Yan and Jiexi Wang*

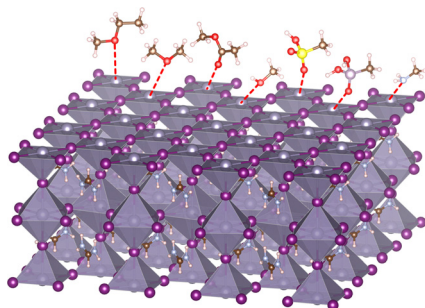
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A comprehensive investigation of the Sr_3AsX_3 (X = F/Cl/Br) inorganic cubic perovskites' strain-induced structural, electronic, optical, and mechanical properties with solar cell applications

Avijit Ghosh,* Mohammad Fokhrul Islam Buian, Nondon Lal Dey, Most. Sadia Islam Ria, Abdullah AL Baki, Asif Ahammad Miaze, Nasser S. Awwad, Rabiul Islam Chowdhury Robin and Hala A. Ibrahim

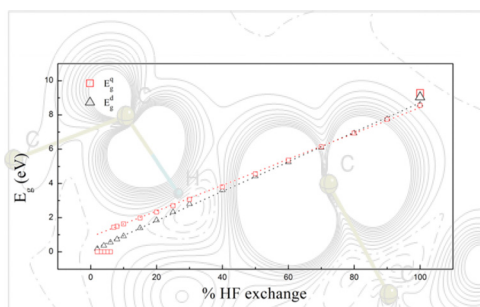
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A first-principles study of organic Lewis bases for passivating tin-based perovskite solar cells

Oscar J. Allen, Zhenzhen Wu,* Jian Kang, Jack J. Hinsch, Shiwei Yin* and Yun Wang*

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The role of the exact Hartree-Fock exchange in the investigation of defects in crystalline systems

Alexander Platonenko,* Francesco Gentile, Khaled E. El-Kelany and Roberto Dovesi

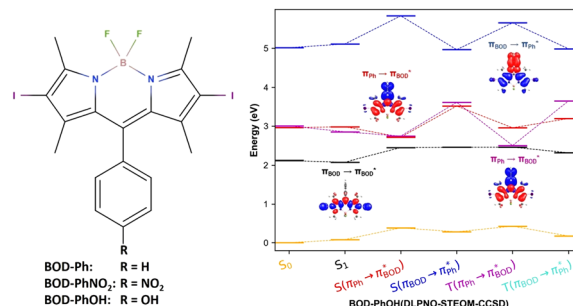


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Singlet and triplet excited states of a series of BODIPY dyes as calculated by TDDFT and DLPNO-STEOM-CCSD methods

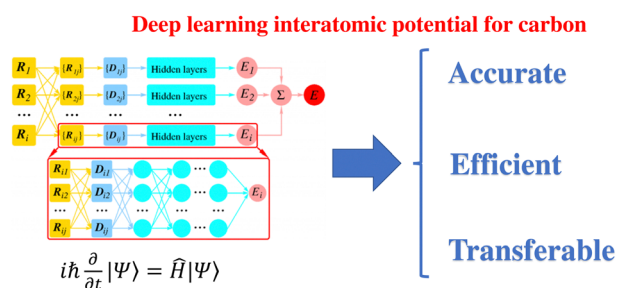
Aoussaj Sbai and Julien Guthmuller*



25936

Exploring the phase change and structure of carbon using a deep learning interatomic potential

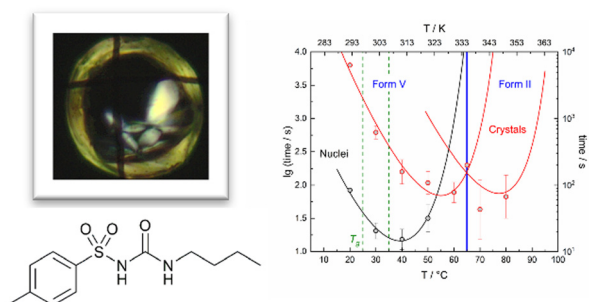
Kai Chen, Riyi Yang, Zhefeng Wang, Wuyan Zhao, Youmin Xu, Huaijun Sun, Chao Zhang, Songyou Wang,* Kaiming Ho, Cai-Zhuang Wang and Wan-Sheng Su*



