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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

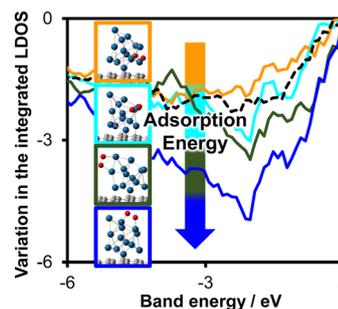


RESEARCH PAPERS

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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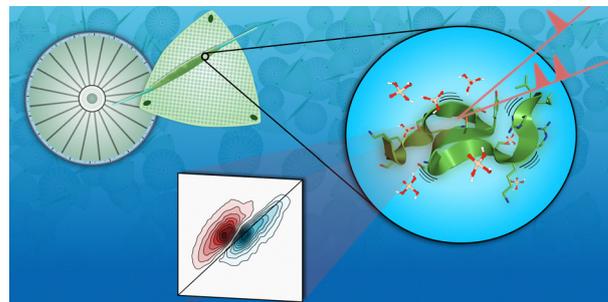


RESEARCH PAPERS

18538

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

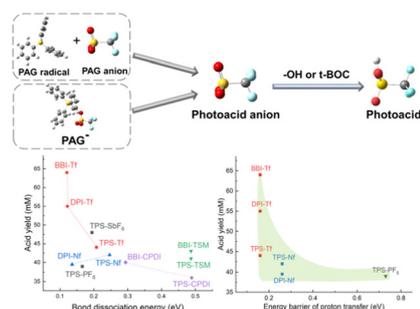
Asger Berg Thomassen, Thomas L. C. Jansen* and Tobias Weidner*



18547

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

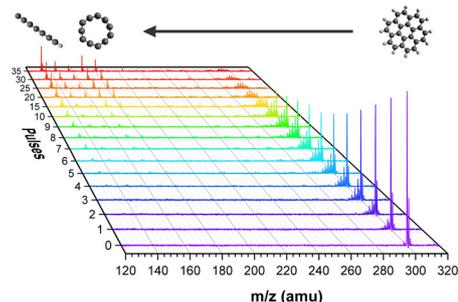
Chengbin Fu, Kun Du, Jie Xue, Hanshen Xin, Jianhua Zhang and Haoyuan Li*



18557

Laser-induced fragmentation of coronene cations

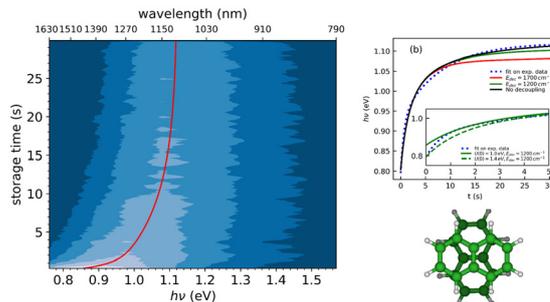
Sanjana Panchagnula, Jerry Kamer, Alessandra Candian, Helgi R. Hrodmarsson, Harold Linnartz, Jordy Bouwman* and Alexander G. G. M. Tielens



18571

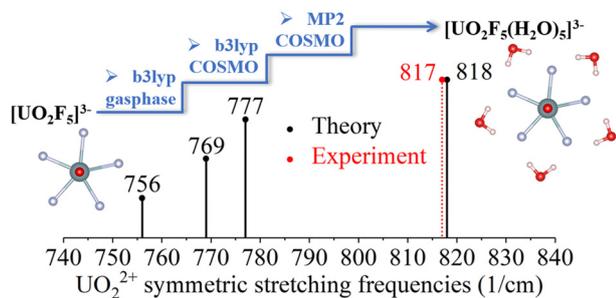
Near-infrared absorption and radiative cooling of naphthalene dimers ($C_{10}H_8$)₂

