

IN THIS ISSUE

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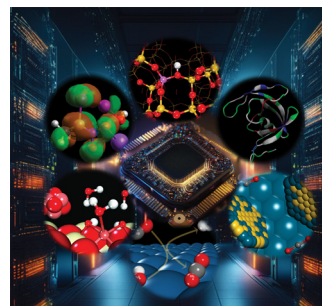
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pp. 20782–20793.
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EDITORIAL

20775

Computational modelling in catalytic science

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

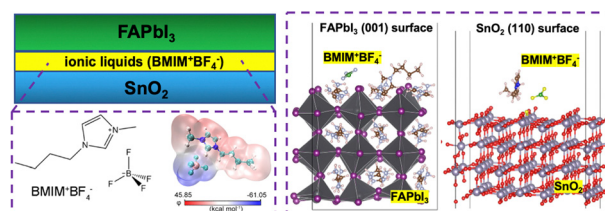


COMMUNICATION

20777

Unraveling the dynamic behaviors of BF₄-based ionic liquids at the SnO₂/FAPbI₃ interface using *ab initio* molecular dynamics simulations

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



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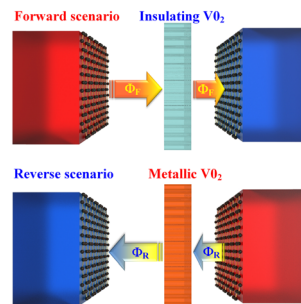


RESEARCH PAPERS

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

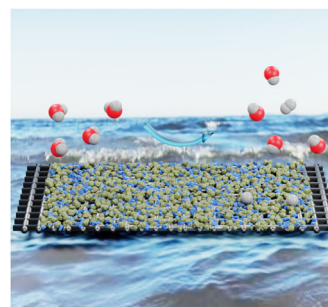
Ming-Jian He, Xue Guo, Hong Qi,* Zhi-Heng Zheng,*
Mauro Antezza and He-Ping Tan



20794

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

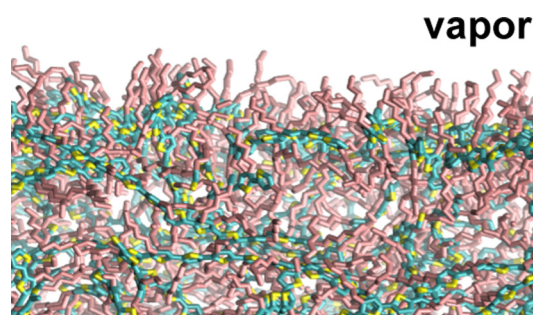
Xiuyu Wu, Alexis Piñeiro-García, Mouna Rafei,
Nicolas Boulanger, Esdras Josué Canto-Aguilar and
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Accumulation and ordering of P3HT oligomers at the liquid–vapor interface with implications for thin-film morphology

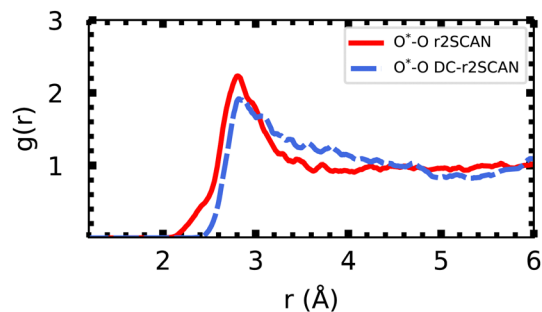
Jakub K. Sowa, Thomas C. Allen and Peter J. Rossky*



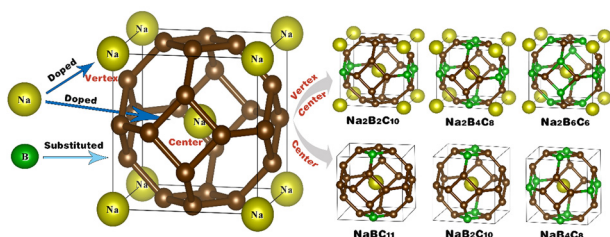
20817

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

Fabian Belleflamme and Jürg Hutter*



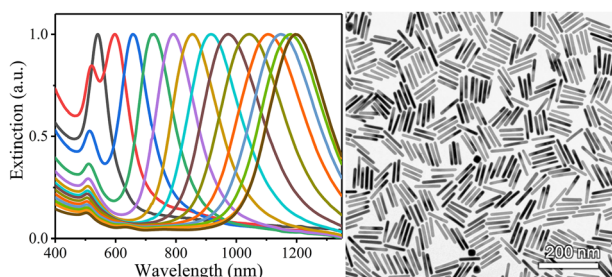
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Prediction of potential hard sodium carbaboride compounds assuming sp³-bonded covalent clathrates