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Nucleation, crystal growth, nuclei stability, and polymorph selection in supercooled tolbutamide melt

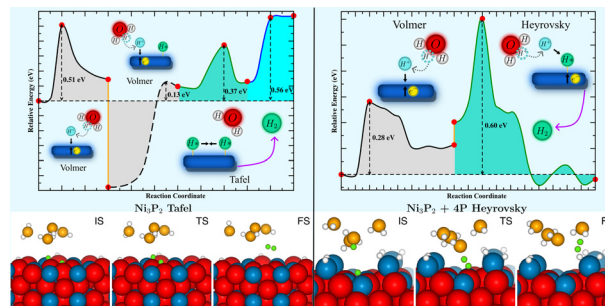
Ruslan A. Andrianov, Tatiana A. Morozova, Daniil S. Snetkov, Ilyas I. Nizamov, Christoph Schick and Timur A. Mukhametzyanov*



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Reaction modelling of hydrogen evolution on nickel phosphide catalysts: density functional investigation

Syam Sadan, Ingeborg-Helene Svenum, Sander Ø. Hanslin and Jaakko Akola*



Matthew E. Potter,* Hamish Cavaye,
Joshua J. M. Le Brocq, Luke L. Daemen and
Yongqiang Cheng

Tamuna Bakhiiia, Andrey Toropov, Iurii Nevolin,
Konstantin Maslakov, Anna Romanchuk* and
Stepan Kalmykov

$X_1 = X_2 = \text{H}$ - Fluorescein
 $X_1 = \text{H}, X_2 = \text{Br}$ - 2Br-fluorescein
 $X_1 = \text{Br}, X_2 = \text{H}$ - Eosin
 $X_1 = X_2 = \text{I}$ - Erythrosine

The diagram illustrates the photophysical processes of the fluorophores. The energy levels are shown as S_0 (ground state), S_1 (first excited singlet state), and T_1 (first excited triplet state). The processes are: Absorption ($S_0 \rightarrow S_1$), Fluorescence ($S_1 \rightarrow S_0$), and Phosphorescence ($T_1 \rightarrow S_0$). The Intersystem Crossing (ISC) is shown as a transition from S_1 to T_1 .

The right panel shows the rate constant of thermal conversion (s^{-1}) versus the spin-orbit coupling matrix element (cm^{-1}). The blue curve represents the rate constant for $S_1 \rightarrow T_1$ ISC, and the red curve represents the rate constant for $T_1 \rightarrow S_0$ ISC. The data points are shown as blue circles and red circles, respectively.

N. Ibrayev,* E. Seliverstova, R. Valiev, A. Aymagambetova
and D. Sundholm

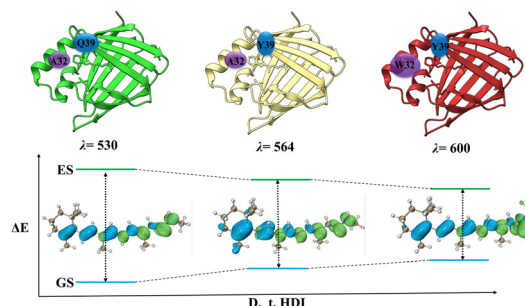
Weijia Xu, Haoyang Xu, Meifang Zhu and Jin Wen*

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Charge transfer characteristics in rhodopsin mimics during photoexcitation

