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EDITORIAL

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Molecular dynamics in the gas phase

Henning Zettergren* and Alicja Domaracka

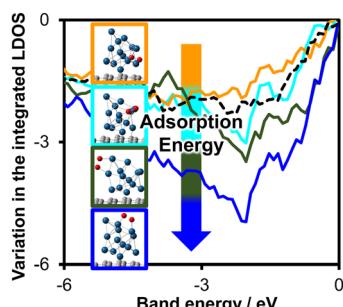


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Characterization of changes in the electronic structure of platinum sub-nanoclusters supported on graphene induced by oxygen adsorption

Hinoki Hirase, Kenji Iida* and Jun-ya Hasegawa*



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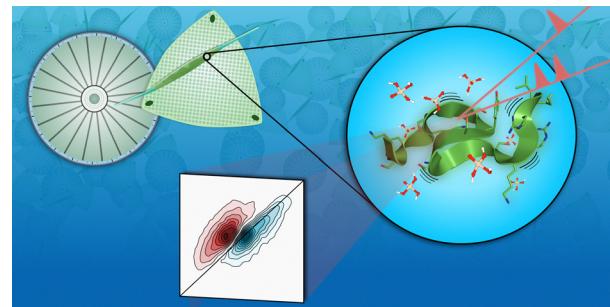
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The secondary structure of diatom silaffin peptide R5 determined by two-dimensional infrared spectroscopy

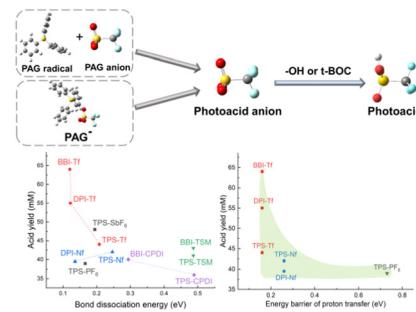
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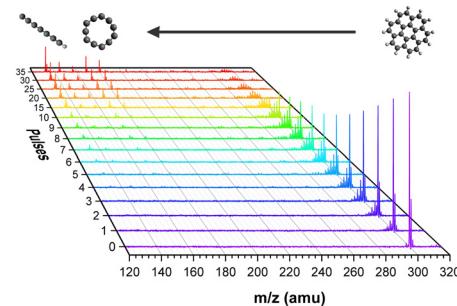
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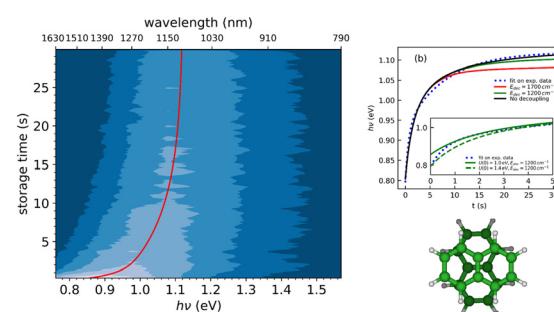
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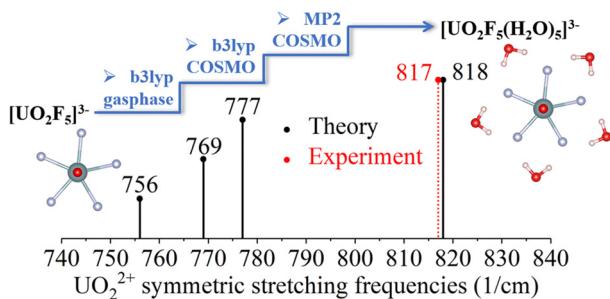
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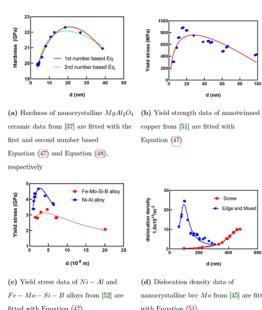
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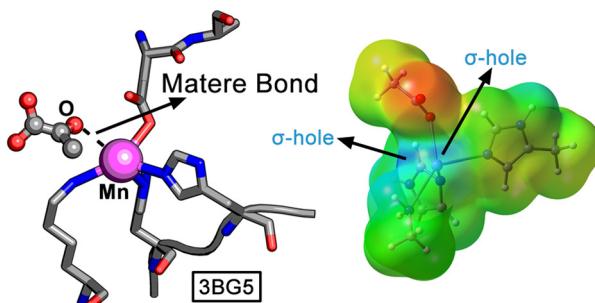
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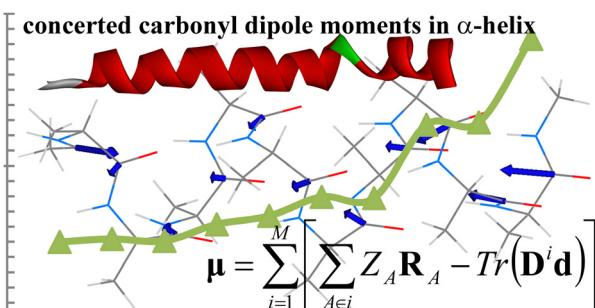
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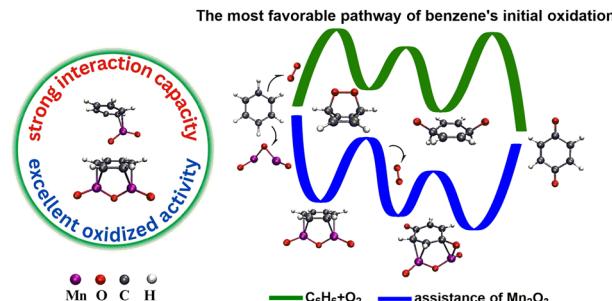


