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IN THIS ISSUE

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Cover
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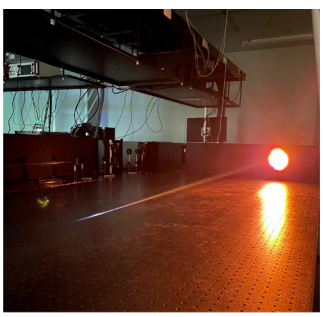
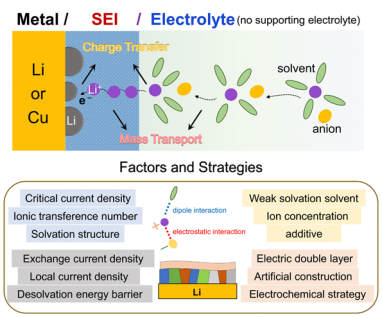
REVIEWS





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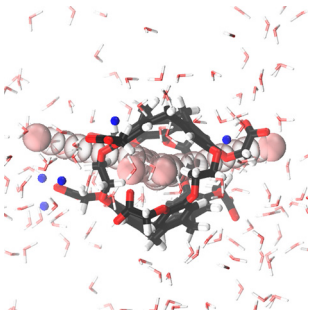

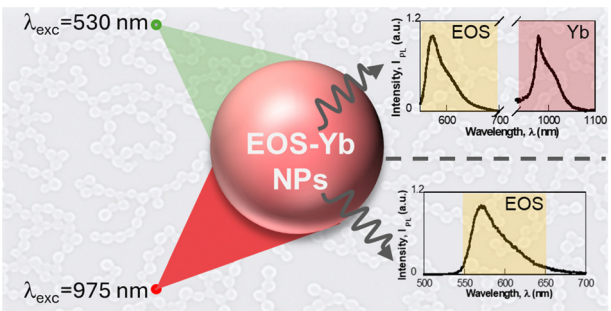

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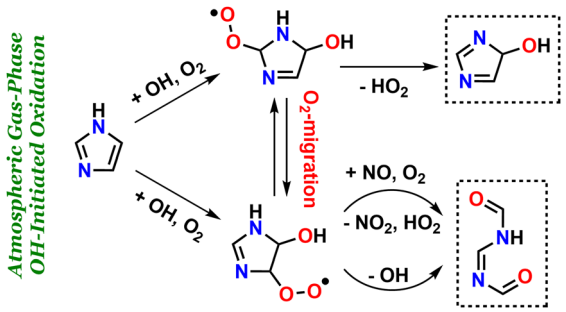

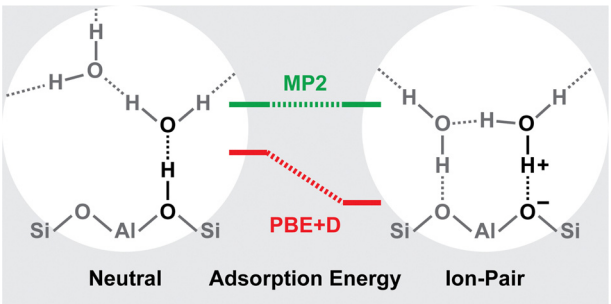

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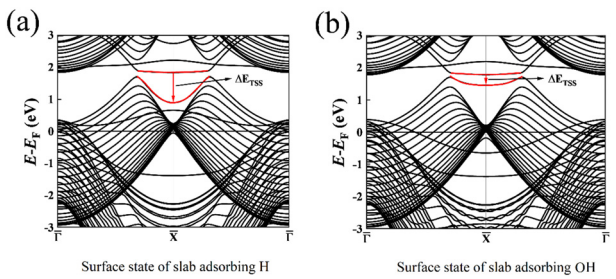
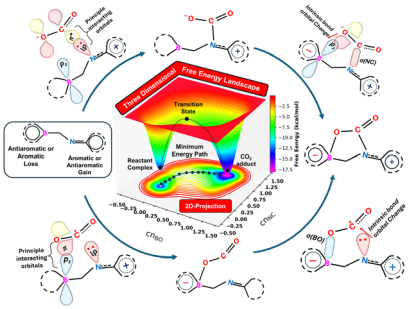


