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Cover

See Kenji Iida, Jun-ya Hasegawa *et al.*, pp. 18530–18537. Image reproduced by permission of Kenji Iida and Jun-ya Hasegawa from *Phys. Chem. Chem. Phys.*, 2024, 26, 18530.



Inside cover

See Thomas L. C. Jansen, Tobias Weidner *et al.*, pp. 18538–18546. Image reproduced by permission of Inge Heise Thomassen from *Phys. Chem. Chem. Phys.*, 2024, 26, 18538.

EDITORIAL

18529

Molecular dynamics in the gas phase

Henning Zettergren* and Alicja Domaracka

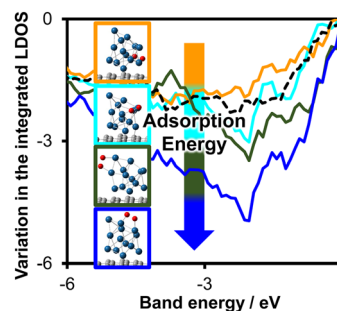


RESEARCH PAPERS

18530

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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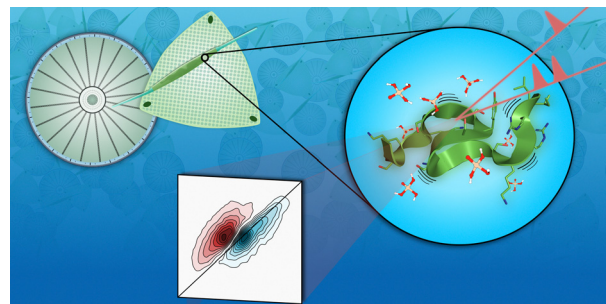


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18538

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

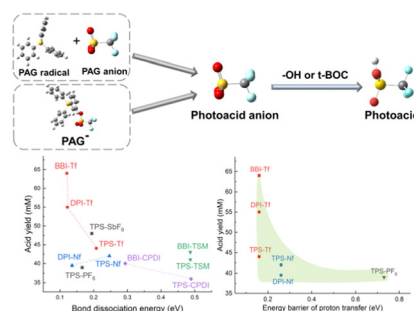
Asger Berg Thomassen, Thomas L. C. Jansen* and Tobias Weidner*



18547

Mechanisms of acid generation from ionic photoacid generators for extreme ultraviolet and electron beam lithography

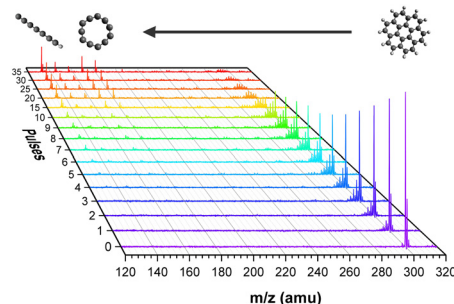
Chengbin Fu, Kun Du, Jie Xue, Hanshen Xin, Jianhua Zhang and Haoyuan Li*



18557

Laser-induced fragmentation of coronene cations

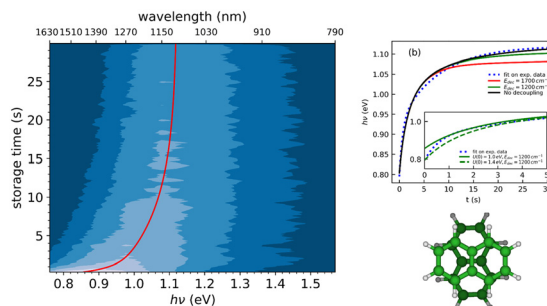
Sanjana Panchagnula, Jerry Kamer, Alessandra Candian, Helgi R. Hrodmarsson, Harold Linnartz, Jordy Bouwman* and Alexander G. G. M. Tielens



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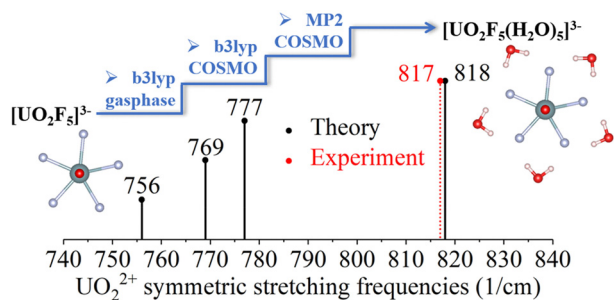
Near-infrared absorption and radiative cooling of naphthalene dimers ($C_{10}H_8$)₂

