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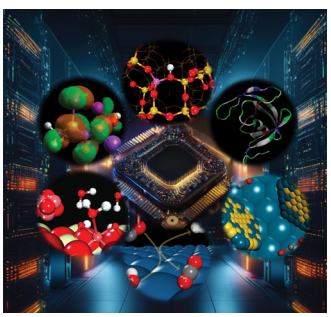
Cover
See Hong Qi, Zhi-Heng Zheng *et al.*, pp. 20782–20793. Image reproduced by permission of Hong Qi from *Phys. Chem. Chem. Phys.*, 2023, **25**, 20782.

EDITORIAL

20775

Computational modelling in catalytic science

C. Richard A. Catlow,* Arunabhiram Chutia* and Matthew G. Quesne*

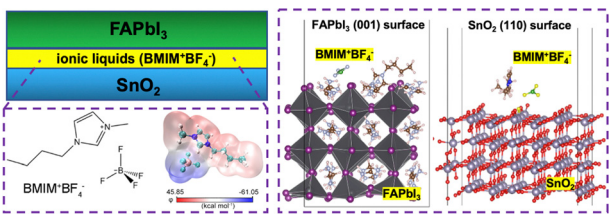


COMMUNICATION

20777

Unraveling the dynamic behaviors of BF_4-based ionic liquids at the SnO_2/$FAPbI_3$ interface using *ab initio* molecular dynamics simulations

Jinge Han, Hongbin Xiao,* Yanru Guo, Xue Liu, Zhigang Zang and Ru Li*



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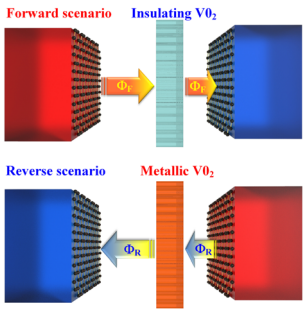
Performance improvement of three-body radiative diodes driven by graphene surface plasmon polaritons

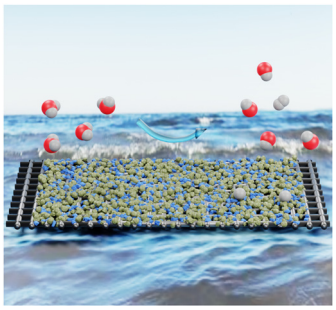
Ming-Jian He, Xue Guo, Hong Qi,* Zhi-Heng Zheng,* Mauro Antezza and He-Ping Tan



20794

Scalable production of foam-like nickel–molybdenum coatings *via* plasma spraying as bifunctional electrocatalysts for water splitting

Xiuyu Wu, Alexis Piñeiro-García, Mouna Rafei, Nicolas Boulanger, Esdras Josué Canto-Aguilar and Eduardo Gracia-Espino*



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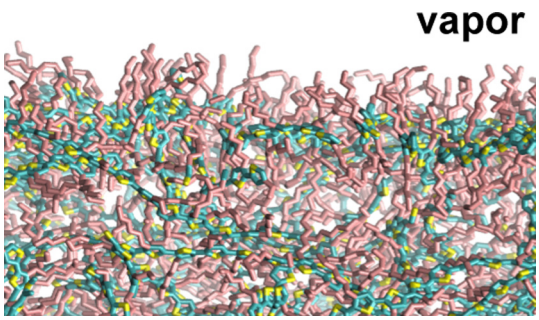
Accumulation and ordering of P3HT oligomers at the liquid–vapor interface with implications for thin-film morphology

Jakub K. Sowa, Thomas C. Allen and Peter J. Rossky*



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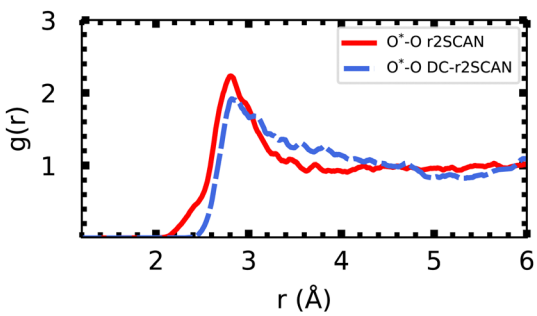
Radicals in aqueous solution: assessment of density-corrected SCAN functional