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A theoretical study of the oxidation of benzene by manganese oxide clusters: formation of quinone intermediates

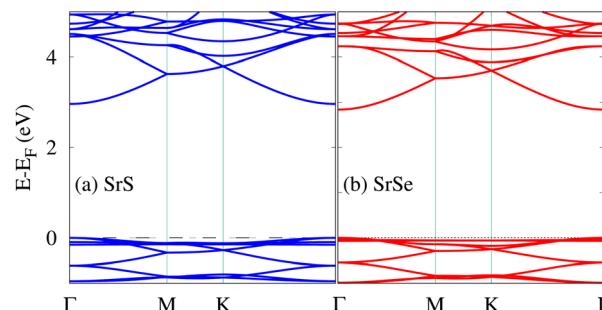
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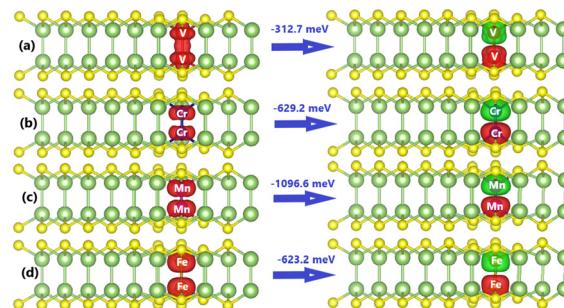
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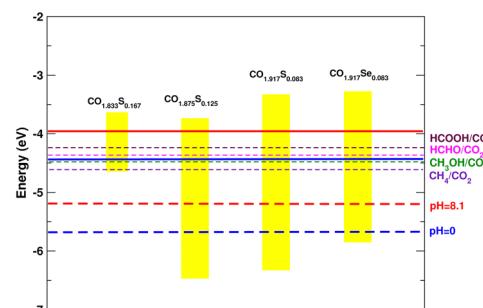
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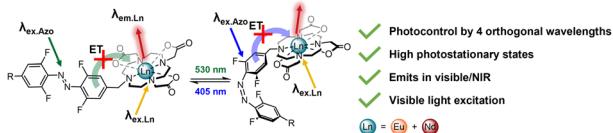
Exploration of isoelectronic substitution in graphene dioxide for photocatalytic and photovoltaic applications – an *ab-initio* study