Jérôme Bernard,* Serge Martin, Abdulaziz Al-Mogeeth, Christine Joblin, MingChao Ji, Henning Zettergren, Henrik Cederquist, Mark H. Sockett, Suvasthika Indrajith, Léo Dontot, Fernand Spiegelman, Dominique Toubanc and Mathias Rapacioli



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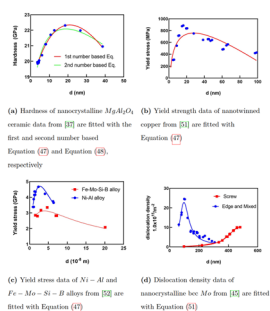
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Systematic Raman spectroscopic study of the complexation of uranyl with fluoride

Yating Yang, Qian Liu,* Youshi Lan, Qianci Zhang, Liyang Zhu, Suliang Yang, Guoxin Tian, Xiaoyan Cao* and Michael Dolg*

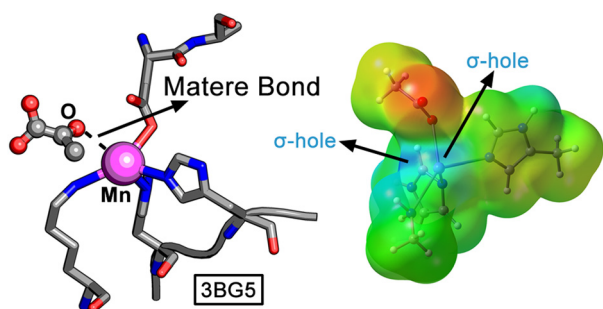
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Dislocation phenomena described with free volume concept and Eyring's rate process theory

Tian Hao* and Ting Hao

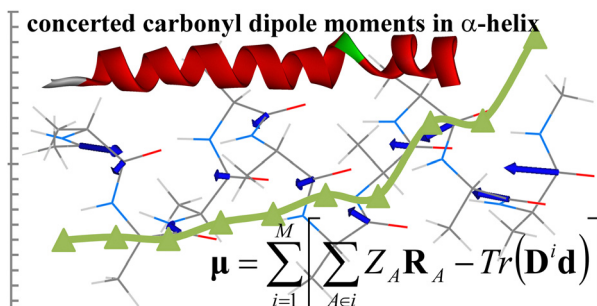
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Manganese mater bonds in biological systems: PDB inspection and DFT calculations

Sergi Burguera, Akshay Kumar Sahu, Michael Jordan Chávez Romero, Himansu S. Biswal* and Antonio Bauzá*

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Partition analysis of dipole moments in solution applied to functional groups in polypeptide motifs

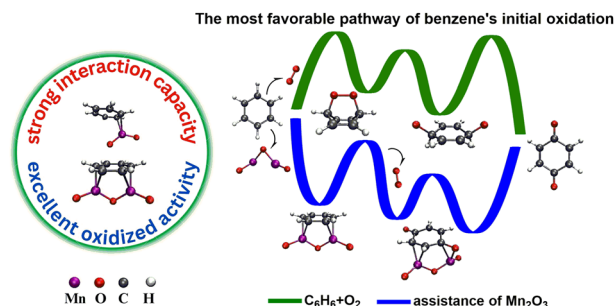
Dmitri G. Fedorov



18629

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

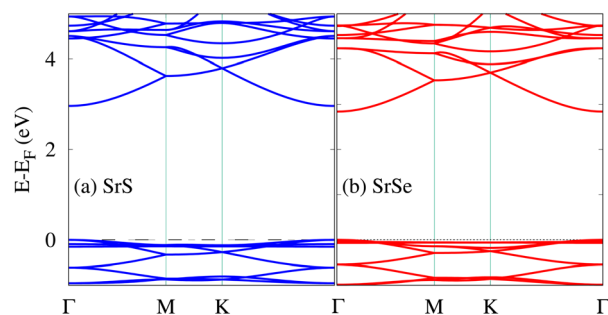
Giang Huong Thi Vu, Thuy Thi Phan, Tho Huu Nguyen, Thang Minh Le, Minh Tho Nguyen and Hue Minh Thi Nguyen*