Fabian Belleflamme and Jürg Hutter*



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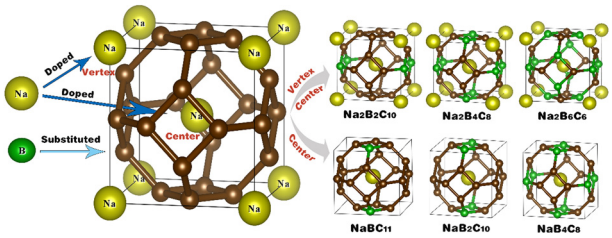
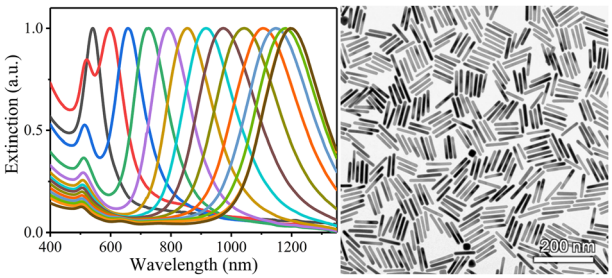


Prediction of potential hard sodium carbaboride compounds assuming sp^3-bonded covalent clathrates

Ailing Liu, Xiaoran Cheng, Xingyu Wang, Yutong Zou and Miao Zhang*

20843



Controlled synthesis of monodisperse gold nanorods with a small diameter of around 10 nm and largest plasmon wavelength of 1200 nm

Anhua Wei, Jingfang OuYang, Yuyang Guo, Suju Jiang, Feifei Chen, Jun Huang, Qi Xiao and Zihua Wu*

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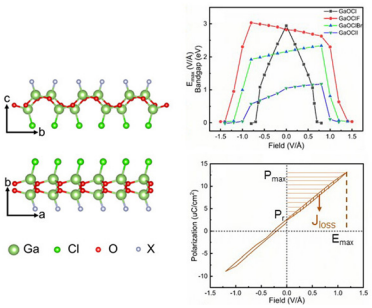
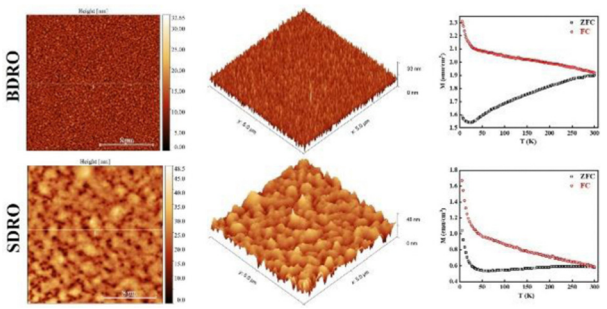


Janus GaOClX (X = F, Br, and I) monolayers as predicted using first-principles calculations: a novel class of nanodielectrics with superior energy storage properties

Shujuan Jiang and Guangping Zheng*

20863



Integrated experimental and theoretical studies on structural and magnetic properties of thin films of double perovskite ruthenates: Ba_2DyRuO_6 & Sr_2DyRuO_6

Sahil Dani, Rakesh Kumar, Hitesh Sharma, R J Choudhary, Navdeep Goyal, Pawanpreet Kaur and Rabia Pandit*

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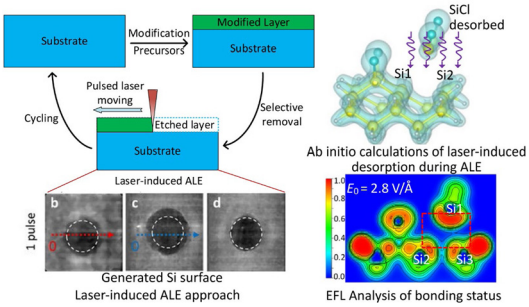
***Ab initio* simulations of ultrashort laser pulse interaction with Cl–Si(100): implications for atomic layer etching**