Variation of topological surface states of nodal line semimetal MgB_2 resulting from adsorption of hydrogen, hydroxide, and water molecules

Pangdong Zhu, Kun Bu,* Ruzhi Wang and Changhao Wang*

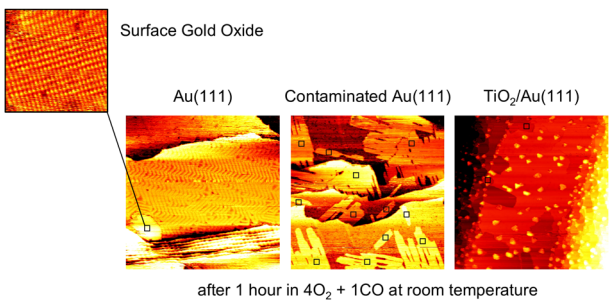
23609



Orbital and free energy landscape expedition towards the unexplored catalytic realm of aromatically modified FLPs for CO_2 sequestration

Mohmmad Faizan, Madhumita Chakraborty, Dinesh Bana and Ravinder Pawar*

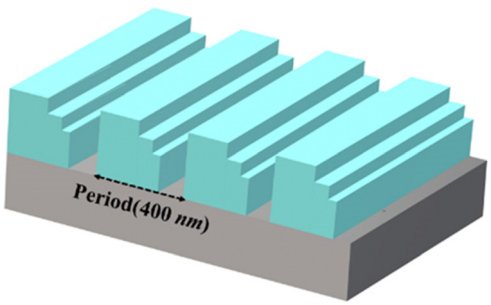
23623



Gold oxide formation on Au(111) under CO oxidation conditions at room temperature

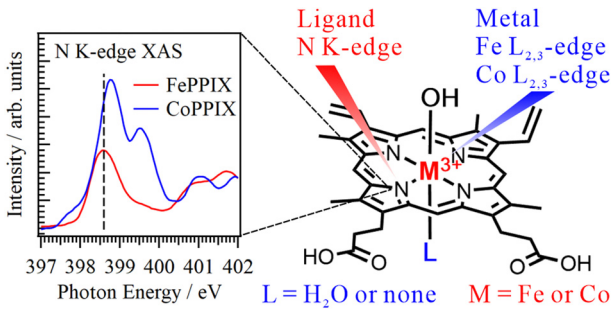
Sabine Wenzel,* Dajo Boden and Irene M. N. Groot

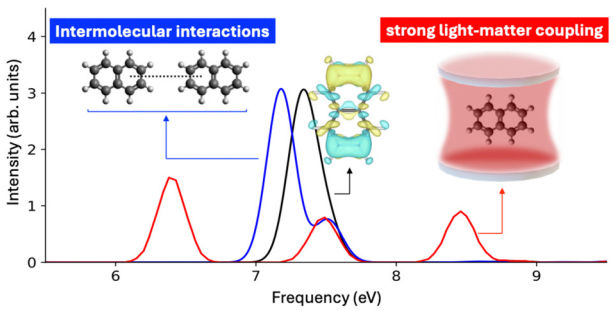
23631

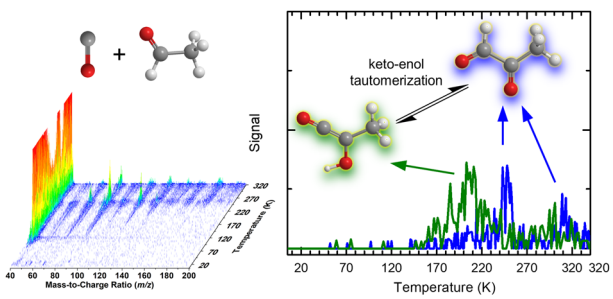


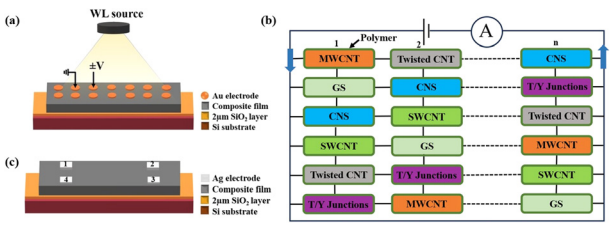
Broadband and weak-dispersion nonlinear response enhancement in the epsilon-near-zero region of a nano-stepped metasurface