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



RESEARCH PAPERS

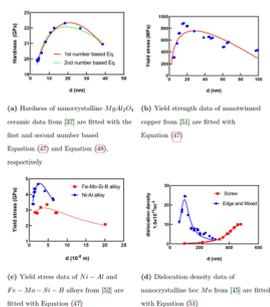
18584



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*

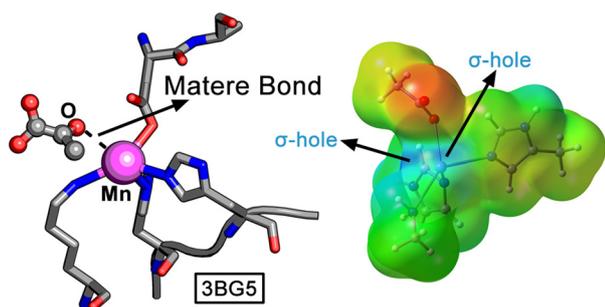
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Dislocation phenomena described with free volume concept and Eyring's rate process theory

Tian Hao* and Ting Hao

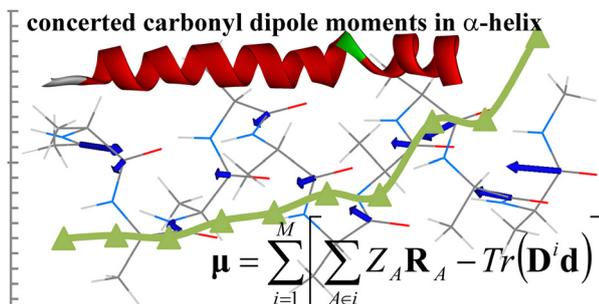
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Manganese matere bonds in biological systems: PDB inspection and DFT calculations

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

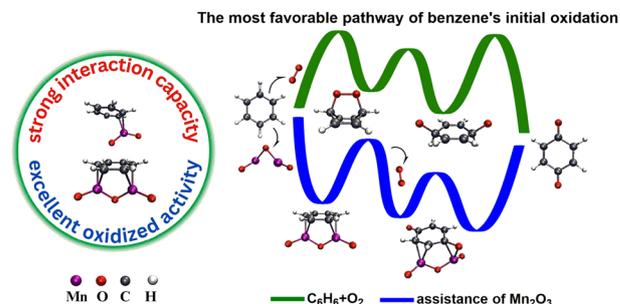
Dmitri G. Fedorov



18629

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

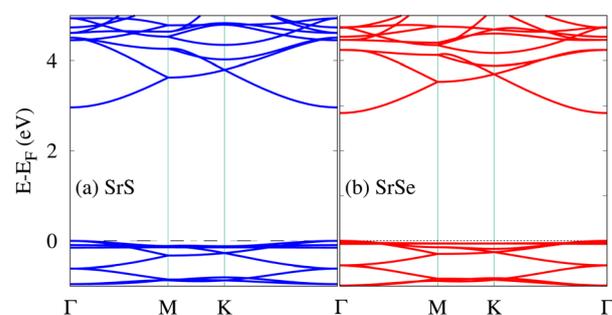
Giang Huong Thi Vu, Thuy Thi Phan, Tho Huu Nguyen, Thang Minh Le, Minh Tho Nguyen and Hue Minh Thi Nguyen*



18649

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

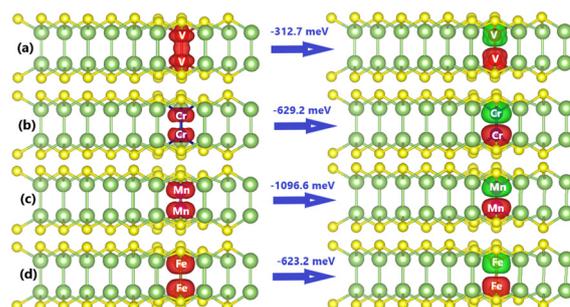
Nzar Rauf Abdullah,* Botan Jawdat Abdullah,* Rangeen Othman Salih, Hemn Gharib Hussein and Vidar Gudmundsson



18657

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

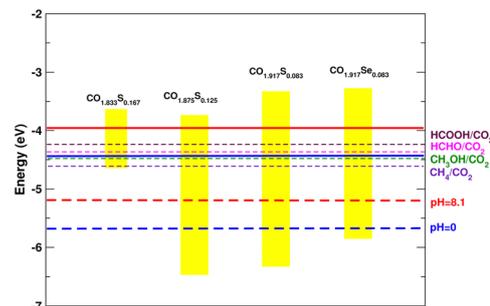
D. M. Hoat,* Nguyen Thanh Tien, Duy Khanh Nguyen and J. Guerrero-Sanchez



