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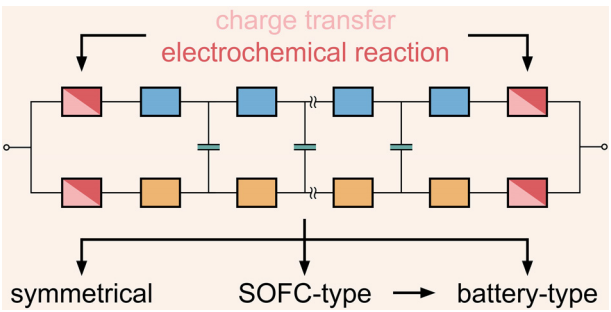
TUTORIAL REVIEW

15068

Transmission line revisited – the impedance of mixed ionic and electronic conductors

Andreas E. Bumberger, Andreas Nenning and Juergen Fleig*

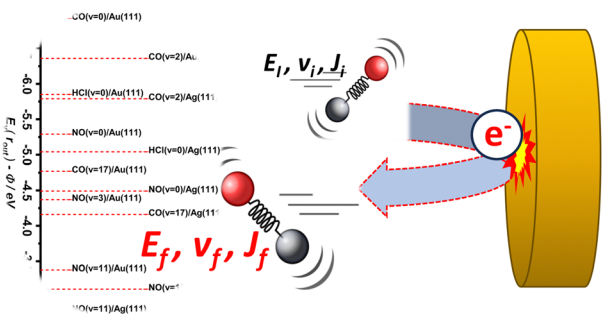


PERSPECTIVE

15090

Vibrational energy transfer in collisions of molecules with metal surfaces

Igor Rahinov,* Alexander Kandratsenka, Tim Schäfer, Pranav Shirhatti, Kai Golibrzuch and Alec M. Wodtke*



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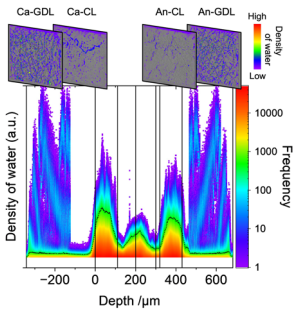
COMMUNICATIONS

15115

In situ 3D X-ray imaging of water distribution in each layer of a membrane electrode assembly of a polymer electrolyte fuel cell

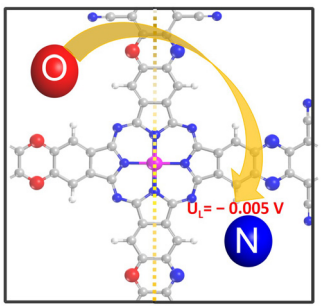
Hirosuke Matsui,* Tomoro Ohta, Takahiro Nakamura, Tomoya Uruga and Mizuki Tada*



15120

A two-dimensional covalent organic framework with single-atom manganese for electrochemical NO reduction: a computational study

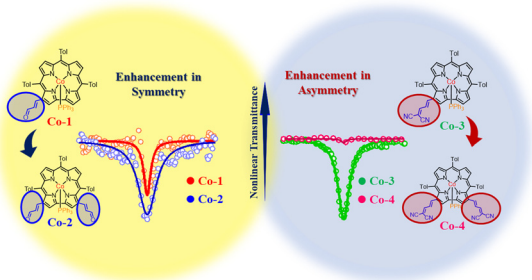
Jing Yu, Yu Wang* and Yafei Li*



15125

Structurally influenced optical nonlinearities and ultrafast dynamics in β-acroleyl- and β-dicyanobutadienyl-appended cobalt corroles

Inderpal Yadav, Jitendra Nath Acharyya, G. Vijaya Prakash* and Muniappan Sankar*

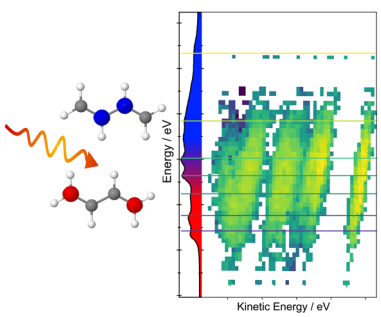


RESEARCH PAPERS

15130

Deconvolution of the X-ray absorption spectrum of _trans_-1,3-butadiene with resonant Auger spectroscopy

David M. P. Holland, Jiří Suchan, Jiří Janoš, Camila Bacellar, Ludmila Leroy, Thomas R. Barillot, Luca Longetti, Marcello Coreno, Monica de Simone, Cesare Grazioli, Majed Chergui, Eva Muchová* and Rebecca A. Ingle*



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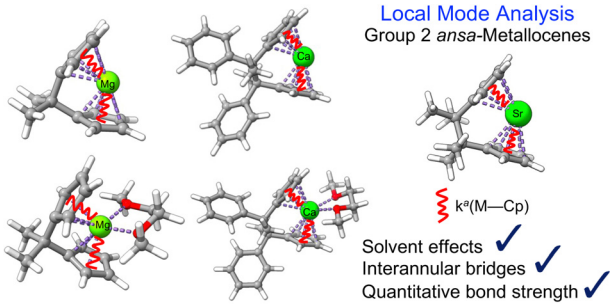
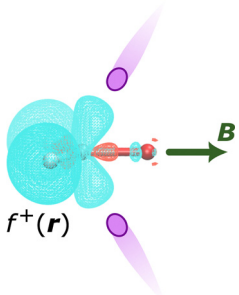


Metal–ring interactions in group 2 *ansa*-metallocenes: assessed with the local vibrational mode theory

Juliana J. Antonio and Elfi Kraka*

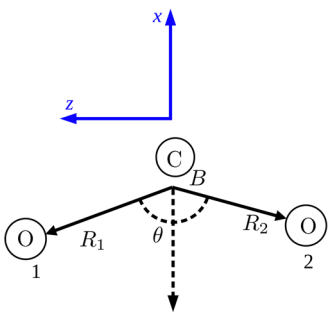
15156



Symmetry and reactivity of π-systems in electric and magnetic fields: a perspective from conceptual DFT

Meilani Wibowo-Teale,* Bang C. Huynh,* Andrew M. Wibowo-Teale, Frank De Proft and Paul Geerlings*