18649

Stability and electronic, phononic, thermal and optical properties of SrX (X = S, Se) nanosheets based on AIMD and DFT computations

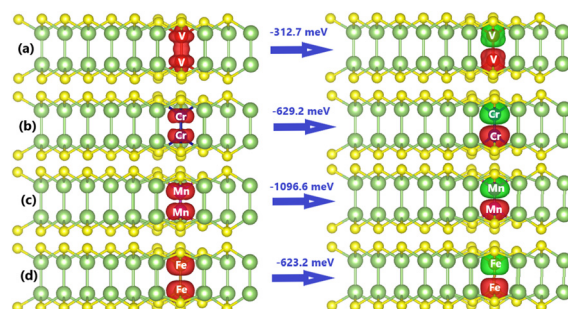
Nzar Rauf Abdullah,* Botan Jawdat Abdullah,* Rangeen Othman Salih, Hemn Gharib Hussein and Vidar Gudmundsson



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Antiferromagnetism in GaS monolayer doped with TM–TM atom pairs (TM = V, Cr, Mn, and Fe)

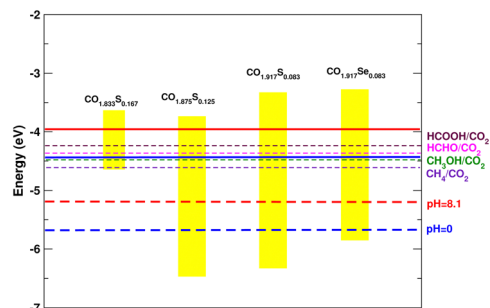
D. M. Hoat,* Nguyen Thanh Tien, Duy Khanh Nguyen and J. Guerrero-Sanchez



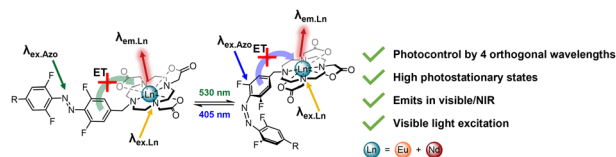
18667

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

Santy M Thomas and P. Ravindran*



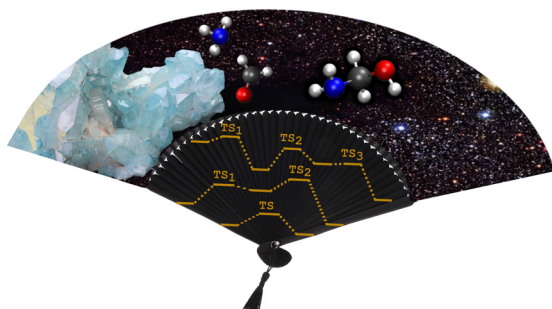
18683



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*

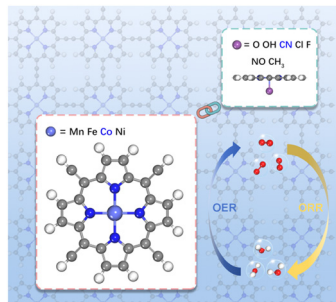
18692



In-depth exploration of catalytic sites on amorphous solid water: I. The astro-synthesis of aminomethanol

Giulia M. Bovolenta, Gabriela Silva-Vera, Stefano Bovino, German Molpeceres, Johannes Kästner and Stefan Vogt-Geisse*

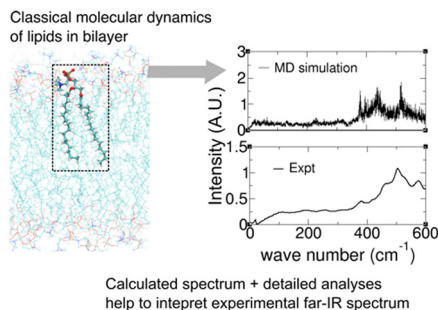
18707



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

Tianze Xu, Tianyang Liu* and Yu Jing*

18715



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

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

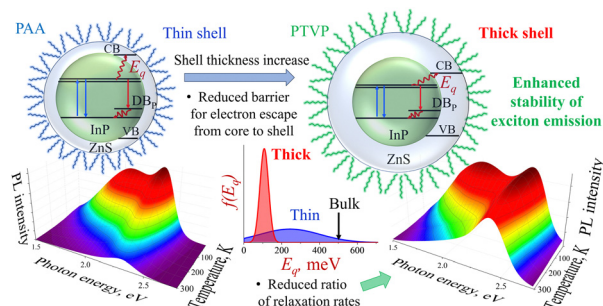


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Thermally assisted optical processes in InP/ZnS quantum dots