18667

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

Santy M Thomas and P. Ravindran*



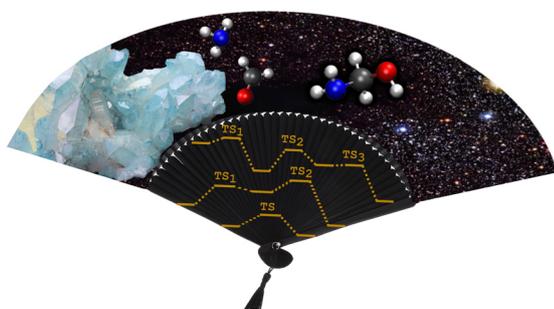
18683



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*

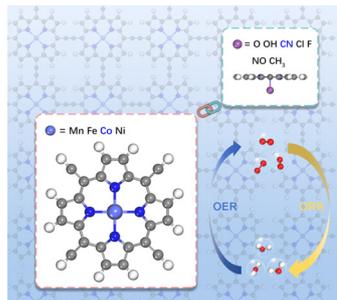
18692



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*

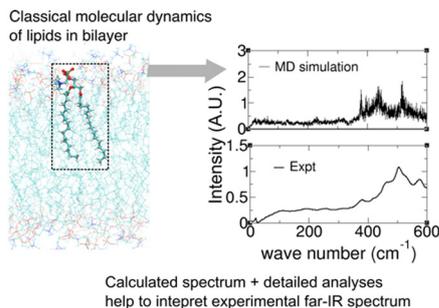
18707



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*

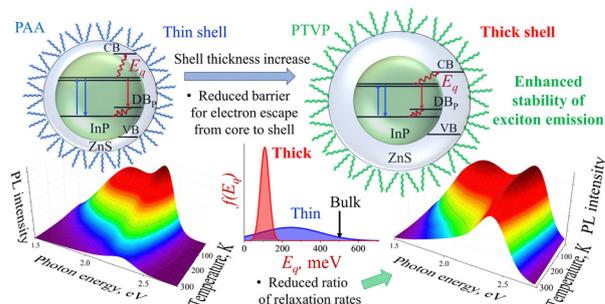


RESEARCH PAPERS

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Thermally assisted optical processes in InP/ZnS quantum dots

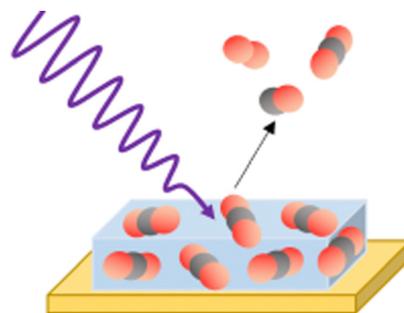
Sergey Savchenko, Alexander Vokhmintsev, Maksim Karabanalov, Yanning Zhang, Ahmed Henaish, Arup Neogi* and Ilya Weinstein



18741

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

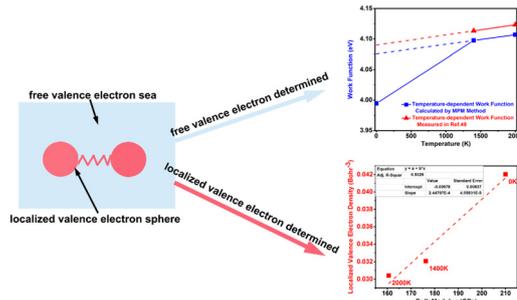
Antoine B. Hacquard,* Daniela Torres-Díaz, Romain Basalgète, Delfina Toulouse, Géraldine Féraud, Samuel Del Fré, Jennifer A. Noble, Laurent Philippe, Xavier Michaut, Jean-Hugues Fillion, Anne Lafosse, Lionel Amiaud and Mathieu Bertin



18753

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

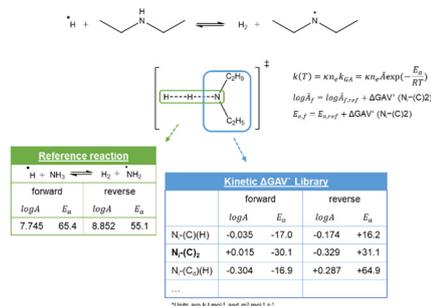
Guomin Hua,* Patricio Mendez and Xinglong Dong