Yanxin Lu, Jiahui Zheng, Feilian Zhang, Qiqi Guo, Yunfei Song, Jiannan Dong and Yihang Chen*









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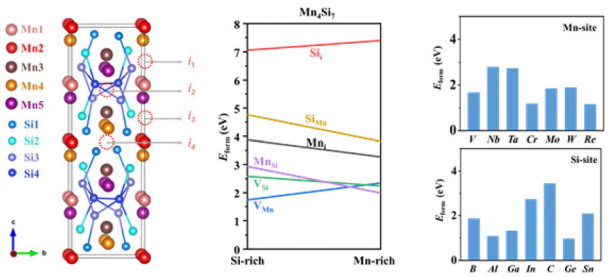
A first-principles study of the electronic structure and point defects in higher manganese silicide Mn_4Si_7

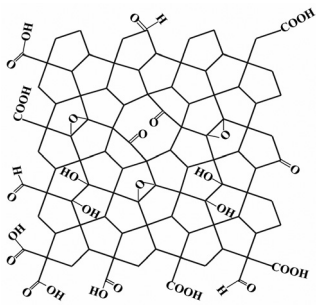
Jun Chai,* Guangshu Li, Mingping He and Hangjia Shen



23730

Regulation of C=C bonds in penta-graphene by oxidative functionalization: a prototype of penta-graphene oxide (PGO)

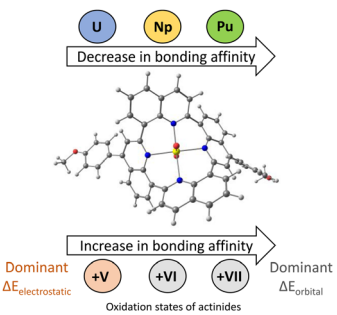
Kaixuan Jin and Xiaojie Liu*



23739

High-valent actinyl (AnO_2^{2+}; An = U, Np and Pu) complexation with TEtraQuinoline (TEQ) ligand – a DFT study

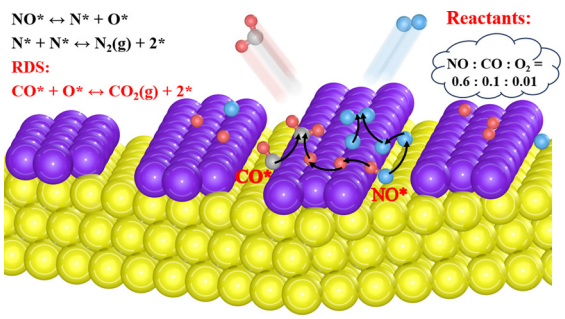
Abigail Jennifer G and Elumalai Varathan*



23754

Design and screening of bimetallic catalysts for nitric oxide reduction by CO: a study of kinetic Monte Carlo simulation based on first-principles calculations

Caimu Wang, Renyi Li and Wei Guo*



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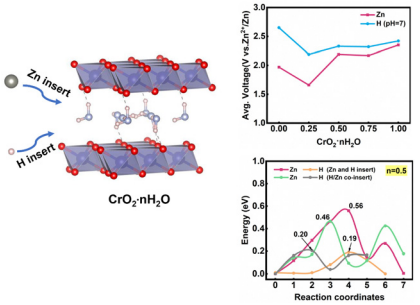
23811

Layered $CrO_2{\cdot}nH_2O$ as a cathode material for aqueous zinc-ion batteries: *ab initio* study

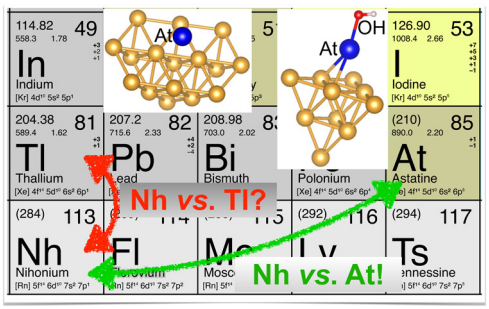
Lu Liu, Zixi He, Binghan Wu, Hongjia Song,* Xiangli Zhong, Jinbin Wang, Daifeng Zou and Juanjuan Cheng*