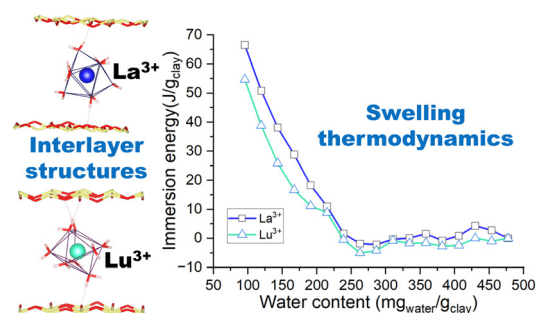
Yongnan Hu, Gaoshang Li, Siteng Zhao, Jin Dai, Xubiao Peng* and Qing Zhao*



26012

Structure and mobility of rare earth ions in interlayer space of montmorillonite: a molecular dynamics study

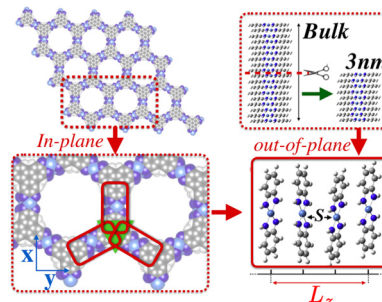
Caorui Wang, Yingchun Zhang and Xiandong Liu*



26022

Tailoring van der Waals interactions in ultra-thin two dimensional metal–organic frameworks (MOFs) for photoconductive applications

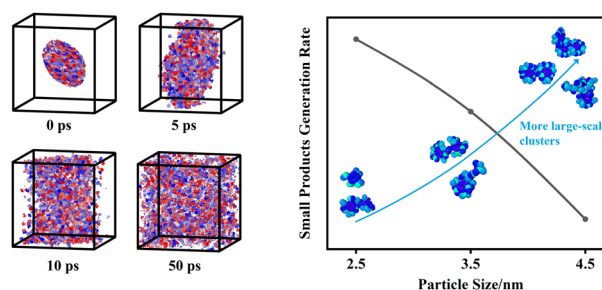
David Dell'Angelo,* Ioannis Karamanis, Mohammad Reza Saeb, Lavinia Balan* and Michael Badawi*



26030

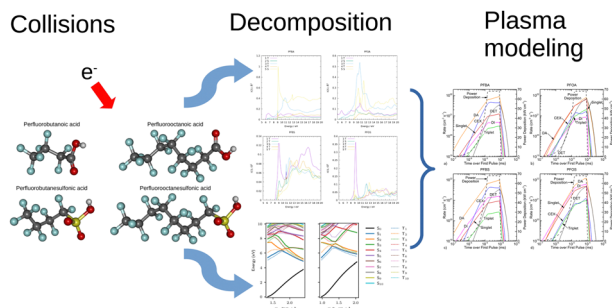
Size effect on the pyrolysis of 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) nanoparticles: a ReaxFF molecular dynamics study

Jialu Guan, Guanchen Dong, Jing Lv, Libo Zhang, Guangcheng Yang, Xiaona Huang* and Linghua Tan*



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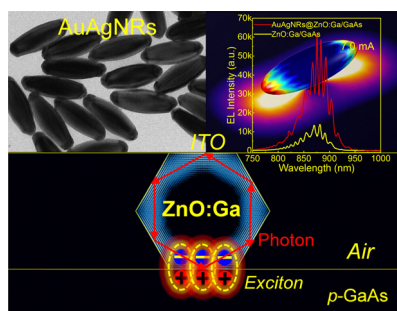
26037



Fundamental data for modeling electron-induced processes in plasma remediation of perfluoroalkyl substances

Marin Sapunar, Mackenzie Meyer, Harindranath B. Ambalampitiya, Mark J. Kushner and Zdeněk Mašín*