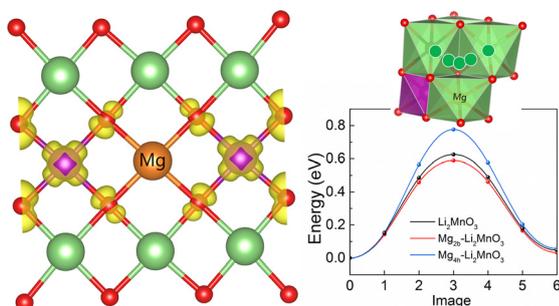
18763

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*



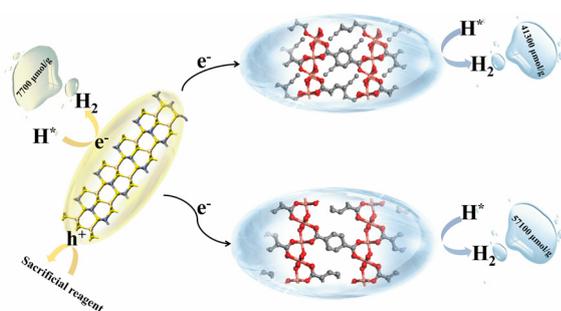
18776



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

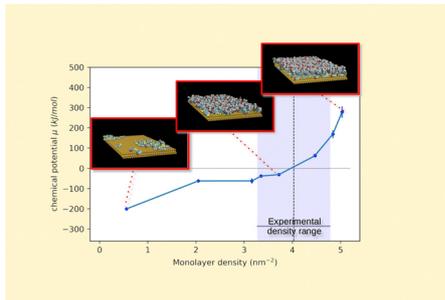
18788



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

Youlin Wu, Yiming Xie and Zhiliang Jin*

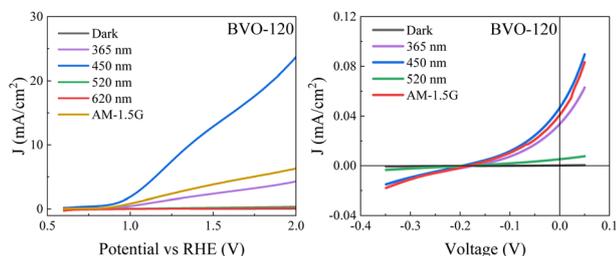
18799



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

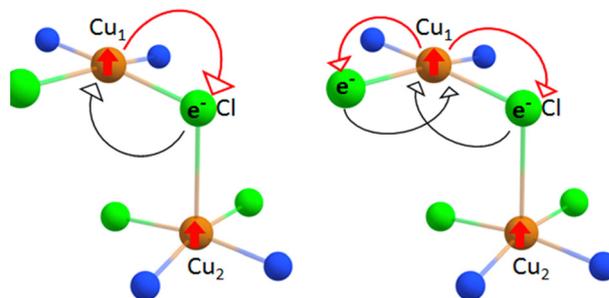
Lei Shi, Wenyue Zhao, Nan Zhang, Zhao Wang, Wenjing Hua, Xiaoxia Yang, Weidong Fei* and Yu Zhao*



18816

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

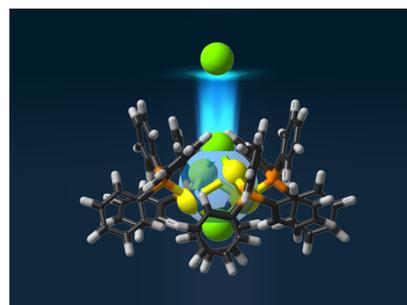
Bharadwaj Chowdary Mummaneni, Sihuai Chen, Wolfgang Hübner and Georgios Lefkidis*



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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 ($\text{X} = \text{Cl}^-, \text{Br}^-, \text{I}^-$)

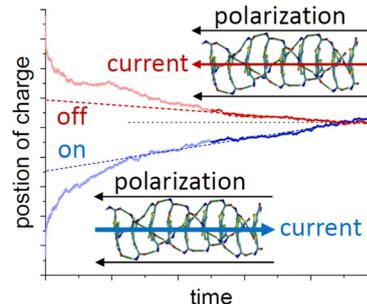
Raul Guajardo-Maturana, Peter. L. Rodríguez-Kessler and Alvaro Muñoz-Castro*



18837

Theory for nonlinear conductivity switching in semiconducting organic ferroelectrics