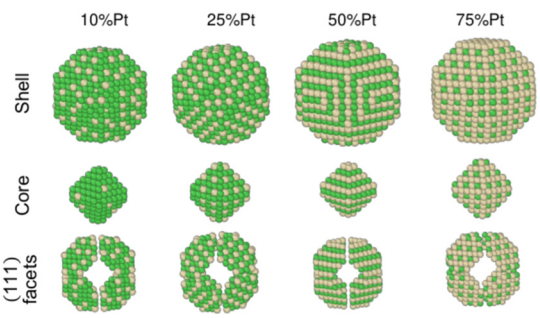
15181



A two-step quadrature-based variational calculation of ro-vibrational levels and wavefunctions of CO_2 using a bisector-*x* molecule-fixed frame

Xiao-Gang Wang and Tucker Carrington Jr

15192



Size and shape effects on chemical ordering in Ni–Pt nanoalloys

Pamela Camilos,* Céline Varvenne and Christine Mottet

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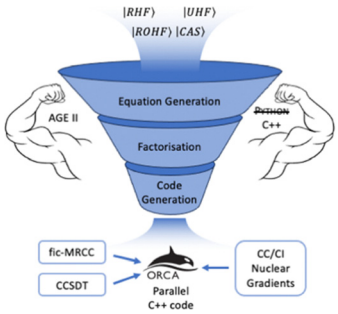
15205

Code generation in ORCA: progress, efficiency and tight integration

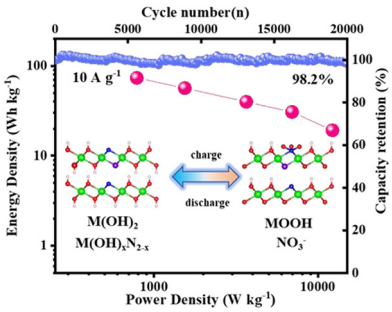
Marvin H. Lechner,* Anastasios Papadopoulos,* Kantharuban Sivalingam, Alexander A. Auer, Axel Koslowski, Ute Becker, Frank Wennmohs and Frank Neese*



15221

Achieving high-capacity aqueous supercapacitors *via* anion-doped construction of dual redox centers in $Ni_xCo_{1-x}SeO_3$

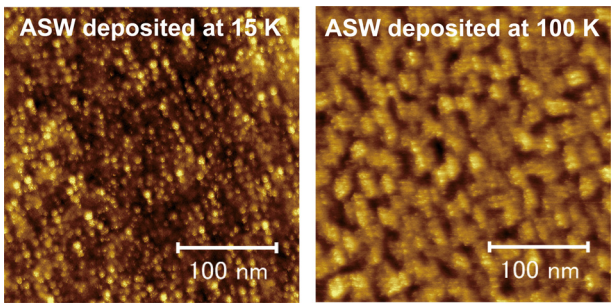
Tao Li, Jinyue Song, Hongguang Fan, Yanpeng Wang, Yusheng Luo, Chenchen Shao, Qingping Li and Wei Liu*



15232

Atomic force microscopy observation of surface morphologies and measurements of local contact potential differences of amorphous solid water samples deposited at 15 and 100 K

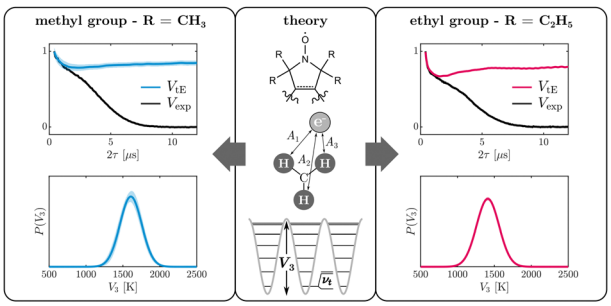
Takuto Tomaru, Hiroshi Hidaka,* Akira Kouchi and Naoki Watanabe



15240

Exploring tunneling ESEEM beyond methyl groups in nitroxides at low temperatures

Andrea Eggeling, Thacien Ngendahimana, Gunnar Jeschke,* Gareth R. Eaton and Sandra S. Eaton*



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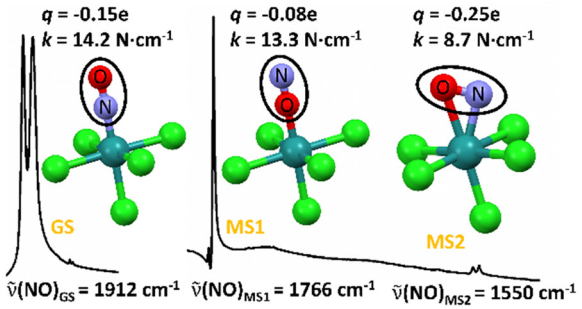
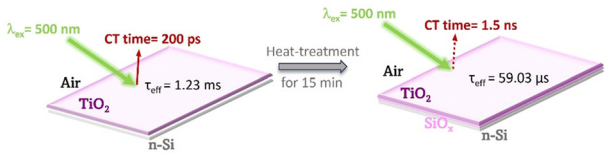


Local force constants and charges of the nitrosyl ligand in photoinduced NO linkage isomers in a prototypical ruthenium nitrosyl complex

Artem A. Mikhailov,* Axel Gansmüller, Krzysztof A. Konieczny, Sébastien Pillet, Gennadiy Kostin, Peter Klüfers, Theo Woike and Dominik Schaniel*

15268



Contactless analysis of surface passivation and charge transfer at the TiO_2–Si interface

Ramsha Khan, Xiaolong Liu, Ville Vähänissi, Harri Ali-Löytty, Hannu P. Pasanen, Hele Savin* and Nikolai V. Tkachenko*

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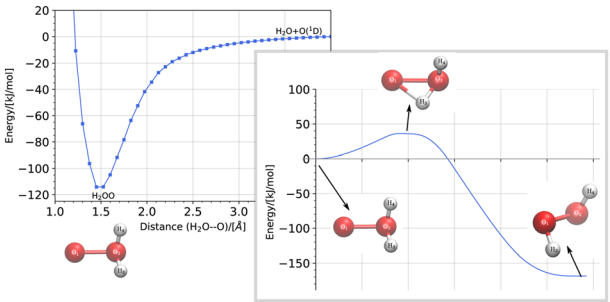
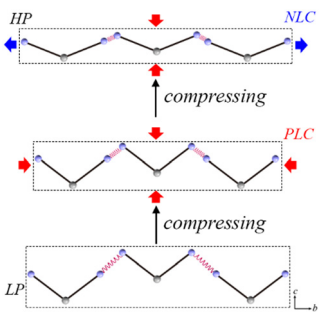