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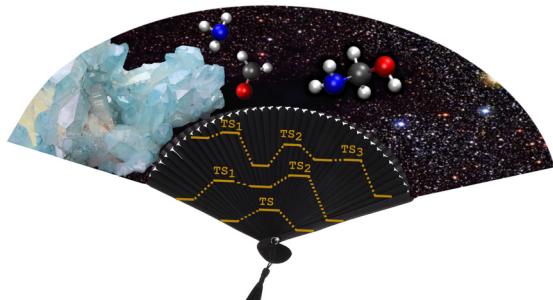
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Photoswitchable luminescent lanthanide complexes controlled and interrogated by four orthogonal wavelengths of light

Charlie H. Simms, Villads R. M. Nielsen, Thomas Just Sørensen, Stephen Faulkner* and Matthew J. Langton*

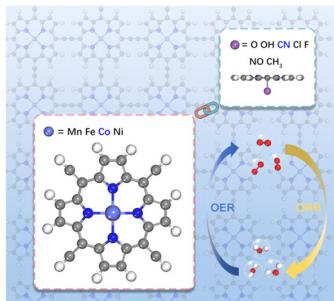
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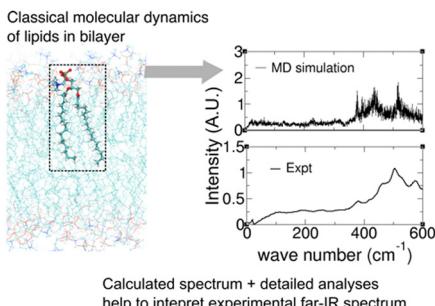
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Bifunctional oxygen reduction/evolution reaction electrocatalysts achieved by axial ligand modulation on two-dimensional porphyrin frameworks

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Molecular dynamics simulations reliably identify vibrational modes in far-IR spectra of phospholipids

Choon-Peng Chng, Annette Dowd, Adam Mechler* and K. Jimmy Hsia*

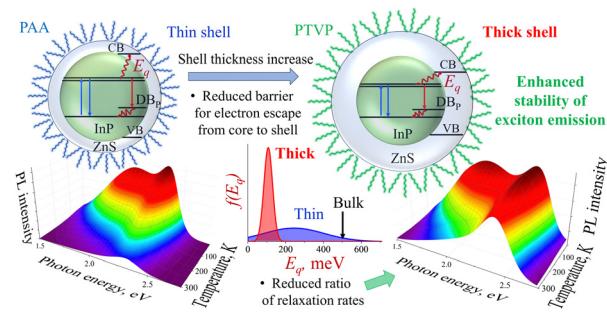


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Thermally assisted optical processes in InP/ZnS quantum dots

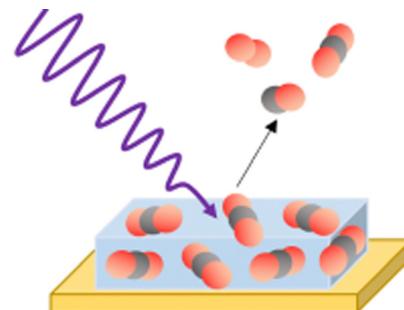
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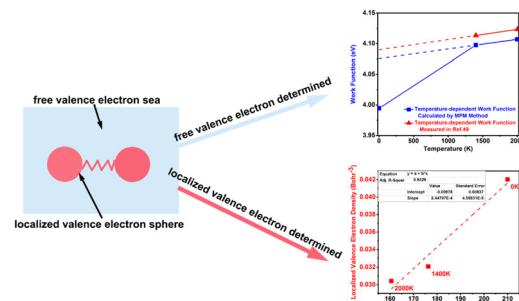
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Temperature-dependent work function, thermionic emission and bulk modulus of TiC: a study on the identification of free valence electrons and localized valence electrons and their roles played in carbides