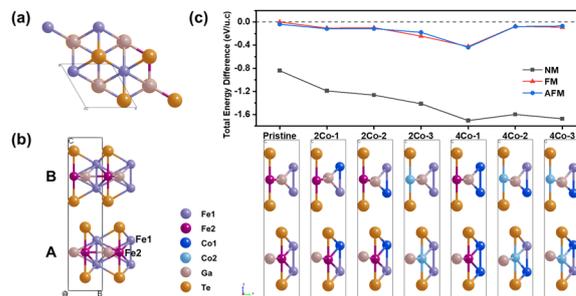
Till Johann, Weiwei Xie, Sara Roosta, Marcus Elstner and Martijn Kemerink*



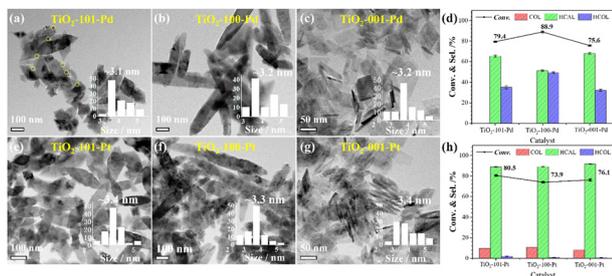
18847

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*



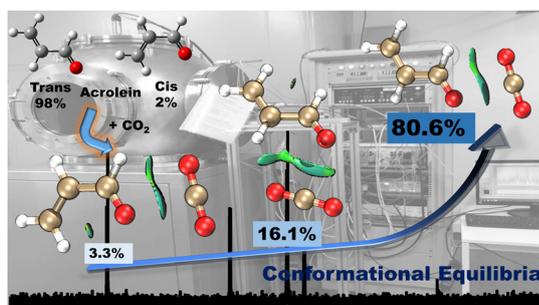
18854



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*

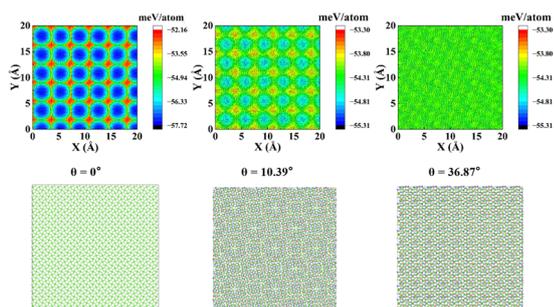
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Conformational equilibria in acrolein–CO₂: the crucial contribution of $n \rightarrow \pi^*$ interactions unveiled by rotational spectroscopy

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

18871

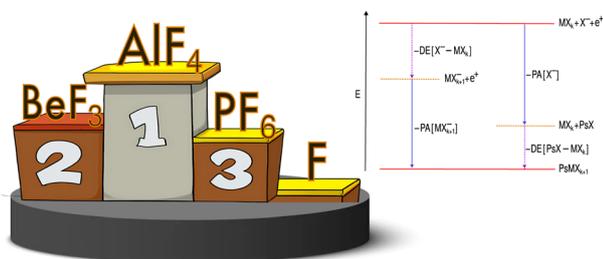


Structural superlubricity at the interface of penta-BN₂

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

18881

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*

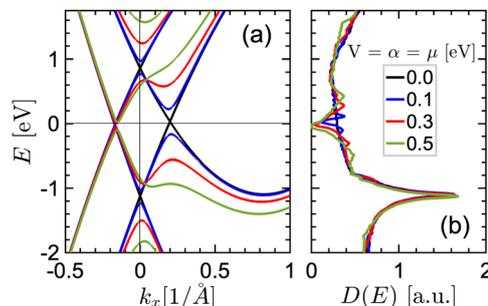


RESEARCH PAPERS

18892

Electronic phase transition in bilayer $P6mmm$ borophene

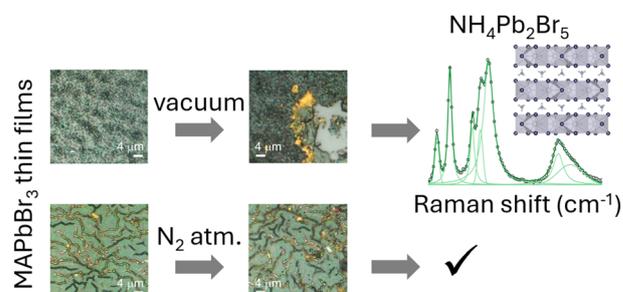
Nguyen N. Hieu, Huynh V. Phuc and Bui D. Hoi*