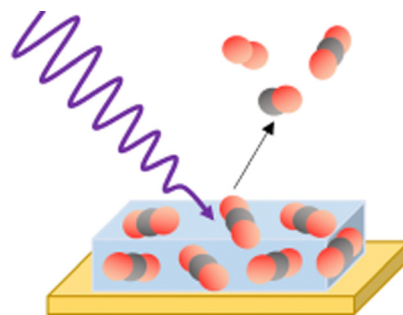
Sergey Savchenko, Alexander Vokhmintsev, Maksim Karabanalov, Yanning Zhang, Ahmed Henaish, Arup Neogi* and Ilya Weinstein



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Flux and fluence effects on the vacuum-UV photodesorption and photoprocessing of CO₂ ices

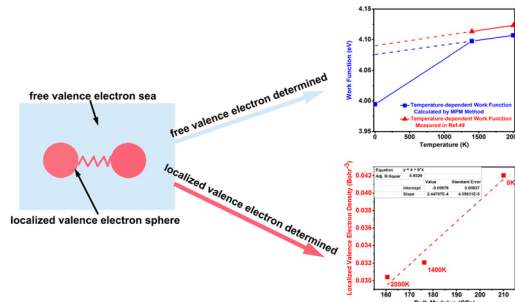
Antoine B. Hacquard,* Daniela Torres-Díaz, Romain Basalgète, Delfina Toulouse, Géraldine Féraud, Samuel Del Fré, Jennifer A. Noble, Laurent Philippe, Xavier Michaut, Jean-Hugues Fillion, Anne Lafosse, Lionel Amiaud and Mathieu Bertin



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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

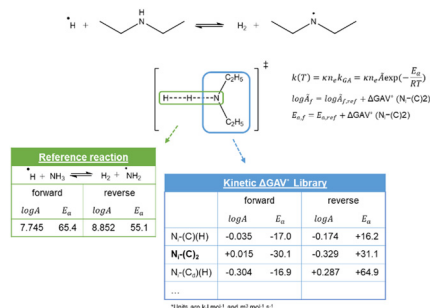
Guomin Hua,* Patricio Mendez and Xinglong Dong



18763

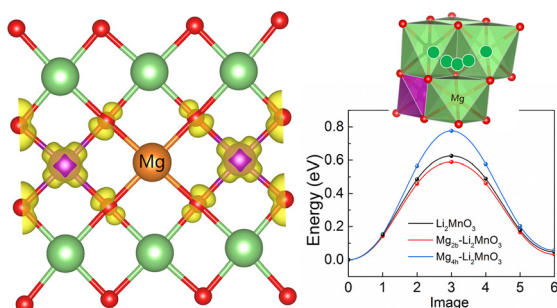
Modeling the kinetics of hydrogen abstraction reactions in nitrogen-containing compounds via group additivity

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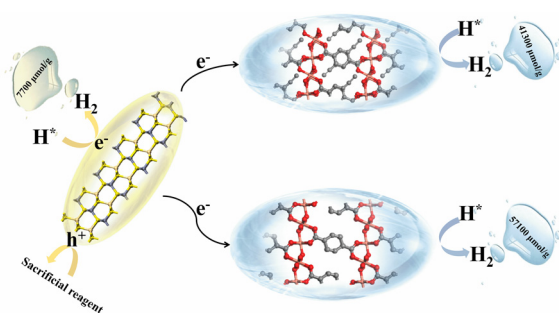
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Understanding the electrochemical properties of Mg-doped Li_2MnO_3 : first-principles calculations

Ziquan Zeng, Jianchuan Wang,* Shiwei Zhang, Bo Han, Feng Dang, Songlin Li and Yong Du

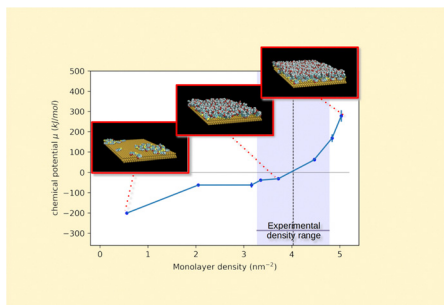
18788



Spherical 2-acetylene-(copper metal–organic framework) preparation and efficient photocatalytic hydrogen evolution over combined bimetallic sulfides