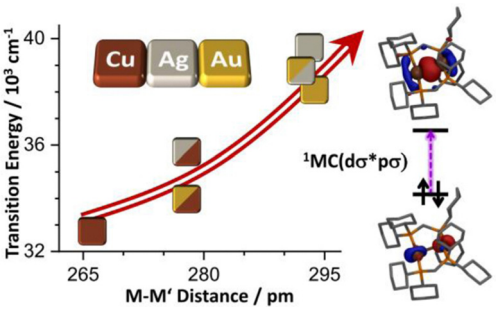
Peizhi Wang and Fengzhou Fang*



20880

Electronic spectroscopy of homo- and heterometallic binuclear coinage metal phosphine complexes in isolation

Marcel J. P. Schmitt, Sebastian V. Kruppa, Simon P. Walg, Werner R. Thiel, Wim Klopper* and Christoph Riehn*



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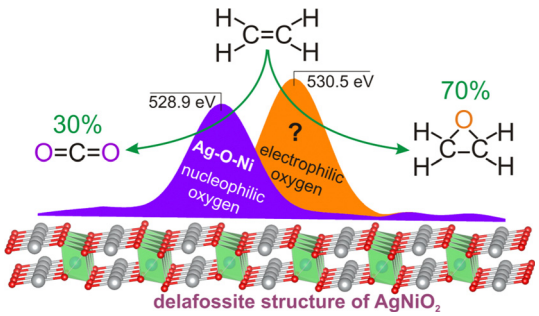
Room temperature epoxidation of ethylene over delafossite-based $AgNiO_2$ nanoparticles

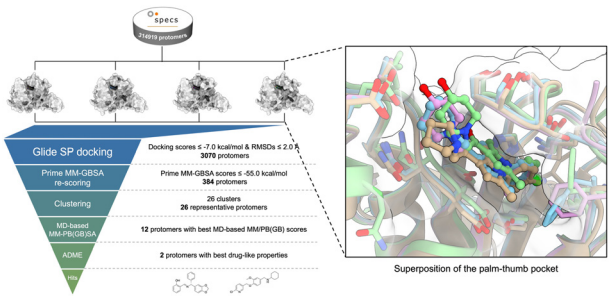
Dmitry A. Svintsitskiy,* Mikhail K. Lazarev, Elena M. Slavinskaya, Elizaveta A. Fedorova, Tatyana Yu. Kardash, Svetlana V. Cherepanova and Andrei I. Boronin



20903

***In silico* screening and computational evaluation of novel promising USP14 inhibitors targeting the palm–thumb pocket**

Tianhao Wang, Jianbo Tong,* Xing Zhang, Hao Luo, Lei Xu and Zhe Wang*



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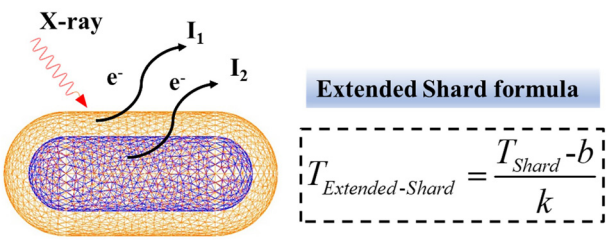

A theoretical characterization method for non-spherical core–shell nanoparticles by XPS

J. M. Gong, M. S. S. Khan, B. Da,* H. Yoshikawa, S. Tanuma and Z. J. Ding*

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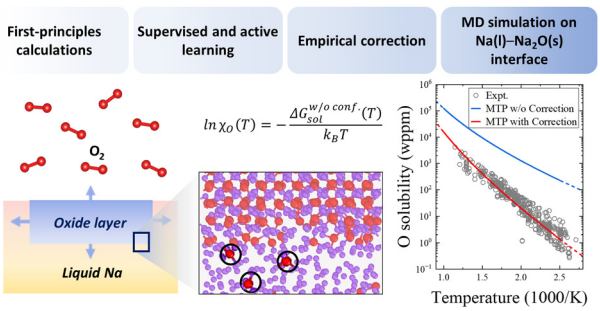

Temperature dependence of O solubility in liquid Na by atomistic simulation of Na(l)–Na_2O(s) interfaces using corrected machine learning potential: a step towards simulating Na combustion