Unraveling the interaction between singlet state atomic oxygen O(^{1}D) and water: toward the formation of oxywater and hydrogen peroxide

Jos Suijker and Behnaz Bagheri*

15286



Hydrogen-bond-modulated negative linear compressibility in a V-shaped molecular crystal

Qingxin Zeng,* Wenbo Qiu, Chengxi Li, Yan Sun, Jian Hao and Yinwei Li*

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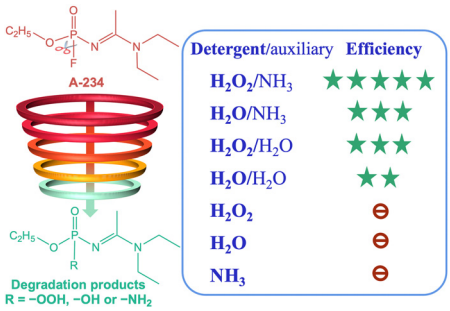
Elucidating the degradation mechanism of the nerve agent A-234 using various detergents: a theoretical investigation

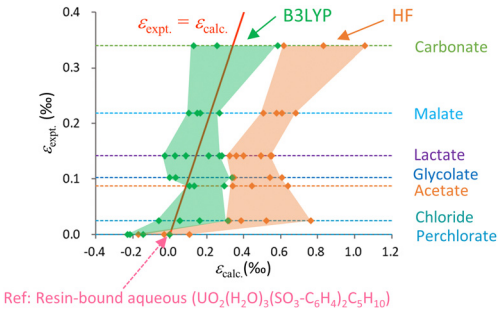
Rongxin Shi, Lin Zhang, Denghui Ma and Zexing Cao*



15301

Electron correlation effects on uranium isotope fractionation in U(VI)–U(VI) and U(IV)–U(VI) equilibrium isotopic exchange systems

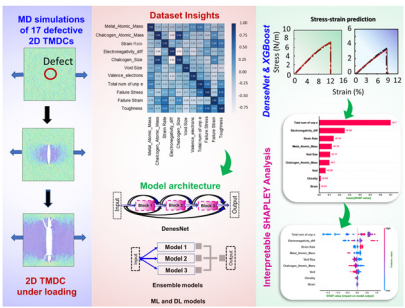
Ataru Sato, Masahiko Hada and Minori Abe*



15316

Machine learning predicted inelasticity in defective two-dimensional transition metal dichalcogenides using SHAP analysis

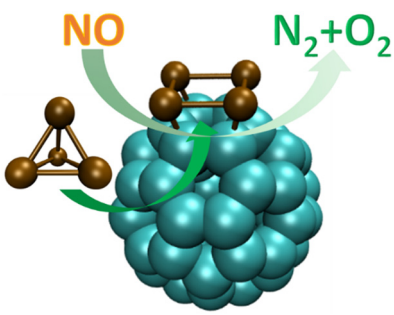
Ankit Anuragi, Ankit Das, Akash Baski, Vinay Maithani and Sankha Mukherjee*



15332

Direct reduction of NO into N_2 catalyzed by fullerene-supported rhodium clusters

Ruomeng Li, Ya-Ke Li,* Jianzhi Xu and Gao-Lei Hou*



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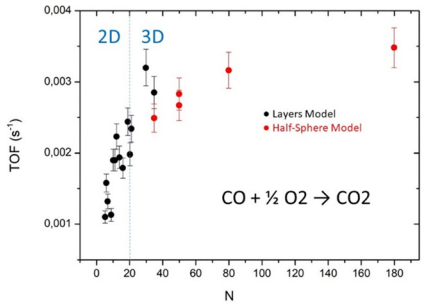
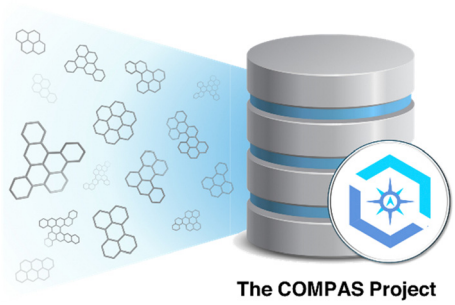


A molecular beam study of CO oxidation on Pd clusters supported on alumina: the effect of cluster size

Georges Sitja* and Claude R. Henry*

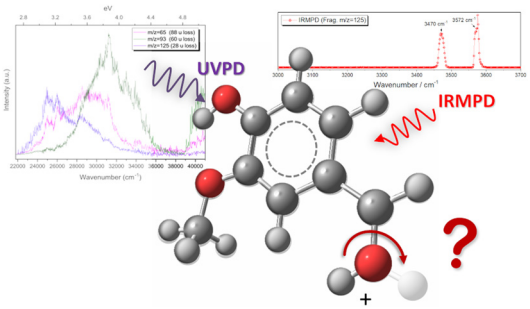
15344



COMPAS-3: a dataset of *peri*-condensed polybenzenoid hydrocarbons

Alexandra Wahab and Renana Gershoni-Poranne*

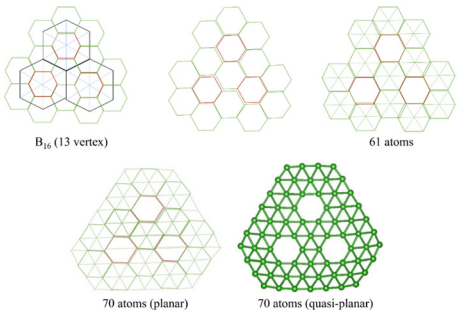
15358



Vibrational and electronic spectra of protonated vanillin: exploring protonation sites and isomerisation

Alejandro Gutiérrez-Quintanilla, Baptiste Moge, Isabelle Compagnon and Jennifer A. Noble*

15369



A topological path to the formation of a quasi-planar B_{70} boron cluster and its dianion

Pinaki Saha, Fernando Buendía, Long Van Duong and Minh Tho Nguyen*

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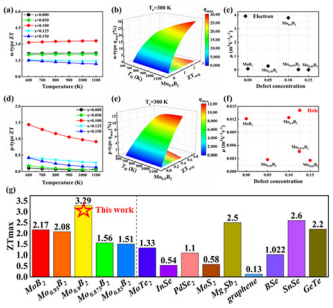
15376

Two-dimensional $Mo_{1-x}B_2$ with ordered metal vacancies obtained for advanced thermoelectric applications based on first-principles calculations