Youlin Wu, Yiming Xie and Zhiliang Jin*

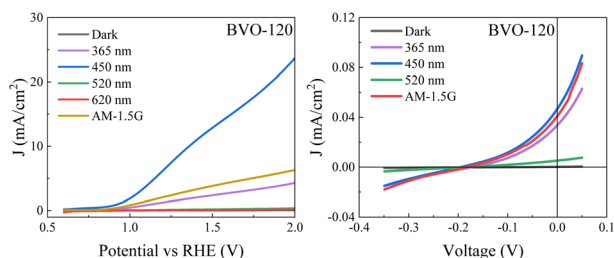
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The thermodynamics of self-assembled monolayer formation: a computational and experimental study of thiols on a flat gold surface

Alberto Zoccante,* Eleonora Cara, Federico Ferrarese Lupi, Philipp Hönicke, Yves Kayser, Burkhard Beckhoff, Petr Klapetek, Davide Marchi and Maurizio Cossi

18808



Photovoltaic-enhanced water splitting properties of low-temperature-synthesized BiVO_4 photoanode films

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

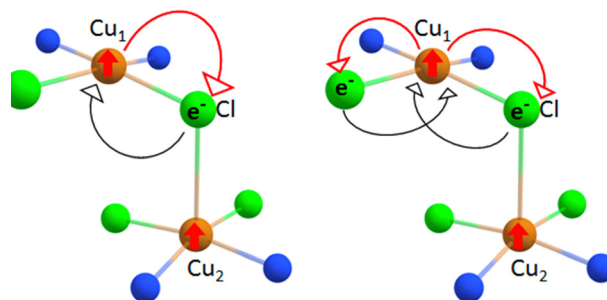


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Investigation of the exact spin channels in laser-induced spin dynamics in two mononuclear Cu(II) complexes

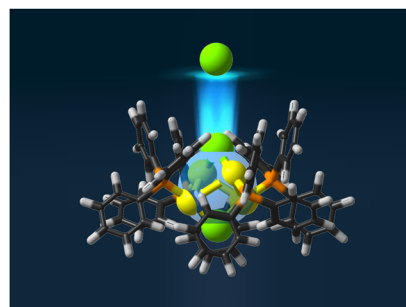
Bharadwaj Chowdary Mummaneni, Sihuai Chen, Wolfgang Hübner and Georgios Lefkidis*



18828

On the halide aggregation into the $[\text{Au}_4(\text{PPh}_3)_4]^{4+}$ cluster core. Insights from structural, optical and interaction energy analysis in $[(\text{Ph}_3\text{PAu})_4\text{X}_2]^{2+}$ and $[(\text{Ph}_3\text{PAu})_4\text{X}]^{3+}$ species ($\text{X} = \text{Cl}^-, \text{Br}^-, \text{I}^-$)

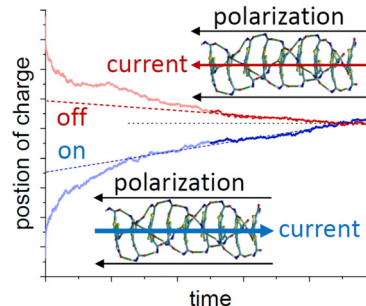
Raul Guajardo-Maturana, Peter. L. Rodríguez-Kessler and Alvaro Muñoz-Castro*



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Theory for nonlinear conductivity switching in semiconducting organic ferroelectrics

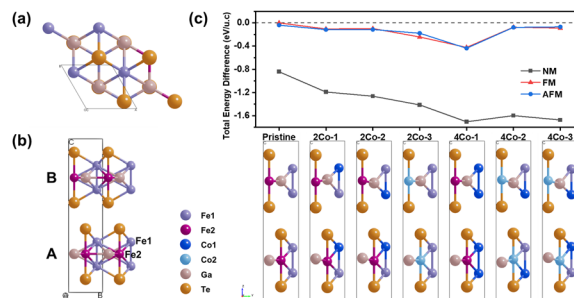
Till Johann, Weiwei Xie, Sara Roosta, Marcus Elstner and Martijn Kemerink*