Chaeyeong Kim and Takuji Oda*

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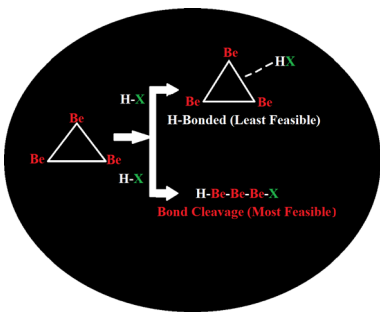

Three-membered beryllium ring, Be_3: not just a hydrogen bond acceptor

Lakhya J. Mazumder and Ankur K. Guha*

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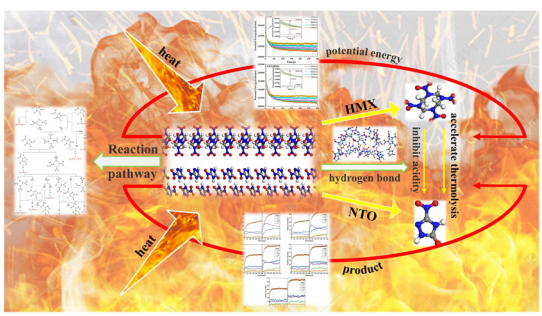

Multi-aspect simulation insight on thermolysis mechanism and interaction of NTO/HMX-based plastic-bonded explosives: a new conception of the mixed explosive model

Xiaofeng Yuan, Ying Huang, Shuhai Zhang,* Ruijun Gou, Shuangfei Zhu and Qianjin Guo

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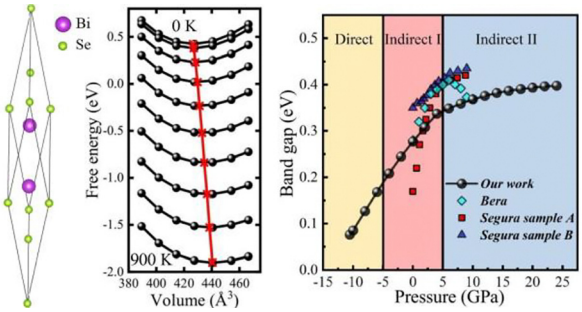
Effects of pressure and temperature on topological electronic materials X_2Y_3 (X = As, Sb, Bi; Y = Se, Te) using first-principles

Le Fang, Chen Chen, Xionggang Lu* and Wei Ren*



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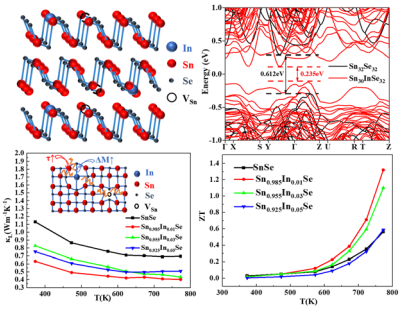
Significantly improved thermoelectric performance of SnSe originating from collaborative adjustment between valence and conduction bands, mass fluctuations, and local strain

Shuai Wang, Hang Yuan, Chunhui Li, HongQuan Liu,* Yi-jie Gu* and YanFang Wang



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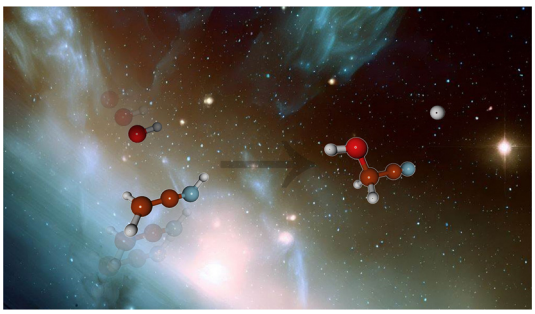
Gas-phase formation of glycolonitrile in the interstellar medium

Luis Guerrero-Méndez, Anxo Lema-Saavedra, Elena Jiménez, Antonio Fernández-Ramos* and Emilio Martínez-Núñez*