18898

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

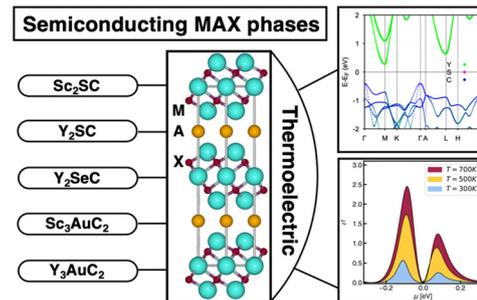
Valentina Carpenella, Fabrizio Messina, Jessica Barichello, Fabio Matteocci, Paolo Postorino, Caterina Petrillo, Alessandro Nucara, Danilo Dini and Claudia Fasolato*



18907

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

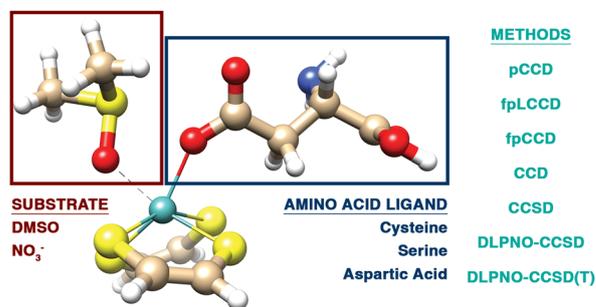
Mohammad Khazaei,* Iraj Maleki,* Namitha Anna Koshi, Ahmad Ranjbar, Nanxi Miao, Junjie Wang,* Rasoul Khaledialidusti, Thomas D. Kühne, Seung-Cheol Lee, Satadeep Bhattacharjee, Hamid Hosano, S. Mehdi Vaez Allaei, Keivan Esfarjani and Kaoru Ohno



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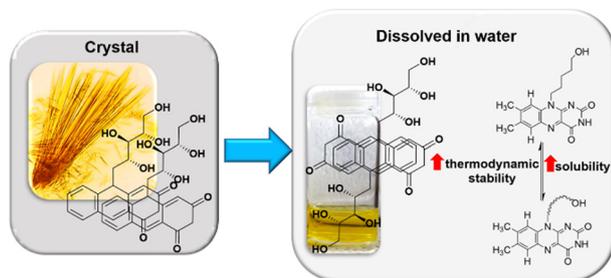
Delving into the catalytic mechanism of molybdenum cofactors: a novel coupled cluster study

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



RESEARCH PAPERS

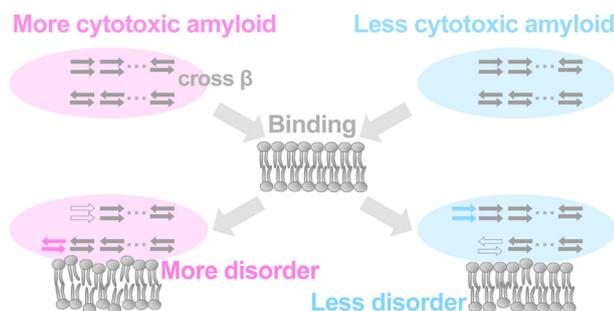
18930



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

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

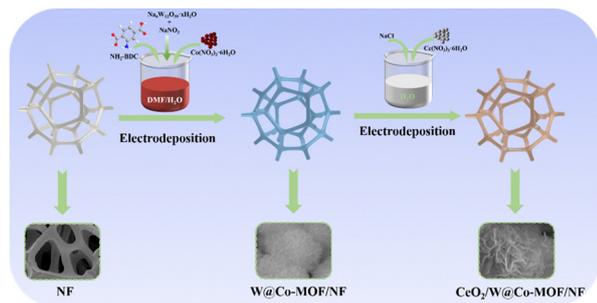
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Phospholipid-induced secondary structural changes of lysozyme polymorphic amyloid fibrils studied using vacuum-ultraviolet circular dichroism