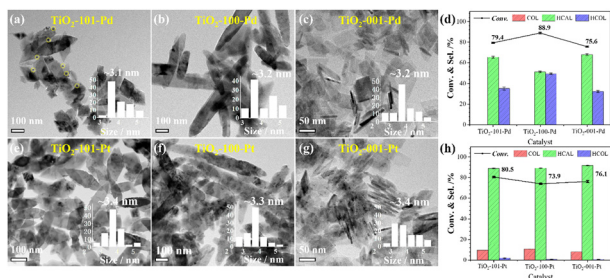
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Tuning the magnetic properties of van der Waals Fe_3GaTe_2 crystals by Co doping

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



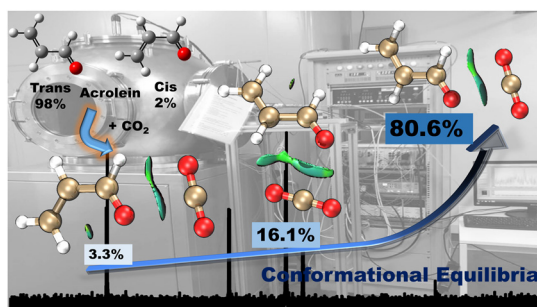
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The nature of crystal facet effect of TiO₂-supported Pd/Pt catalysts on selective hydrogenation of cinnamaldehyde: electron transfer process promoted by interfacial oxygen species

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

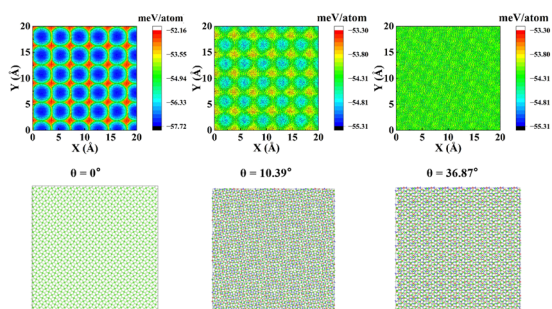
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Conformational equilibria in acrolein–CO₂: the crucial contribution of n → π* interactions unveiled by rotational spectroscopy

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

18871

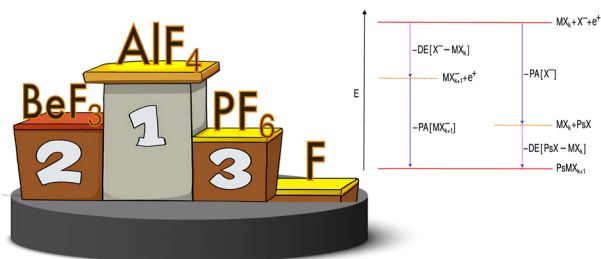


Structural superlubricity at the interface of penta-BN₂

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*

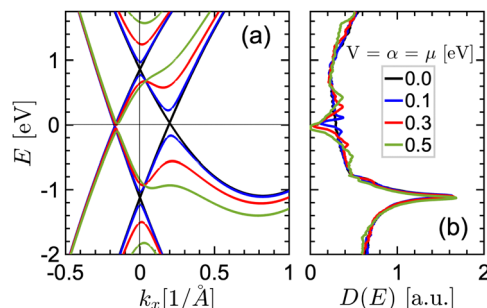


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Electronic phase transition in bilayer $P6mmm$ borophene

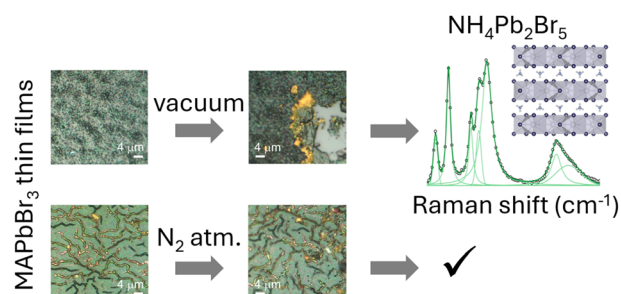
Nguyen N. Hieu, Huynh V. Phuc and Bui D. Hoi*



18898

Physical and chemical properties and degradation of MAPbBr₃ films on transparent substrates