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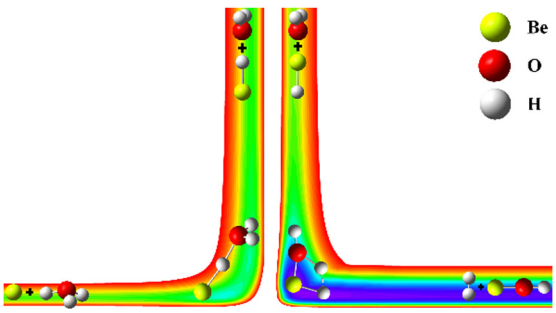
Theoretical studies on the kinetics and dynamics of the $BeH^+ + H_2O$ reaction: comparison with the experiment

Jiaqi Li, Zhao Tu, Haipan Xiang, Yong Li* and Hongwei Song*



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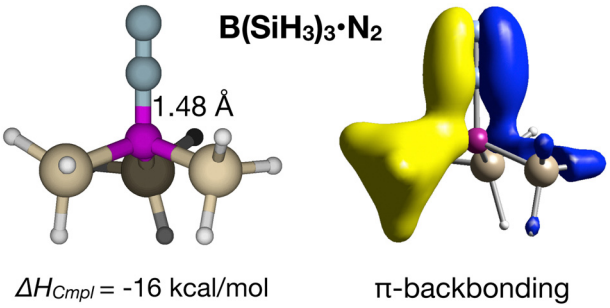
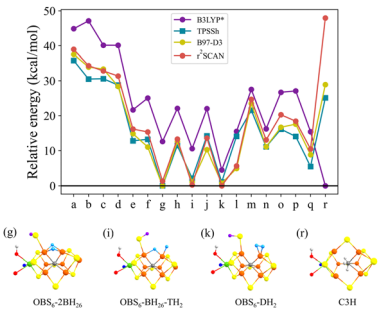


Anomalous π-backbonding in complexes between $B(SiR_3)_3$ and N_2: catalytic activation and breaking of scaling relations

Tore Brinck* and Suman Kalyan Sahoo

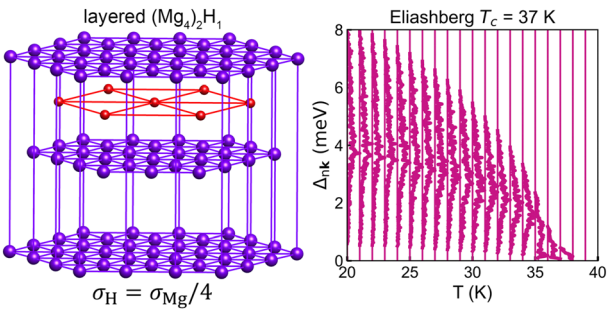
21020



The E_3 state of FeMoco: one hydride, two hydrides or dihydrogen?

Yunjie Pang and Ragnar Bjornsson*

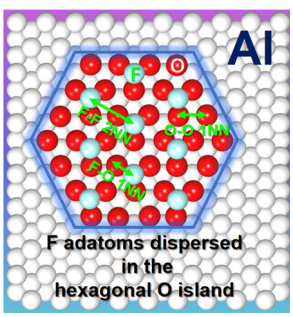
21037



Enhancement for phonon-mediated superconductivity up to 37 K in few-hydrogen metal-bonded layered magnesium hydride under atmospheric pressure

Yong He, Juan Du,* Shi-ming Liu, Chong Tian, Min Zhang, Yao-hui Zhu, Hongxia Zhong, Xinqiang Wang and Jun-jie Shi*

21045



Morphology evolution of the aluminum surface in a fluorine-containing environment

Pengqi Hai, Chao Wu,* Xiangdong Ding* and Yuanjie Li*

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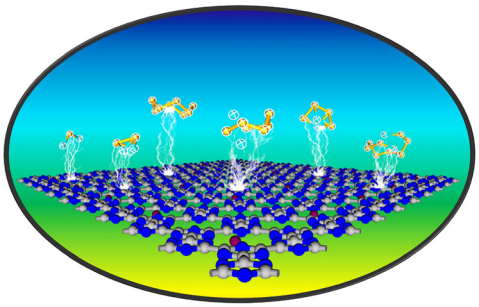
RESEARCH PAPERS

21054

Unveiling the anchoring and catalytic effect of Co@C_3N_3 monolayer as a high-performance selenium host material in lithium–selenium batteries: a first-principles study