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

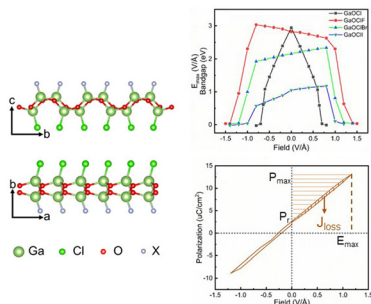
20843



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*

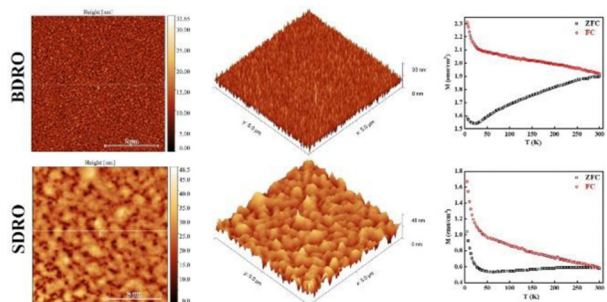
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Janus GaOCIX (X = F, Br, and I) monolayers as predicted using first-principles calculations: a novel class of nanodielectrics with superior energy storage properties

Shujuan Jiang and Guangping Zheng*

20863



Integrated experimental and theoretical studies on structural and magnetic properties of thin films of double perovskite ruthenates: Ba₂DyRuO₆ & Sr₂DyRuO₆

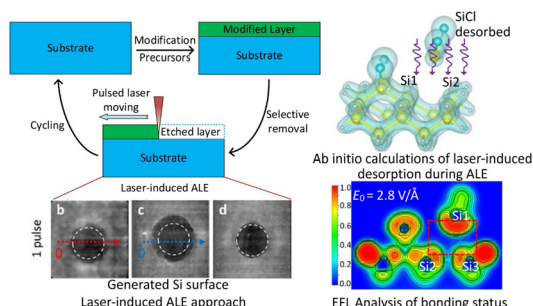
Sahil Dani, Rakesh Kumar, Hitesh Sharma, R J Choudhary, Navdeep Goyal, Pawanpreet Kaur and Rabia Pandit*



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

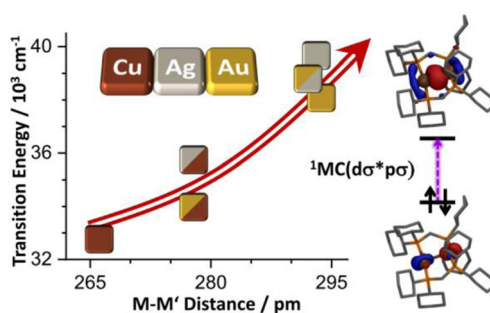
Peizhi Wang and Fengzhou Fang*



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

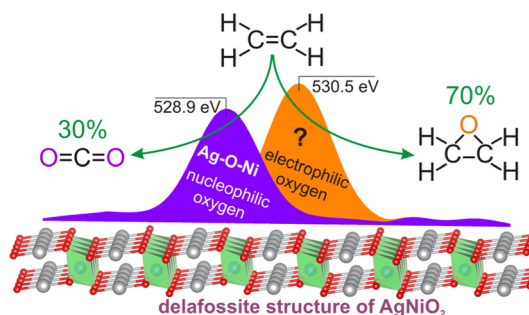
Marcel J. P. Schmitt, Sebastian V. Kruppa, Simon P. Walg, Werner R. Thiel, Wim Klopper* and Christoph Riehn*



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Room temperature epoxidation of ethylene over delafossite-based AgNiO₂ nanoparticles