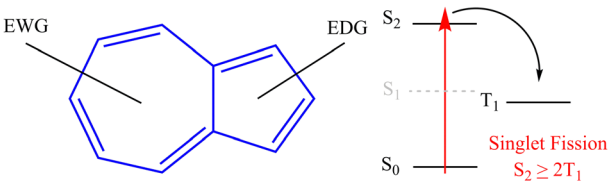
Jie Pu, Ziyu Hu* and Xiaohong Shao*



15386

Designing potentially singlet fission materials with an anti-Kasha behaviour

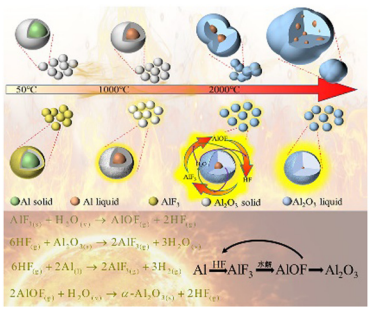
Ricardo Pino-Rios,* Rodrigo Báez-Grez, Dariusz W. Szczepanik and Miquel Solá*



15393

Enhancing the combustion of nAl with AlF_3 coating: gas–solid reaction mechanism for reducing combustion agglomeration of Al powder

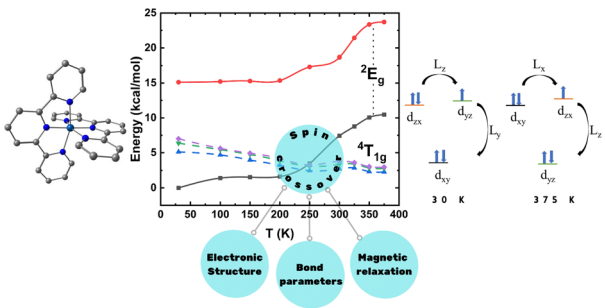
Chen Shen, Shi Yan,* Jie Yao, Hui Ren, Xueyong Guo, Jianxin Nie, Yapeng Ou, Qingjie Jiao and Yunjun Luo



15405

***Ab initio* calculation of magnetic anisotropy and thermal spin transition in the variable temperature crystal conformations of $[Co(terpy)_2]^{2+}$**

Moromi Nath, Shalini Joshi and Sabyashachi Mishra*



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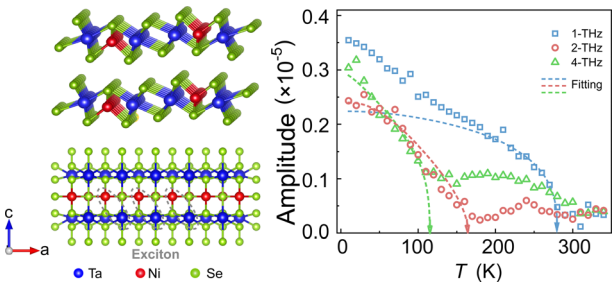
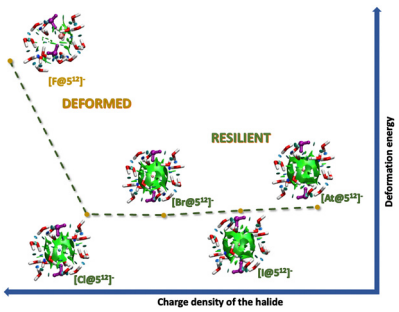


Multiple coherent amplitude modes and exciton–phonon coupling in quasi-one-dimensional excitonic insulator Ta_2NiSe_5

Yaohua Jiang, Yang Mi,* Jia Guo,* Zixuan Wang, Ning Zhang, Bo Liu and Sheng-Nian Luo

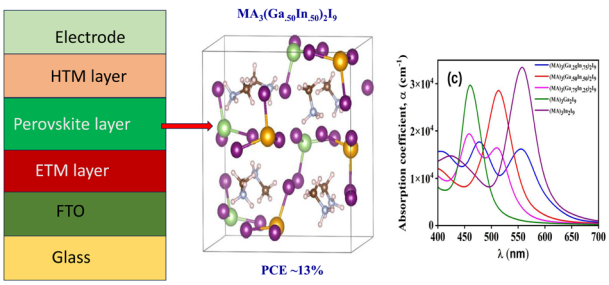
15426



Encapsulation of charged halogens by the 5^{12} water cage

Sara Gómez,* Elizabeth Flórez, Nancy Acelas, Chiara Cappelli, Cacier Hadad and Albeiro Restrepo*

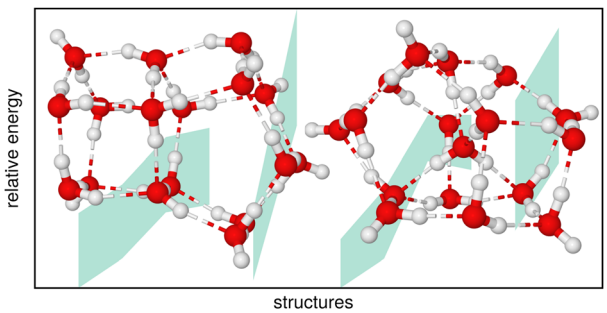
15437



Ga and In-based hybrid halide perovskites as an alternative to Pb: a first principles study

Tridip Chutia, Tanmoy Kalita, Uddipana Saikia and Dhruba Jyoti Kalita*

15445



On the brink of self-hydration: the water heptadecamer

Bernd Hartke

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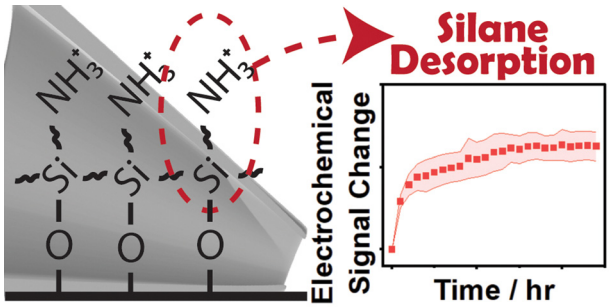
Reproducibility and stability of silane layers in nanoconfined electrochemical systems