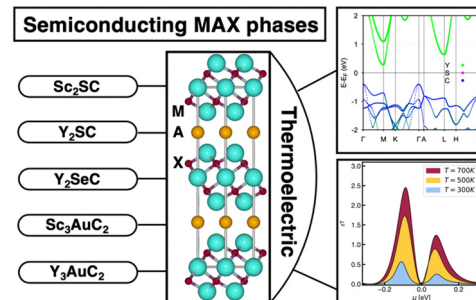
Valentina Carpenella, Fabrizio Messina, Jessica Barichello, Fabio Matteocci, Paolo Postorino, Caterina Petrillo, Alessandro Nucara, Danilo Dini and Claudia Fasolato*



18907

Beyond metals: theoretical discovery of semiconducting MAX phases and their potential application in thermoelectrics

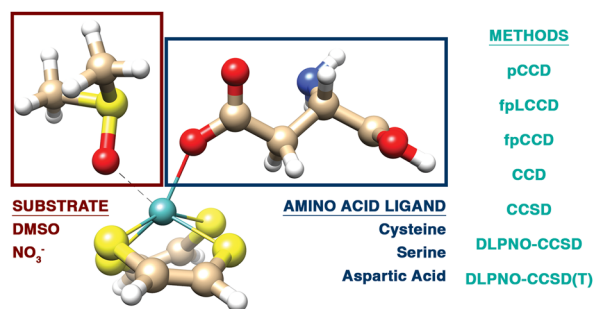
Mohammad Khazaei,* Iraj Maleki,* Namitha Anna Koshi, Ahmad Ranjbar, Nanxi Miao, Junjie Wang,* Rasoul Khaledialidusti, Thomas D. Kühne, Seung-Cheol Lee, Satadeep Bhattacharjee, Hamid Hosano, S. Mehdi Vaez Allaei, Keivan Esfarjani and Kaoru Ohno



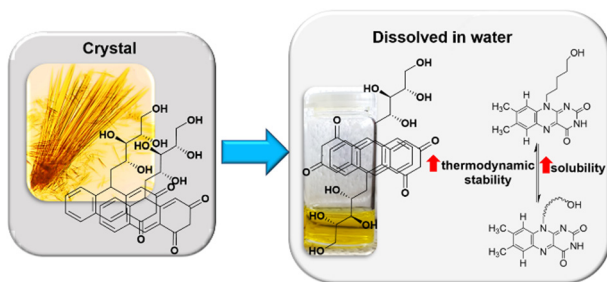
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Delving into the catalytic mechanism of molybdenum cofactors: a novel coupled cluster study

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



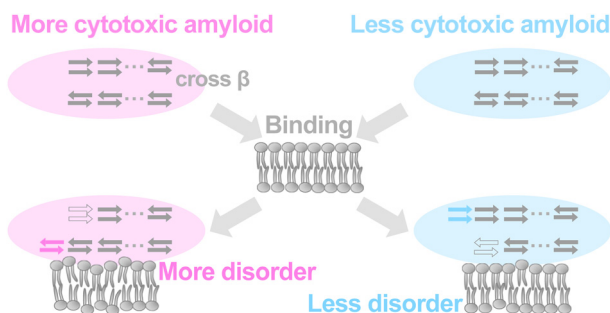
18930



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

Nadja Ulmann,* Johnny Hioe, Didier Touraud, Dominik Horinek and Werner Kunz*

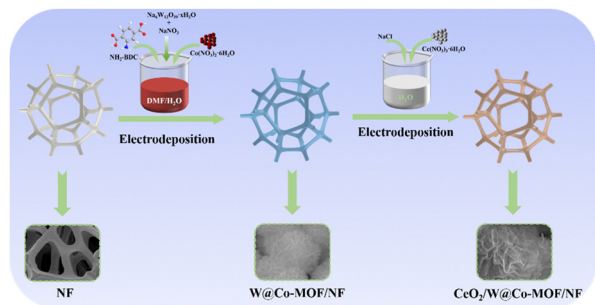
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Phospholipid-induced secondary structural changes of lysozyme polymorphic amyloid fibrils studied using vacuum-ultraviolet circular dichroism