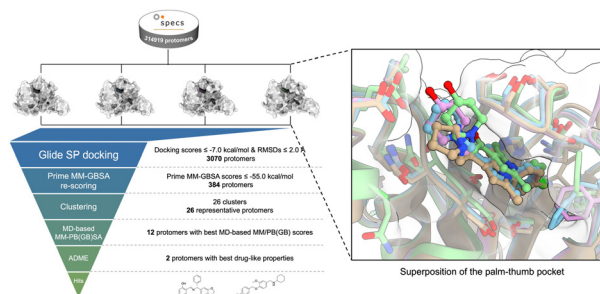
Dmitry A. Svintsitskiy,* Mikhail K. Lazarev, Elena M. Slavinskaya, Elizaveta A. Fedorova, Tatyana Yu. Kardash, Svetlana V. Cherepanova and Andrei I. Boronin



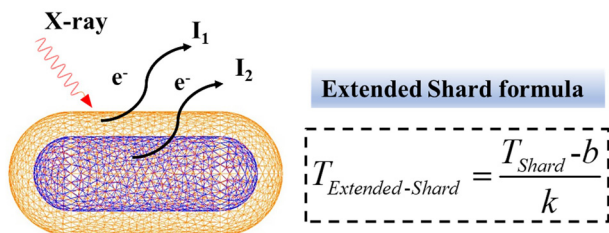
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In silico screening and computational evaluation of novel promising USP14 inhibitors targeting the palm–thumb pocket

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



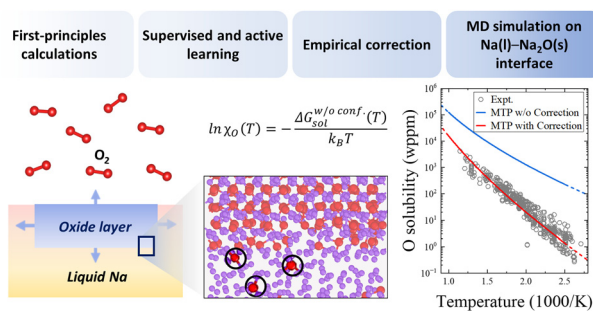
20917



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*

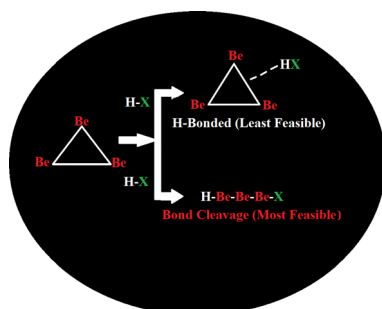
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Temperature dependence of O solubility in liquid Na by atomistic simulation of Na(l)–Na₂O(s) interfaces using corrected machine learning potential: a step towards simulating Na combustion

Chaeyeong Kim and Takuji Oda*

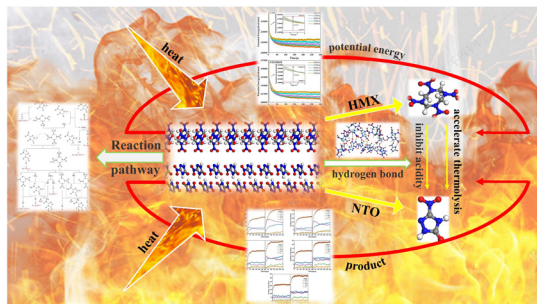
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Three-membered beryllium ring, Be₃: not just a hydrogen bond acceptor

Lakhya J. Mazumder and Ankur K. Guha*

20951



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

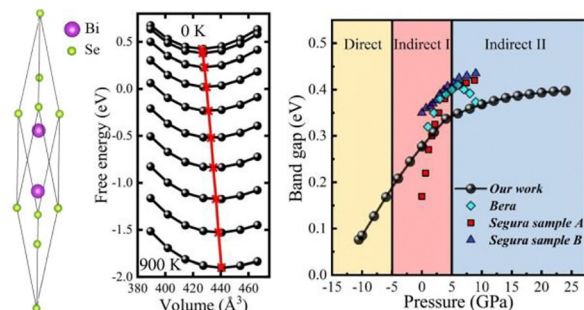


RESEARCH PAPERS

20969

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

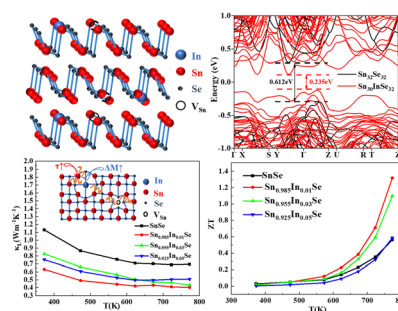
Le Fang, Chen Chen, Xionggang Lu* and Wei Ren*