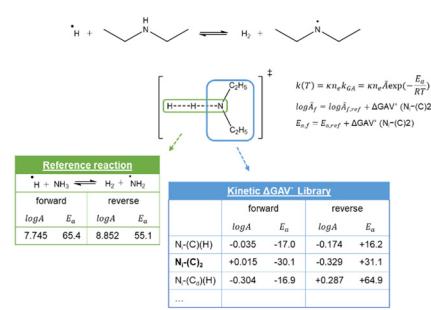
Guomin Hua,* Patricio Mendez and Xinglong Dong



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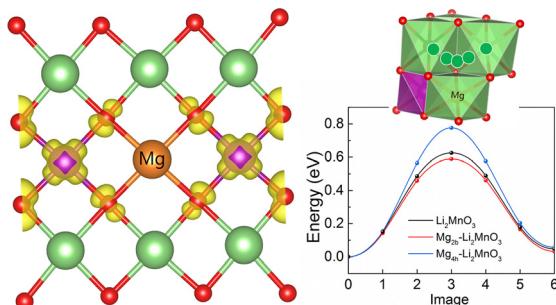
Modeling the kinetics of hydrogen abstraction reactions in nitrogen-containing compounds via group additivity

Cato A. R. Pappijn, Ruben Van de Vijver,
Maarten K. Sabbe, Marie-Françoise Reyniers,
Guy B. Marin and Kevin M. Van Geem*



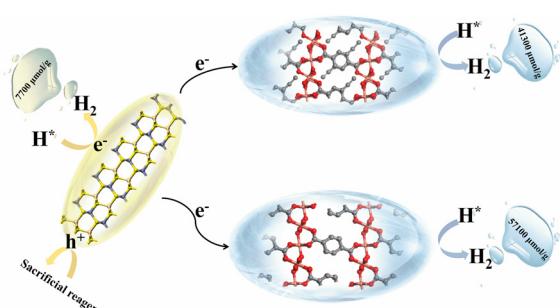
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**Understanding the electrochemical properties of Mg-doped Li_2MnO_3 : first-principles calculations**

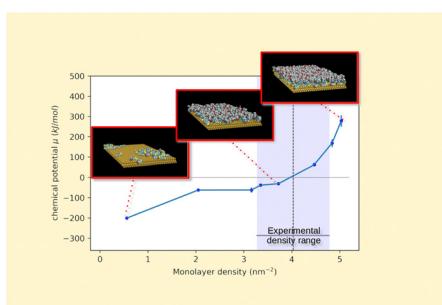
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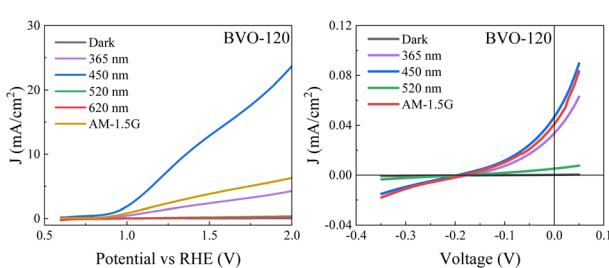
Youlin Wu, Yiming Xie and Zhiliang Jin*

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Lei Shi, Wenyue Zhao, Nan Zhang, Zhao Wang, Wenjing Hua, Xiaoxia Yang, Weidong Fei* and Yu Zhao*

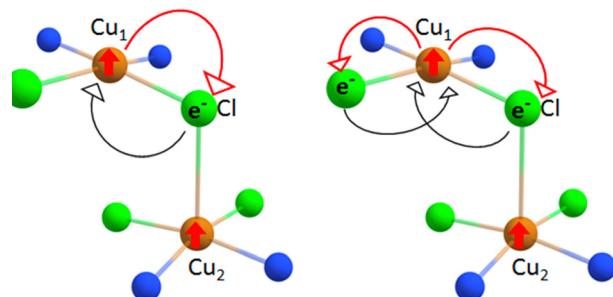


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Investigation of the exact spin channels in laser-induced spin dynamics in two mononuclear Cu(II) complexes