Tatsuhito Matsuo,* Seigi Yamamoto and Koichi Matsuo

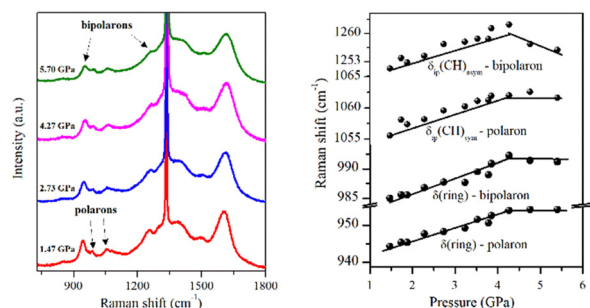
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Facile synthesis of CeO₂-decorated W@Co-MOF heterostructures as a highly active and durable electrocatalyst for overall water splitting

Chang Su, Dan Wang, Wenchang Wang, Naotoshi Mitsuzaki and Zhidong Chen*

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Effect of hydrostatic pressure on charge carriers in a conducting pyrrole-co-poly(pyrrole-3-carboxylic) copolymer

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

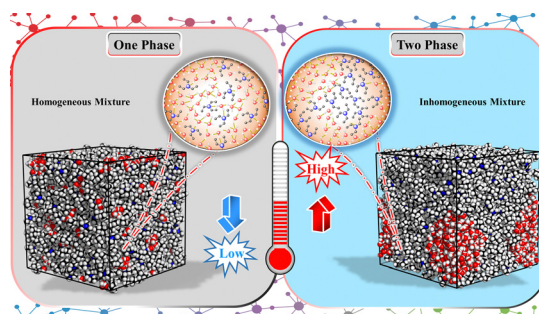


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Unraveling the interplay of temperature with molecular aggregation and miscibility in TEA–water mixtures

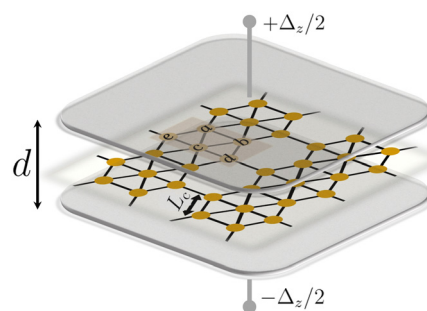
Ravi Singh, Jiwon Seo, Jonghyuk Ryu and Jun-Ho Choi*



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

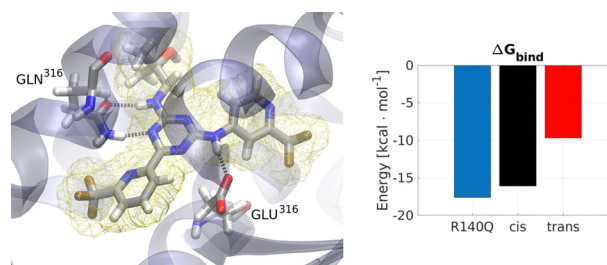
Tran Cong Phong, Huynh V. Phuc and Le T. T. Phuong*



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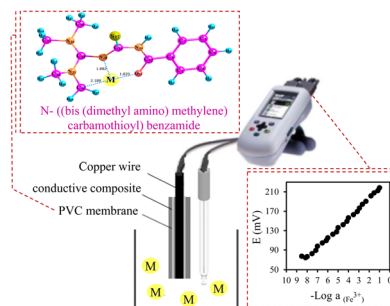
Trans vs. *cis*: a computational study of enasidenib resistance due to IDH2 mutations

Erik Lindahl, Erik Arvidsson and Ran Friedman*

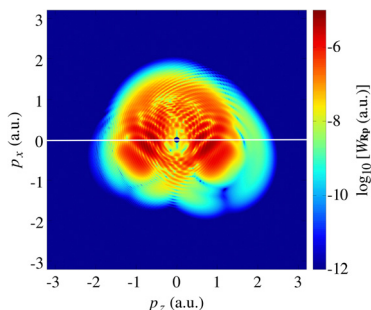


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Comparison of selectivity and sensitivity of various ferric selective electrodes prepared using *N*-((bis(dimethyl amino)methylene)carbamothioyl)benzamide

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

19008



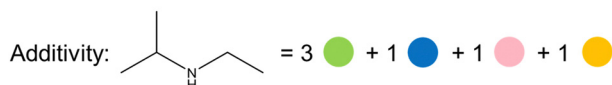
High-order above-threshold ionisation of diatomic molecules by few-cycle bicircular and orthogonally polarised two-colour pulses

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

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- C-(C)(H)₃
- C-(N)(C)₂(H)
- C-(N)(C)(H)₂
- N-(C)₂(H)



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*