23823

Uncovering chemical homology of superheavy elements: a close look at astatine

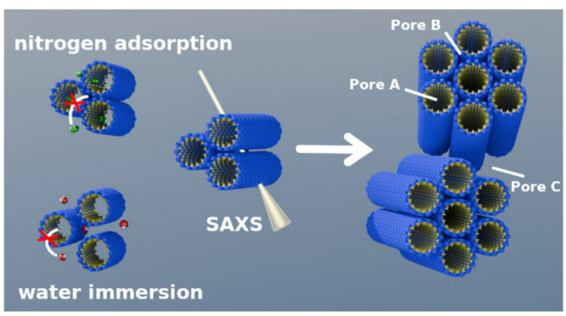
Yuriy A. Demidov, Alexander A. Shalaevsky, Alexander V. Oleynichenko and Alexander A. Rusakov*



23835

Dried hybrid imogolite nanotubes as solids with a changeable surface area: an insight into textural properties based on the correlation between nitrogen gas adsorption, immersion calorimetry into water, and small angle X-ray scattering

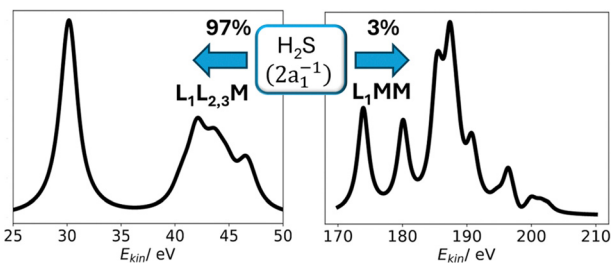
Ali Dhaini, Amine Geneste, Fadwa Alfadel Raad, Pierre Picot, Gaelle Martin-Gassin, Benedicte Prelot, Pierre-Marie Gassin, Philippe Trens, Antoine Thill* and Jerzy Zajac*



23846

Ab initio treatment of molecular Coster–Kronig decay using complex-scaled equation-of-motion coupled-cluster theory

Jan Philipp Drennhaus, Anthuan Ferino-Pérez, Florian Matz and Thomas-C. Jagau*



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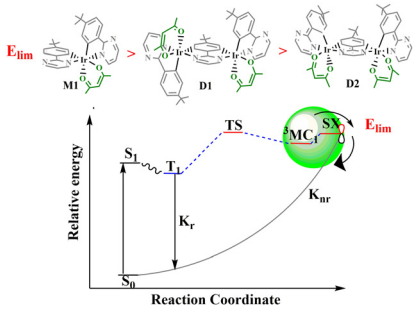