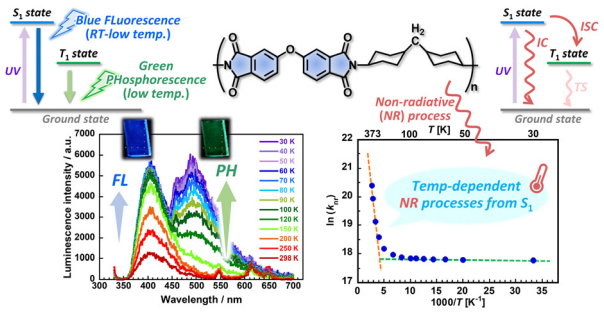
Dominik Duleba, Shekemi Denuga and Robert P. Johnson*



15461

Photophysical analysis of dual fluorescence and phosphorescence emissions observed for semi-aliphatic polyimides at lower temperatures

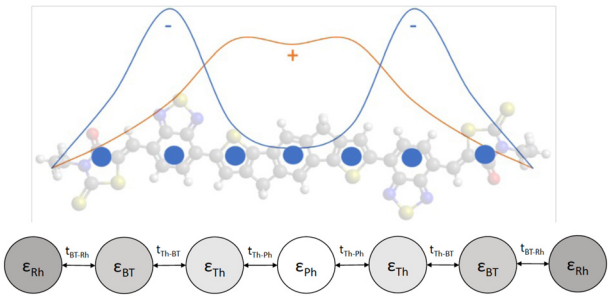
Mayuko Nara, Eisuke Fujiwara, Aurimas Vyšniauskas, Vidmantas Gulbinas* and Shinji Ando*



15472

Tight-binding model predicts exciton energetics and structure for photovoltaic molecules

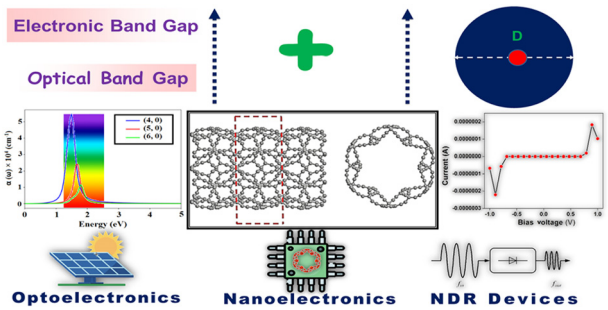
Vishal Jindal, Mohammed K. R. Aldahdooh, Enrique D. Gomez, Michael J. Janik and Scott T. Milner*



15484

Density functional theory study of the electronic and optical properties of pentagraphyne nanotubes

Jyotirmoy Deb, N. Bedamani Singh and Utpal Sarkar*



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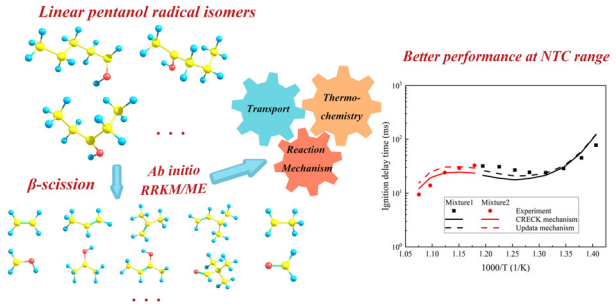
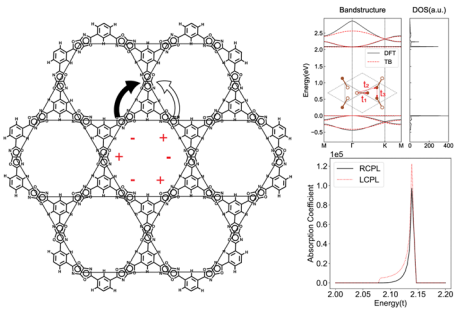
15494



Theoretical investigation on isomerization and decomposition reactions of pentanol radicals–part II: linear pentanol isomers

Yueying Liang, Yuxiang Zhu, Jintao Chen, Xingcai Lu* and Chong-Wen Zhou*

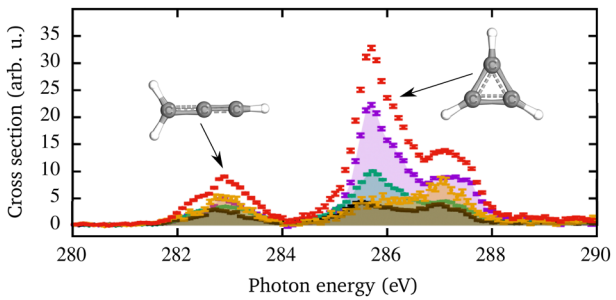
15511



Topology and giant circular dichroism of enantiomorphic Kagome bands in a designed covalent organic framework

Quan Gao, Lei Yang, Zhikuan Wang, Dongmei Li, Bin Cui* and Desheng Liu*

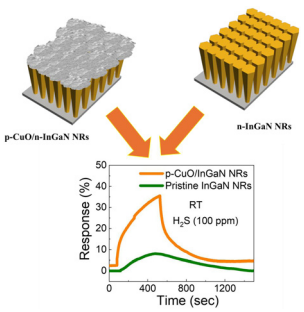
15519



Isomer-specific photofragmentation of $C_3H_3^+$ at the carbon K-edge

Simon Reinwardt, Patrick Cieslik, Ticia Buhr, Alexander Perry-Sassmannshausen, Stefan Schippers, Alfred Müller, Florian Trinter and Michael Martins*

15530



CuO nanostructure-decorated InGaN nanorods for selective H_2S gas detection

Chandrakalavathi Thota, C. Gangadhara, Dhanalakshmi Radhalayam, Ramu Singiri, Na-Hyun Bak, Paruchuri Kondaiah, C. Ningappa, Reddeppa Maddaka* and Moon-Deock Kim*

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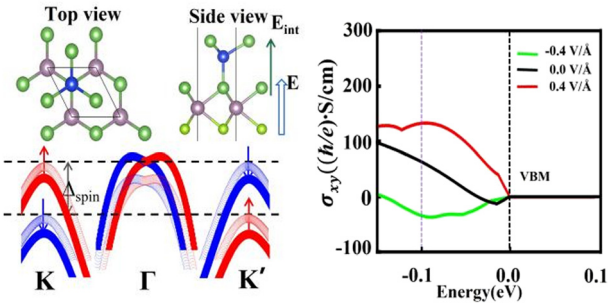
15539

Spin Hall effect modulated by an electric field in asymmetric two-dimensional $MoSiAs_2Se$