20979

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

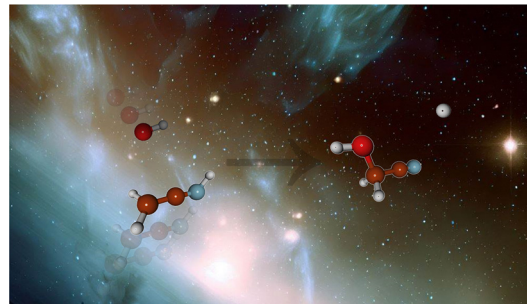
Shuai Wang, Hang Yuan, Chunhui Li, HongQuan Liu,* Yi-jie Gu* and YanFang Wang



20988

Gas-phase formation of glycolonitrile in the interstellar medium

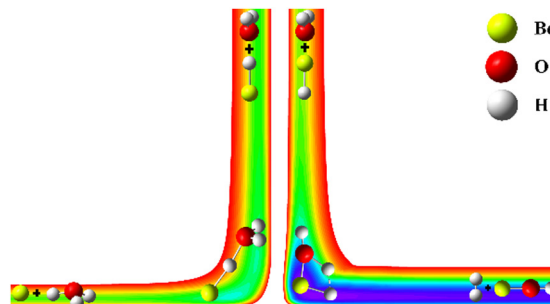
Luis Guerrero-Méndez, Anxo Lema-Saavedra, Elena Jiménez, Antonio Fernández-Ramos* and Emilio Martínez-Núñez*



20997

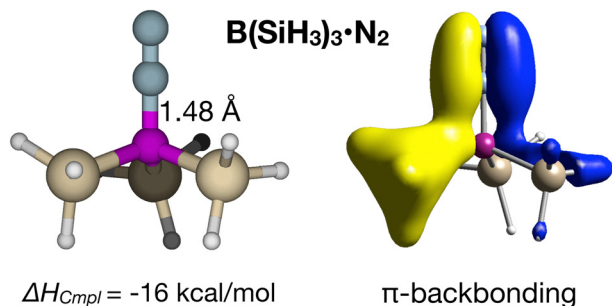
Theoretical studies on the kinetics and dynamics of the $\text{BeH}^+ + \text{H}_2\text{O}$ reaction: comparison with the experiment

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



RESEARCH PAPERS

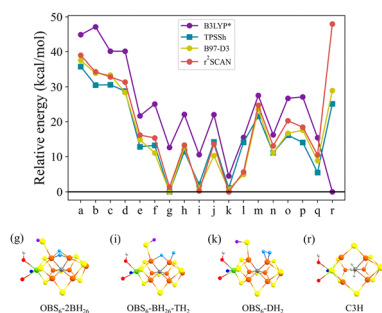
21006



Anomalous π -backbonding in complexes between B(SiR₃)₃ and N₂: catalytic activation and breaking of scaling relations

Tore Brinck* and Suman Kalyan Sahoo

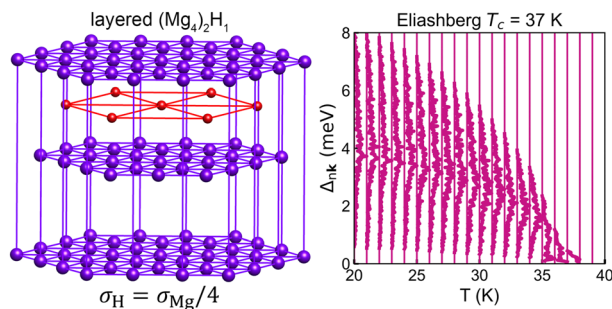
21020



The E₃ state of FeMoco: one hydride, two hydrides or dihydrogen?