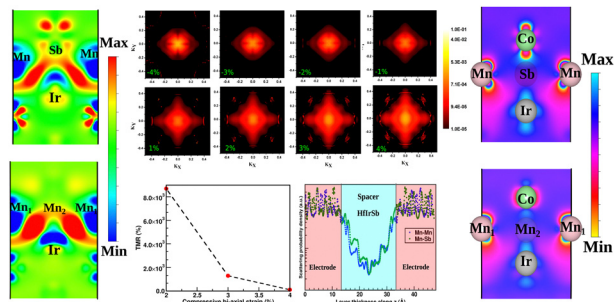
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Plasmonically-boosted exciton–photon coupling strength in a near-infrared LED based on a ZnO:Ga microwire/GaAs heterojunction with surface-coated Au&Ag alloy nanorods

Lixiang Sun, Kai Tang,* Peng Wan, Maosheng Liu, Daning Shi, Caixia Kan and Mingming Jiang*

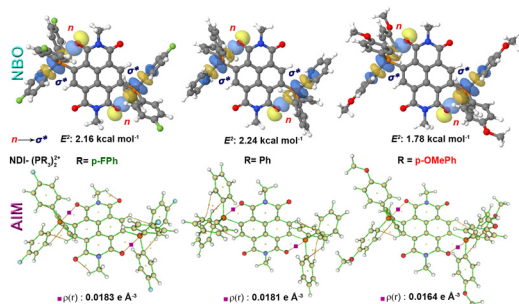
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Spin dependent tunneling and strain sensitivity in a $\text{Co}_2\text{MnSb}/\text{HfIrSb}$ magnetic tunneling junction: a first-principles study

Joydipto Bhattacharya, Ashima Rawat, Ranjit Pati, Aparna Chakrabarti* and Ravindra Pandey

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Unravelling the intramolecular $n \rightarrow \sigma^*$ interaction in ultra-electron deficient naphthalenediimides and their radical ions

Sharvan Kumar, Kalyanashis Mandal, Ajayakumar M. R., Geeta Hundal and Pritam Mukhopadhyay*

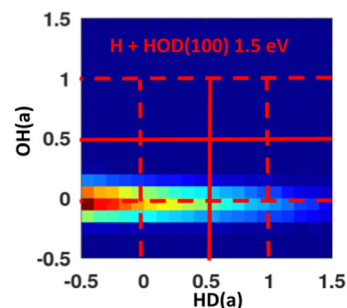


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A quasi-classical study in a quantum spirit of mode specificity of the H + HOD abstraction reaction

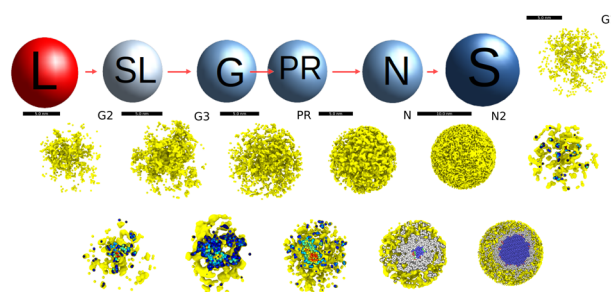
Matthew Braunstein* and Laurent Bonnet



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Resolving heterogeneous particle mobility in deeply quenched liquid iron: an ultra-fast assembly-free two-step nucleation mechanism

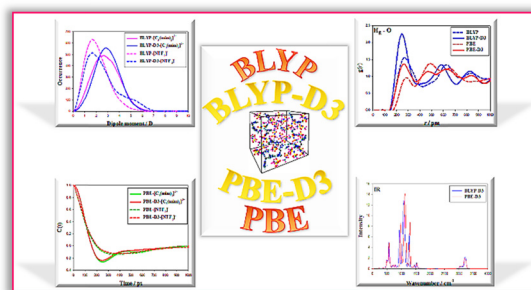
P. Süle



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Comparative assessment of the performance of density functionals and dispersion correction on different properties of dicationic ionic liquids – an *ab initio* molecular dynamics (AIMD) study

Zahra Ostadsharif Memar and Majid Moosavi*



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Reaction pathways leading to HPALD intermediates in the OH-initiated oxidation of isoprene

Péter Szabó,* Zhen Liu, Jean-François Müller, Jeremy N. Harvey and Jozef Peeters*