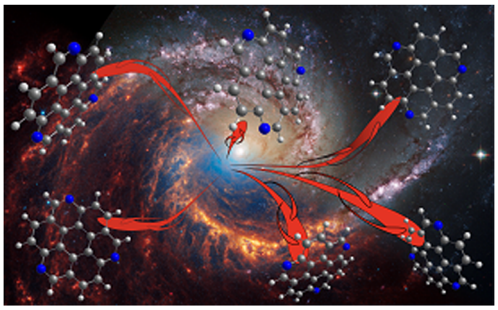
Jinhui Xing, Chao Wu, Shiqi Li, Yuanping Chen, Lizhi Zhang, Yuee Xie,* Jiaren Yuan* and Lichuan Zhang*



15547

Photoprocessing of cationic triazacoronene: dissociation characteristics of polycyclic aromatic nitrogen heterocycles in interstellar environments

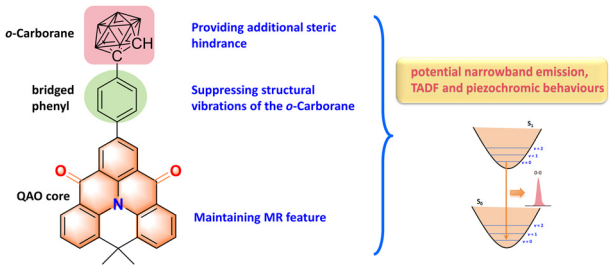
Domenik Schleier,* Jerry Kamer, Andy Jiao, Grégory F. Schneider, Harold Linnartz and Jordy Bouwman*



15559

Narrowband emission from fully-bridged triphenylamine derivatives: insights into effects of structure modification and pressure

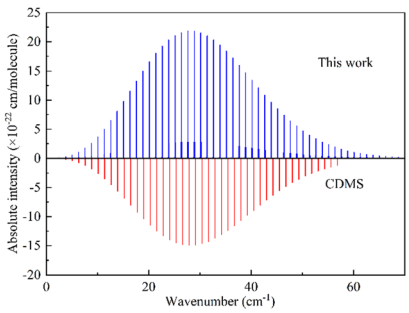
Qing Zhang, Tao Liu, Yuhua Guo, Yujian Zhang, Chunyan Lv,* Yue Zhang* and Zexing Cao*



15569

High-temperature rotation–vibration spectrum of iminosilylene (HNSi)

Ximing Li, Zhi Qin and Linhua Liu*



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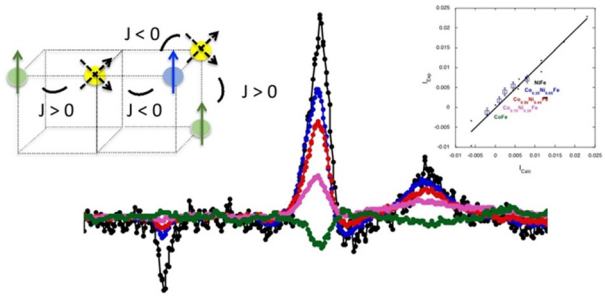
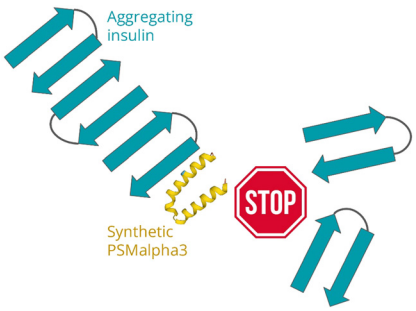
15576



Interplay between transition-metal K-edge XMCD, slight structural distortions and magnetism in a series of trimetallic $(Co_xNi_{(1-x)})_4[Fe(CN)_6]_{3/8}$ Prussian blue analogues

Adama N'Diaye, Amélie Bordage, Lucie Nataf, François Baudelet, Eric Rivière and Anne Bleuzen*

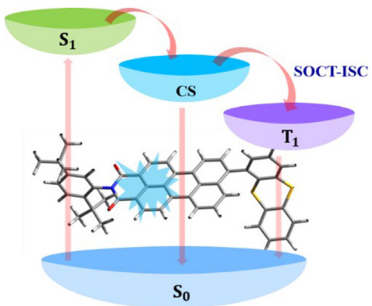
15587



Cytotoxic *Staphylococcus aureus* PSMα3 inhibits the aggregation of human insulin *in vitro*

Aleksandra Kalitnik,* Monika Szefczyk, Alicja W. Wojciechowska, Jakub W. Wojciechowski, Marlena Gąsior-Głogowska, Joanna Olesiak-Bańska and Małgorzata Kotulska*

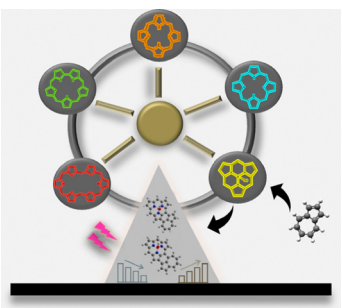
15600



Substitution effects on the photoinduced excited state dynamics of perylenemonoimides in solution and thin films

Suman Dhami, Mst Nasima Khatun, Chaitrali Sengupta, Parameswar Krishnan Iyer* and Ravindra Pandey*

15611



Why does the orientation of azulene affect the two-photon activity of a porphyrinoid–azulene system?

Swati Singh Rajput, Nikita Raghuvanshi, Tejendra Banana, Pooja Yadav and Md. Mehboob Alam*

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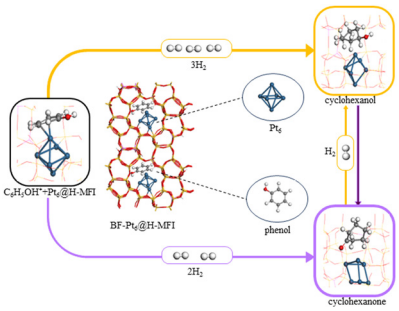
15620

Phenol hydrogenation over H-MFI zeolite encapsulated platinum nanocluster catalyst

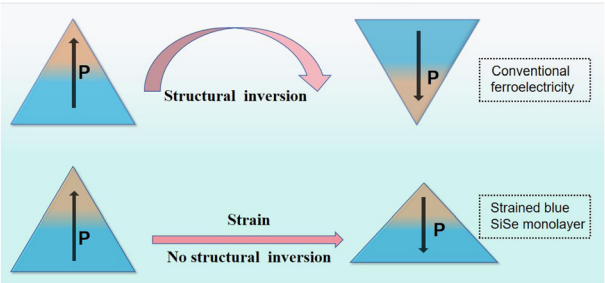
Kexin Wang, Weiwei Zhang* and Donghai Mei*