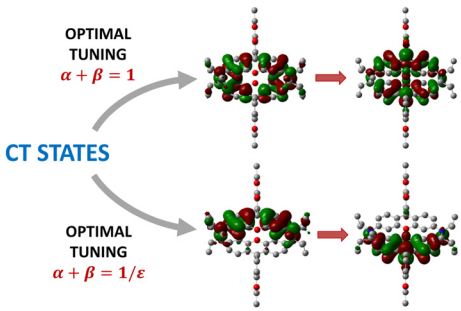

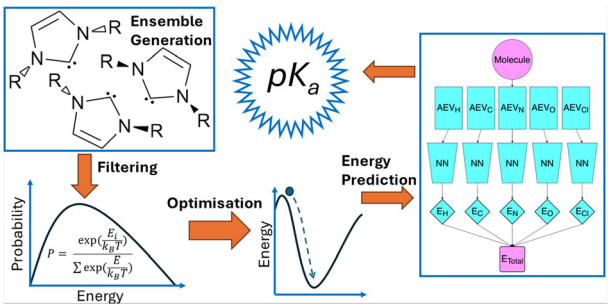

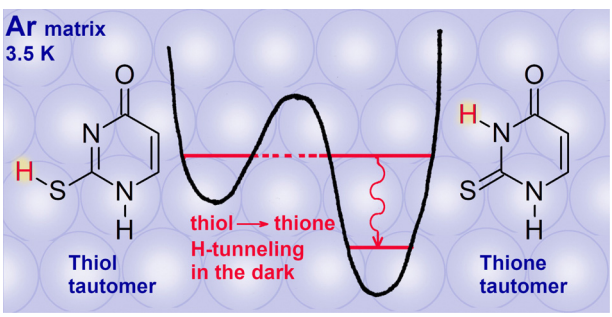

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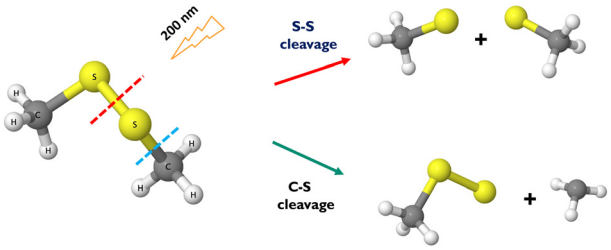

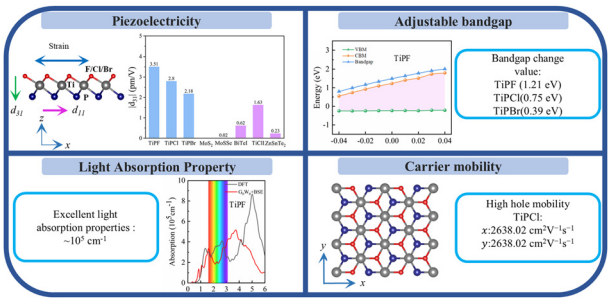

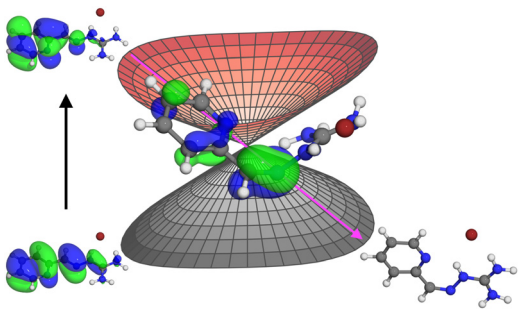

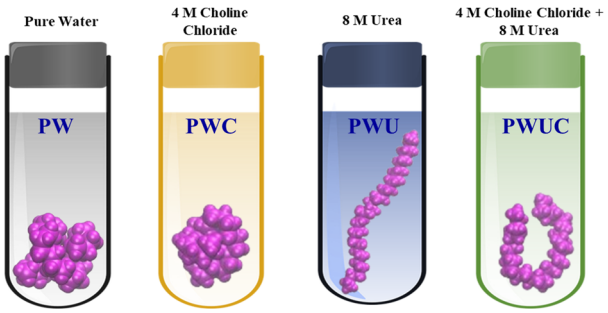

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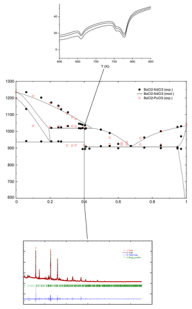
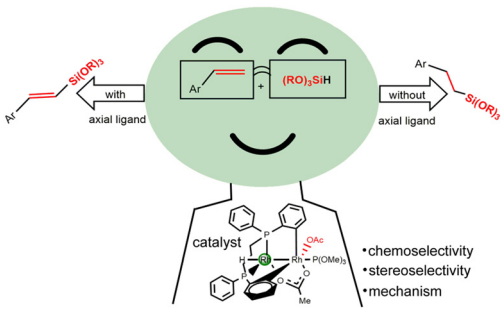
24041



Experimental investigation and thermodynamic modelling assessment of the $AECl_2$–$NdCl_3$ (AE = Sr, Ba) systems