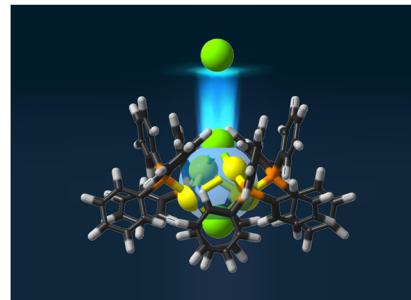
Bharadwaj Chowdary Mummaneni, Sihuai Chen, Wolfgang Hübner and Georgios Lefkidis*



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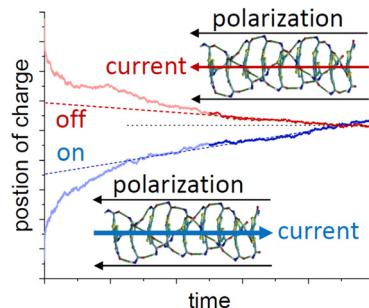
Raul Guajardo-Maturana, Peter. L. Rodriguez-Kessler and Alvaro Muñoz-Castro*



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Theory for nonlinear conductivity switching in semiconducting organic ferroelectrics

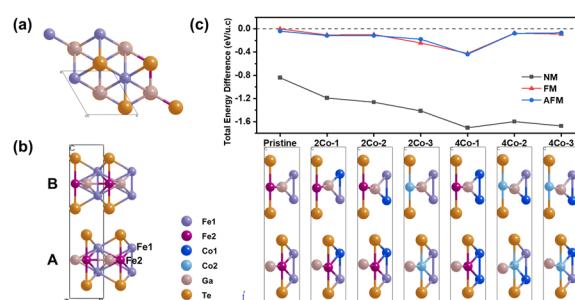
Till Johann, Weiwei Xie, Sara Roosta, Marcus Elstner and Martijn Kemerink*



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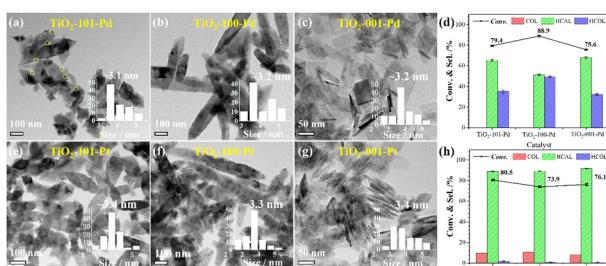
Tuning the magnetic properties of van der Waals Fe_3GaTe_2 crystals by Co doping

Jie Yu, Wen Jin, Gaojie Zhang, Hao Wu, Bichen Xiao, Li Yang and Haixin Chang*



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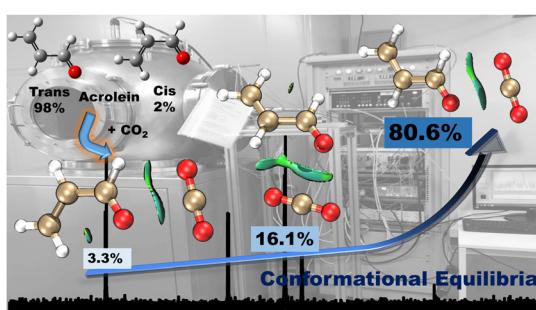
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The nature of crystal facet effect of TiO₂-supported Pd/Pt catalysts on selective hydrogenation of cinnamaldehyde: electron transfer process promoted by interfacial oxygen species

Jia-Feng Zhou, Bo Peng,* Meng Ding, Bing-Qian Shan, Yi-Song Zhu, Laurent Bonneviot, Peng Wu and Kun Zhang*