Yunjie Pang and Ragnar Bjornsson*

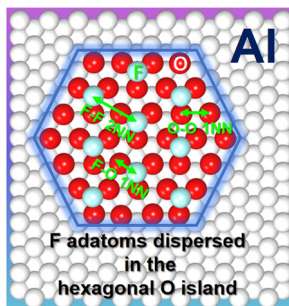
21037



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*

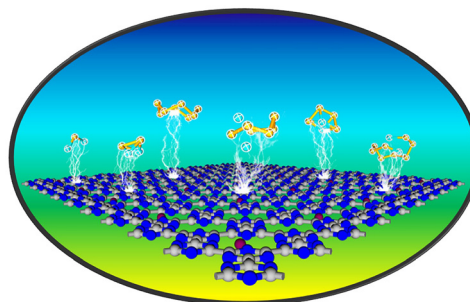


RESEARCH PAPERS

21054

Unveiling the anchoring and catalytic effect of Co@C₃N₃ monolayer as a high-performance selenium host material in lithium–selenium batteries: a first-principles study

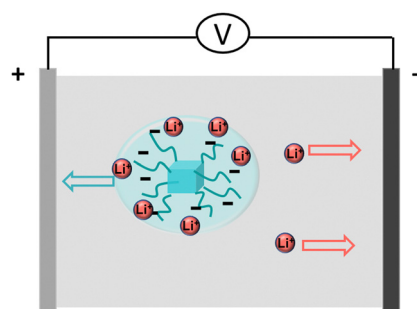
Shuwei Tang,* Wentao Liu, Zehui Yang, Chenchen Liu, Shulin Bai, Jingyi Zhang and Dongming Luo



21065

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

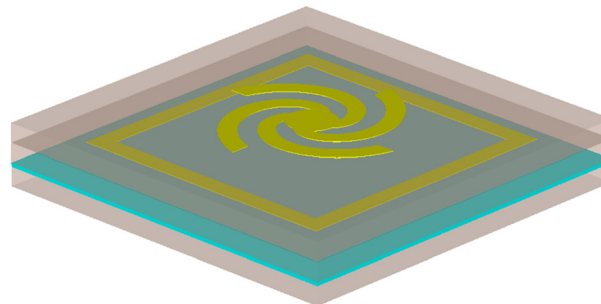
Saheli Chakraborty, David M. Halat, Julia Im, Darby T. Hickson, Jeffrey A. Reimer and Nitash P. Balsara*



21074

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

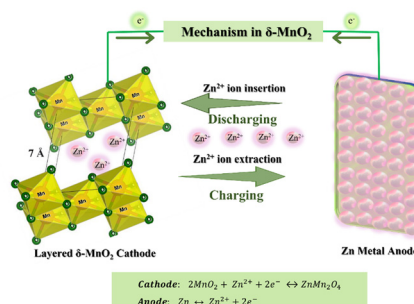
Mingming Chen* and Xue-Xia Yang*



21082

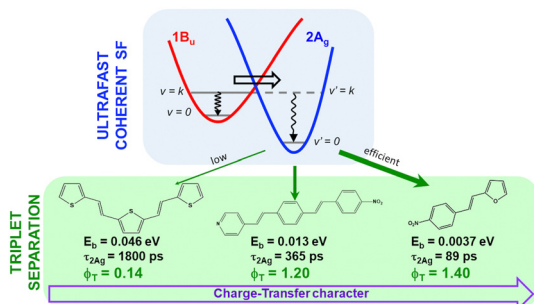
A highly stable δ -MnO₂ cathode with superior electrochemical performance for rechargeable aqueous zinc ion batteries

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



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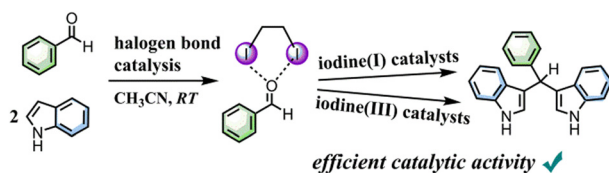
21089



Unveiling the double triplet nature of the $2A_g$ 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*