15629

Strain-induced ferroelectric polarization reversal without undergoing geometric inversion in blue SiSe monolayer

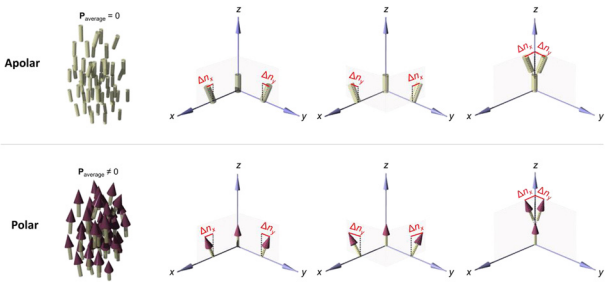
Yan-Dong Guo,* Rui-Jie Meng, Xue-Qin Hu, Li-Yan Lin, Yu-Rong Yang,* Ming-Yu Yang, Yun You, Lan-Qi Zhang, Yi-Long Xu and Xiao-Hong Yan



15637

Extended free-energy functionals for achiral and chiral ferroelectric nematic liquid crystals: theory and simulation

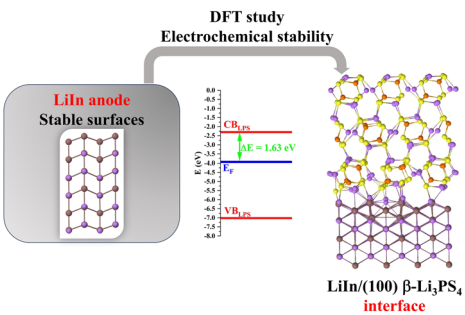
Yu Zou and Satoshi Aya*



15648

A computational study of the negative LiIn modified anode and its interaction with β-Li_3PS_4 solid–electrolyte for battery applications

Naiara Leticia Marana, Fabrizio Silveri, Eduardo de Oliveira Gomes, Lorenzo Donà, Maddalena D'Amore, Eleonora Ascrizzi, Mauro Francesco Sgroi, Lorenzo Maschio and Anna Maria Ferrari*



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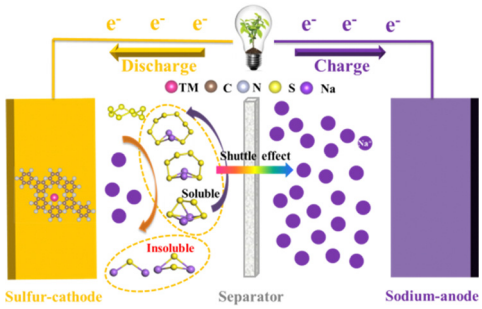
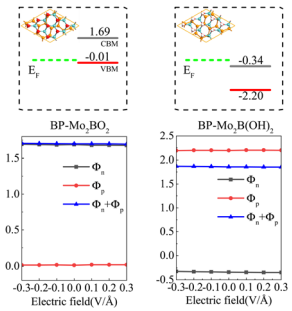
15657



Single-atom catalysts based on C_2N for sulfur cathodes in Na–S batteries: a first-principles study

Wanlin Xu, Tengrui Feng, Jiezhen Xia, Rong Cao and Qi Wu*

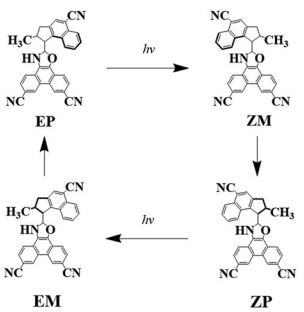
15666



Surface-engineered Mo_2B: a promising electrode material for constructing Ohmic contacts with blue phosphorene for electronic device applications

Jingying Yang, Xiang Liu, Xiaohui Deng, Zhenkun Tang and Liemao Cao*

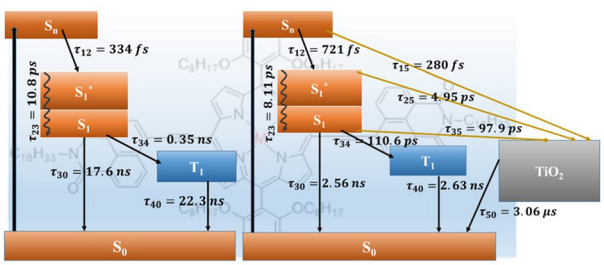
15672



Advanced theoretical design of light-driven molecular rotary motors: enhancing thermal helix inversion and visible-light activation

Weiliang Shi, Jianzheng Ma, Chenwei Jiang* and Tetsuya Taketsugu*

15681



Hot carrier dynamics in metalated porphyrin–naphthalimide thin films

Md Soif Ahmed, Sudhanshu Kumar Nayak, Botta Bhavani, Dipanjan Banerjee, Seelam Prasanthkumar, Lingamallu Giribabu, Venugopal Rao Soma and Sai Santosh Kumar Raavi*

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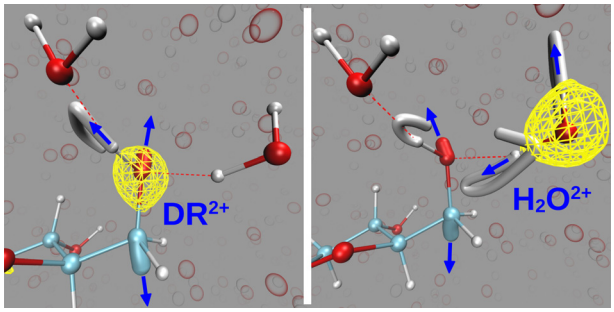
15693

Ultrafast fragmentation of highly-excited doubly-ionized deoxyribose: role of the liquid water environment

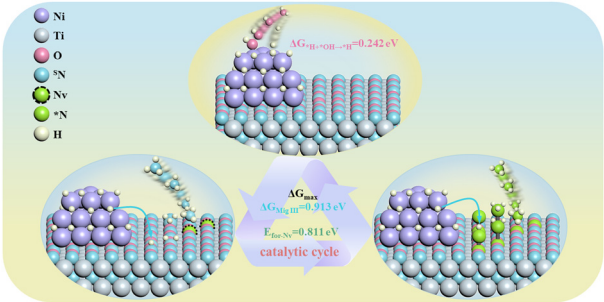
Marie-Anne Hervé du Penhoat,* Alexandre Souchaud, Aashini Rajpal, Rodolphe Vuilleumier, Marie-Pierre Gaigeot, Ivano Tavernelli, Kentaro Fujii, Akinari Yokoya, Sergio Díaz-Tendero and Marie-Françoise Politis