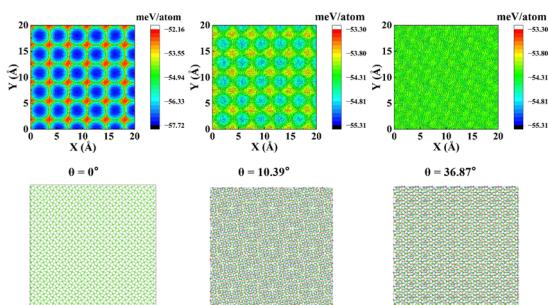
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Conformational equilibria in acrolein–CO₂: the crucial contribution of n → π* interactions unveiled by rotational spectroscopy

Hao Wang, Junhua Chen, Xiao Tian, Chenxu Wang, Junlin Lan, Xingchen Liu, Zhenhua Zhang, Xiaodong Wen and Qian Gou*

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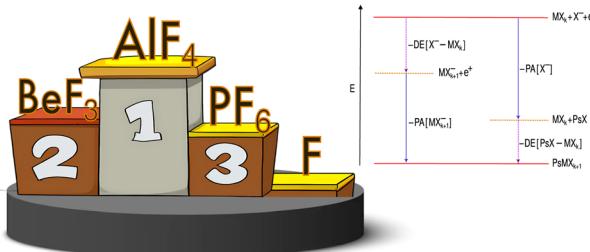


Structural superlubricity at the interface of penta-BN₂

Hao Wang, Hanyue Zhang, Xinqi Zhang, Tengfei Cao, Junqi Shi* and Xiaoli Fan*

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There is a new Ps binding super champion!



Electron superhalogens as positronium superhalogens

Rafael Porras-Roldan, Felix Moncada, Jorge Charry, Marcio Varella, Roberto Flores-Moreno and Andrés Reyes*

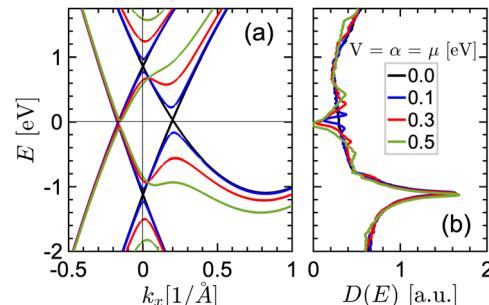


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Electronic phase transition in bilayer *P6mmm* borophene

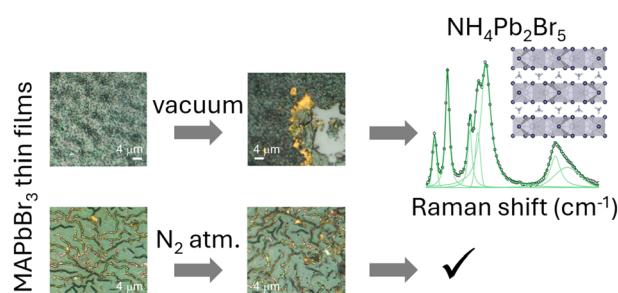
Nguyen N. Hieu, Huynh V. Phuc and Bui D. Hoi*



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Physical and chemical properties and degradation of MAPbBr_3 films on transparent substrates

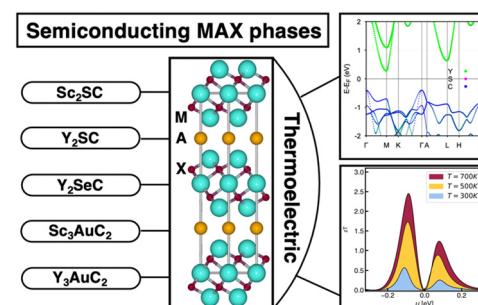
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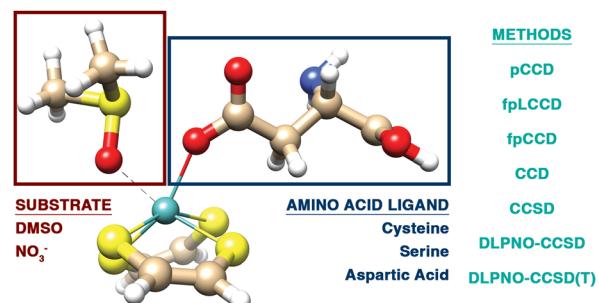
Mohammad Khazaei,* Iraj Maleki,* Namitha Anna Koshi, Ahmad Ranjbar, Nanxi Miao, Junjie Wang,* Rasoul Khaledalidusti, Thomas D. Kühne, Seung-Cheol Lee, Satadeep Bhattacharjee, Hamid Hosano, S. Mehdi Vaez Allaei, Keivan Esfarjani and Kaoru Ohno