D. C. Alders, D. J. Cette, R. J. M. Konings and A. L. Smith*

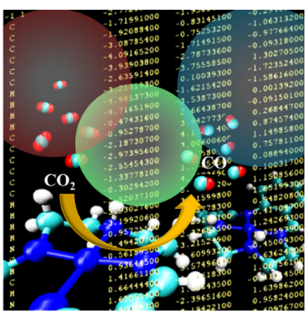
24058



Dirhodium(II) complex catalyzed dehydrosilylation of styrenes: theoretical investigations on the mechanism, selectivity, and ligand effects

Ziying Zhong, Qingzhong Li and Xiaoyan Li*

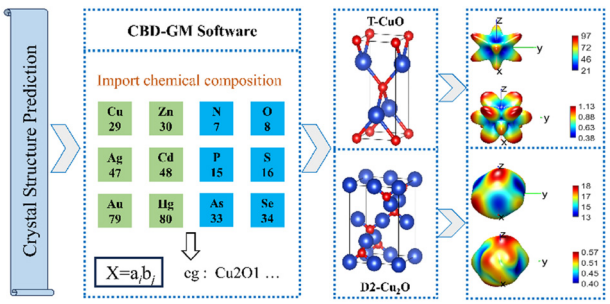
24068



Theoretical study of electrochemical reduction of CO_2 to CO using a nickel-N_4-Schiff base complex

Wilasinee Santiwarodom, Pavee Apilardmongkol, Thanawit Kuamit and Vudhichai Parasuk*

24078



Crystal structure prediction and property calculation of copper–oxygen compounds using innovative search software from first principles

Jinrong Huo, Kai Zhang, Pengfei Liu, Haocong Wei and Chaozheng He*

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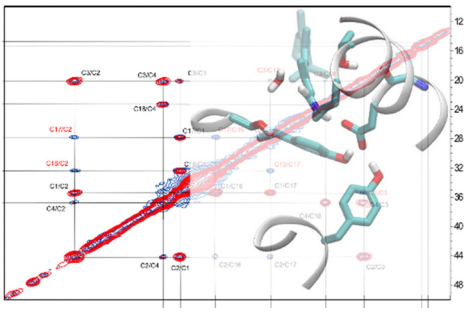

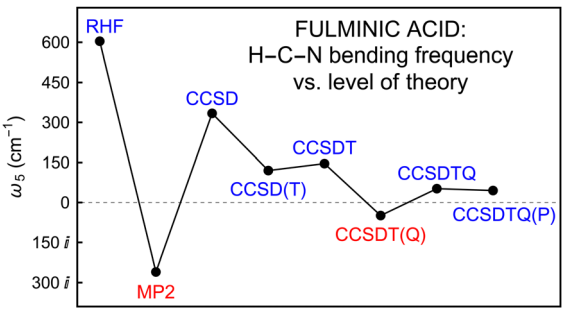

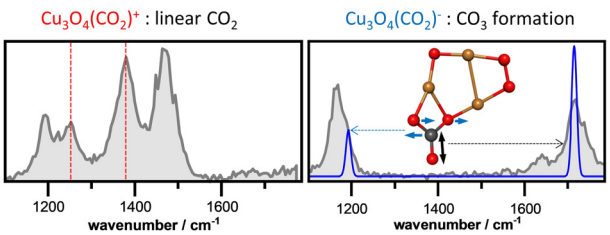

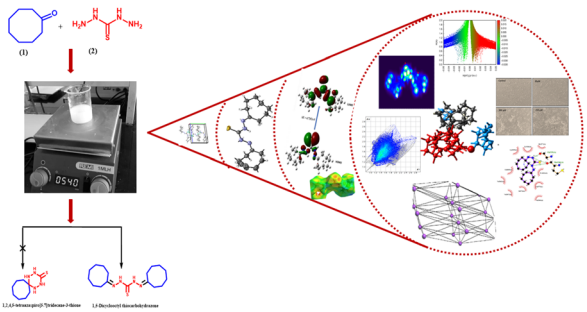

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CORRECTION

24189

Correction: Novel germanene–arsenene and germanene–antimonene lateral heterostructures: interline-dependent electronic and magnetic properties

Chu Viet Ha, Bich Ngoc Nguyen Thi, Pham Quynh Trang, R. Ponce-Pérez, J. Guerrero-Sanchez and D. M. Hoat*