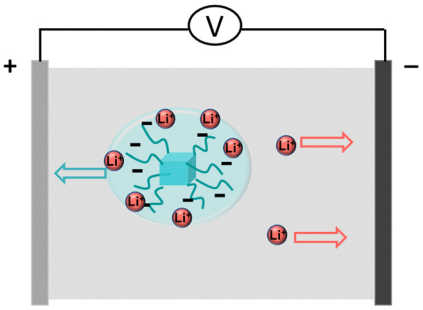
Shuwei Tang,* Wentao Liu, Zehui Yang, Chenchen Liu, Shulin Bai, Jingyi Zhang and Dongming Luo



21065

Lithium transference in electrolytes with star-shaped multivalent anions measured by electrophoretic NMR

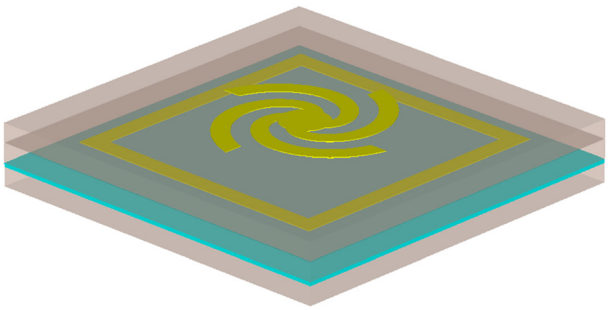
Saheli Chakraborty, David M. Halat, Julia Im, Darby T. Hickson, Jeffrey A. Reimer and Nitash P. Balsara*



21074

Polarization-insensitive electromagnetically induced transparency and its sensing performance based on spoof localized surface plasmons in vanadium dioxide-based terahertz metasurfaces

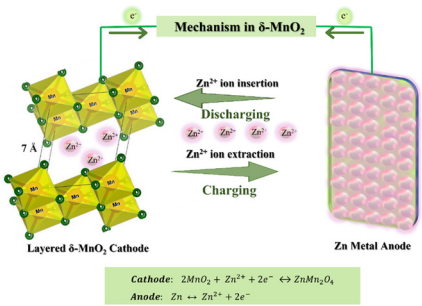
Mingming Chen* and Xue-Xia Yang*



21082

A highly stable δ-MnO_2 cathode with superior electrochemical performance for rechargeable aqueous zinc ion batteries

Priya Yadav, Dimas Putro, Nisha Kumari, Jaekook Kim* and Alok Kumar Rai*



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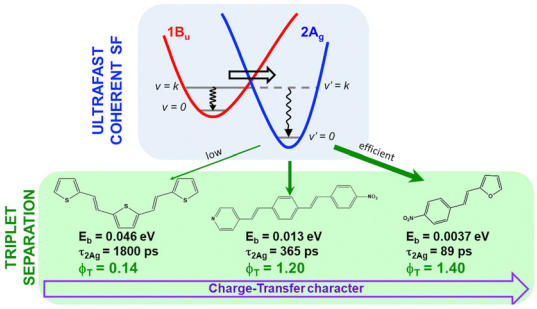
RESEARCH PAPERS

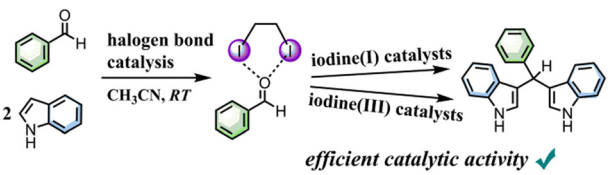
21089



Unveiling the double triplet nature of the 2Ag state in conjugated stilbenoid compounds to achieve efficient singlet fission

Letizia Mencaroni, Martina Alebardi, Fausto Elisei, Irena Škorić, Anna Spalletti and Benedetta Carlotti*

21100



Iodine(I)-based and iodine(III)-based halogen bond catalysis on the Friedel–Crafts reaction: a theoretical study

Chang Zhao, Ying Li, Xiaoyan Li and Yanli Zeng*

CORRECTION

21109

Correction: First-principles modeling of the highly dynamical surface structure of a MoS_2 catalyst with S-vacancies

Po-Yuan Wang, Bo-An Chen, Yu-Chi Lee and Cheng-chau Chiu*

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