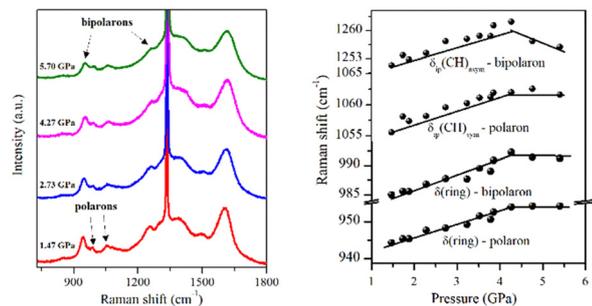
Tatsuhito Matsuo,* Seigi Yamamoto and Koichi Matsuo

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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*

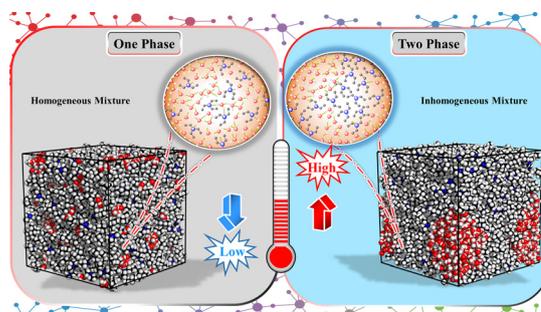


RESEARCH PAPERS

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

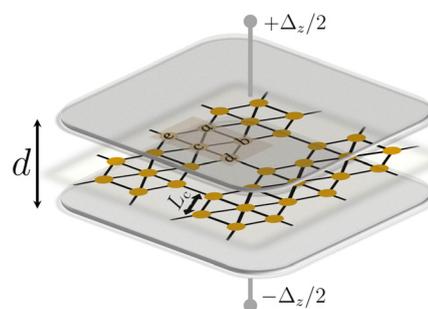
Ravi Singh, Jiwon Seo, Jonghyuk Ryu and Jun-Ho Choi*



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

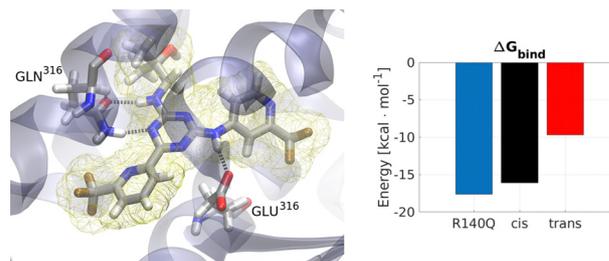
Tran Cong Phong, Huynh V. Phuc and Le T. T. Phuong*



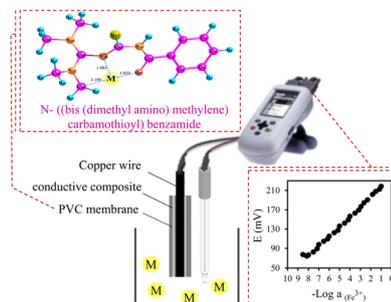
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Trans vs. *cis*: a computational study of enasidenib resistance due to IDH2 mutations

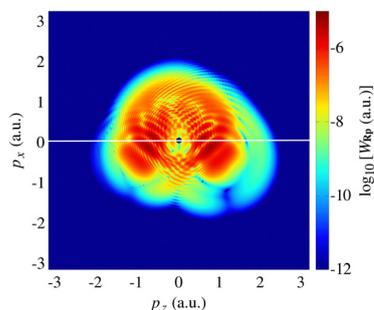
Erik Lindahl, Erik Arvidsson and Ran Friedman*



18997

Comparison of selectivity and sensitivity of various ferric selective electrodes prepared using *N*-((bis(dimethyl amino)methylene)carbamothioyl)benzamideMehrdad Ghaemi, Leila Hajiaghababaei,*
Jamshid Najafpour, Ashraf Sadat Shahvelayati and
Ramin M. A. Tehrani

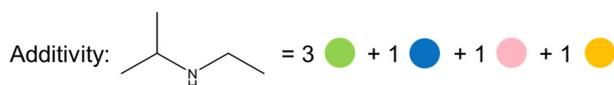
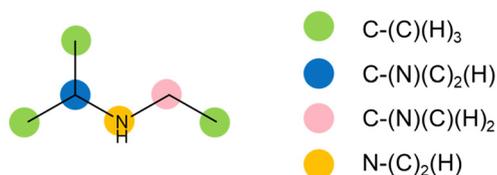
19008



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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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*