15705

***H migration-assisted MvK mechanism for efficient electrochemical NH_3 synthesis over TM–TiNO**

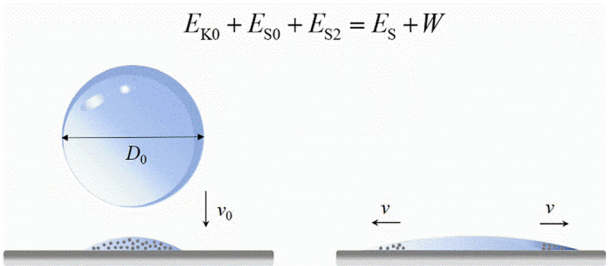
Luyao Cui, Zijun Sun, Yawen Wang, Xuan Jian, Houfen Li, Xiao Zhang, Xiaoming Gao, Rui Li* and Jianxin Liu*



15717

Spreading dynamics of a droplet upon impact with a liquid film containing solid particles

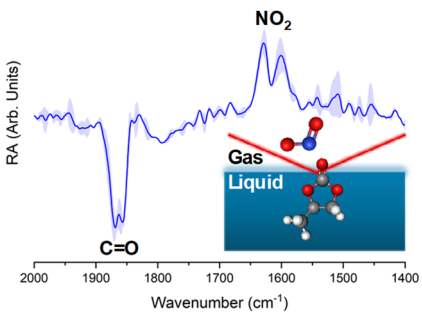
Jiale Wang, Lei Li, Xinlong Lu, Yu Zhou, Jiandong Zhou and Dengwei Jing*



15733

Interfacial carbonyl groups of propylene carbonate facilitate the reversible binding of nitrogen dioxide

Jessica B. Clark and Heather C. Allen*



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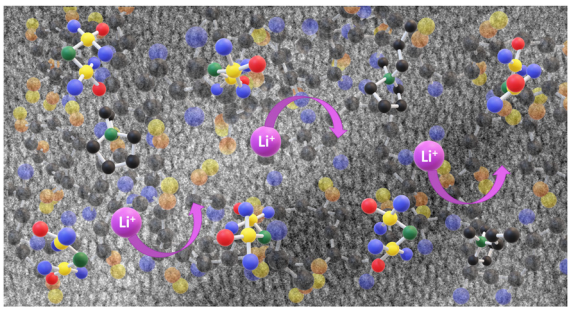
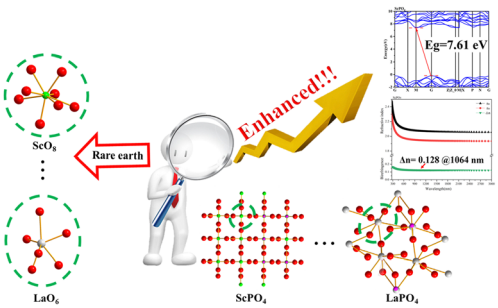


Impact of optimised quasi-block structures on the properties of polymer electrolytes

Greg Rollo-Walker,* Meisam Hasanpoor, Nino Malic, Faezeh Makhlooghi Azad, Luke O'Dell, Jacinta White, John Chiefari and Maria Forsyth

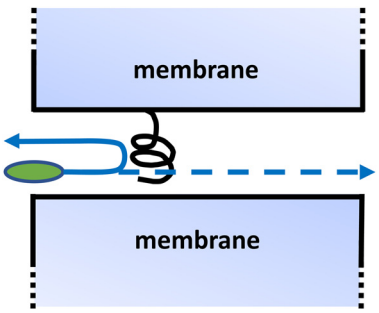
15751



The enhanced bandgap and birefringence of rare-earth phosphates XPO_4 (X = Sc, Y, La, and Lu): a first-principles investigation

Nuerbiye Tuerhong, Hongheng Chen, Mei Hu, Xiuhua Cui, Haiming Duan, Qun Jing* and Zhaohui Chen*

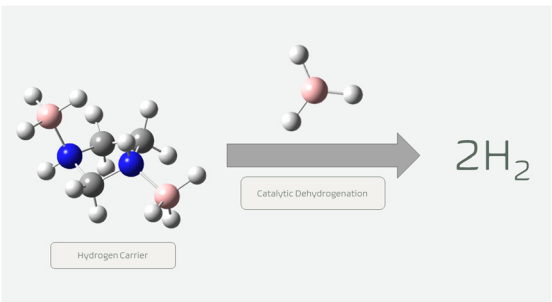
15758



Solute translocation probability, lifetime, and "rectification" in membrane channels with localized constriction

Alexander M. Berezhkovskii and Sergey M. Bezrukov*

15765



Structural and thermochemical investigation of 1,3-bis(λ^4-boraneyl)-1λ^4,3λ^4-imidazolidine adduct for chemical hydrogen storage

Fathima Rifana Mohamed Irfan and Sarah L. Masters*

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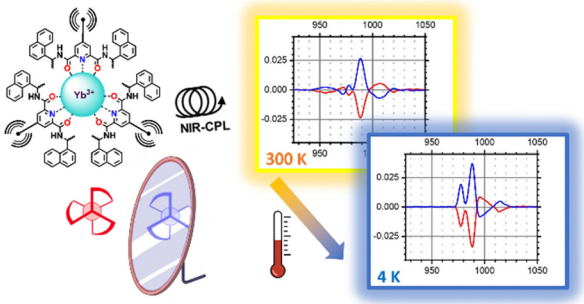
15776

Temperature-dependent NIR-CPL spectra of chiral Yb(III) complexes

Annika Sickinger, Maxime Grasser, Bruno Baguenard, Amina Bensalah-Ledoux, Laure Guy, Anh Thy Bui, Yannick Guyot, Vincent Dorcet, Fabrice Pointillart, Olivier Cador, Stéphan Guy, Olivier Maury, Boris Le Guennic and François Riobé*



CORRECTION

15784

Correction: A topological path to the formation of a quasi-planar B_{70} boron cluster and its dianion

Pinaki Saha, Fernando Buendía, Long Van Duong and Minh Tho Nguyen*