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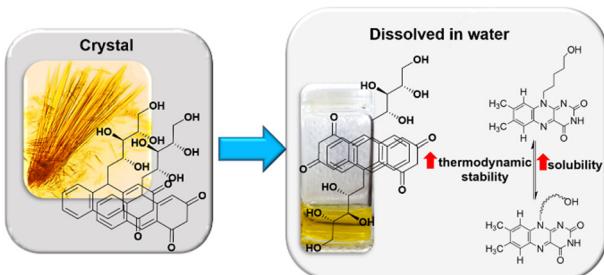
Delving into the catalytic mechanism of molybdenum cofactors: a novel coupled cluster study

Marta Gatyńska,* Matheus Morato F. de Moraes,* Paweł Tecmer and Katharina Boguslawski*



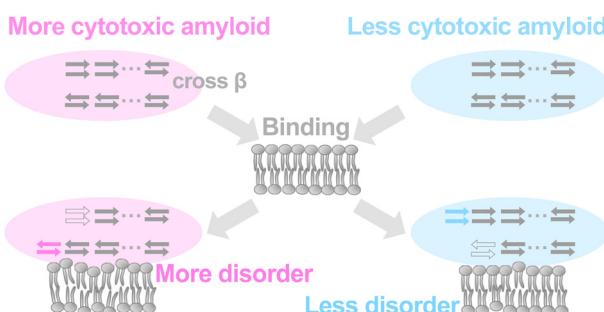
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**Self-association as a solubility limiting factor of riboflavin in aqueous media**

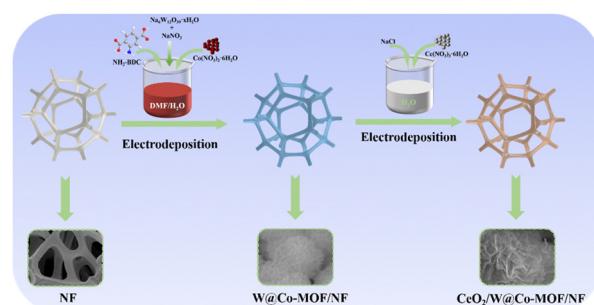
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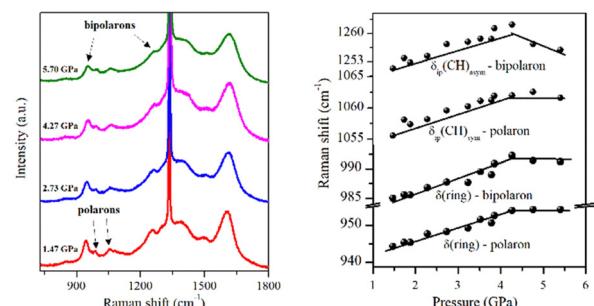
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**Facile synthesis of CeO₂-decorated W@Co-MOF heterostructures as a highly active and durable electrocatalyst for overall water splitting**

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Adam Mizera,* Sylwia Zięba, Michał Bielejewski, Alina T. Dubis and Andrzej Łapiński*

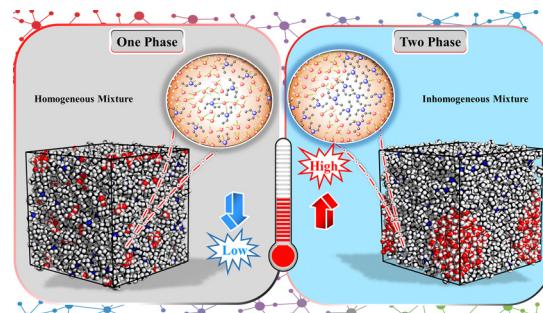


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Unraveling the interplay of temperature with molecular aggregation and miscibility in TEA–water mixtures

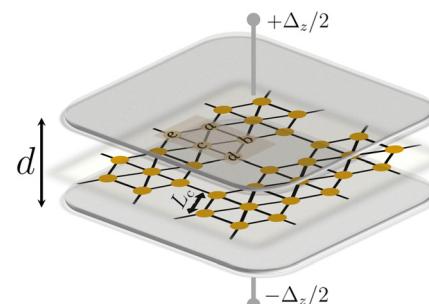
Ravi Singh, Jiwon Seo, Jonghyuk Ryu and Jun-Ho Choi*



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Electron–phonon coupling effect on the optical absorption of gated β_{12} -borophene

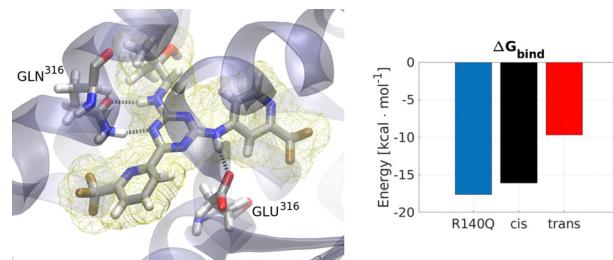
Tran Cong Phong, Huynh V. Phuc and Le T. T. Phuong*



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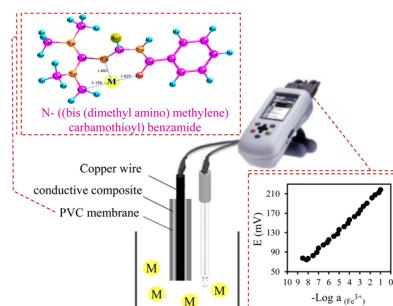
Erik Lindahl, Erik Arvidsson and Ran Friedman*



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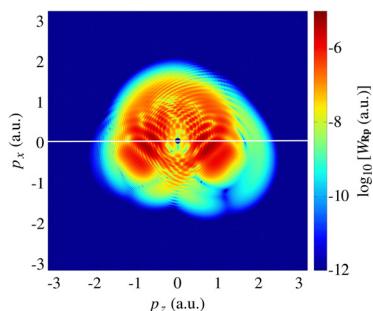
Comparison of selectivity and sensitivity of various ferric selective electrodes prepared using *N*-(*bis*(dimethyl amino)methylene)carbamothioyl)benzamide

Mehrdad Ghaemi, Leila Hajiaghbabaei,* Jamshid Najafpour, Ashraf Sadat Shahvelayati and Ramin M. A. Tehrani



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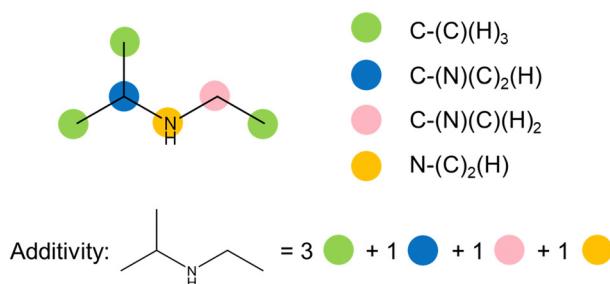
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High-order above-threshold ionisation of diatomic molecules by few-cycle bicircular and orthogonally polarised two-colour pulses

Dino Habibović,* Abdulah S. Jašarević,
Mustafa Busuladžić and Dejan B. Milošević

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Modeling the thermochemistry of nitrogen-containing compounds *via* group additivity

Cato A. R. Pappijn, Ruben Van de Vijver,
Marie-Françoise Reyniers, Maarten K. Sabbe,
Guy B. Marin and Kevin M. Van Geem*

