

IN THIS ISSUE

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Cover

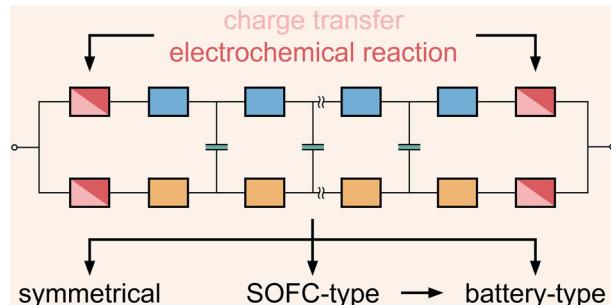
See Eva Muchová,
Rebecca A. Ingle
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Phys. Chem. Chem. Phys.,
2024, 26, 15130.

TUTORIAL REVIEW

15068

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

Andreas E. Bumberger, Andreas Nenning and
Juergen Fleig*

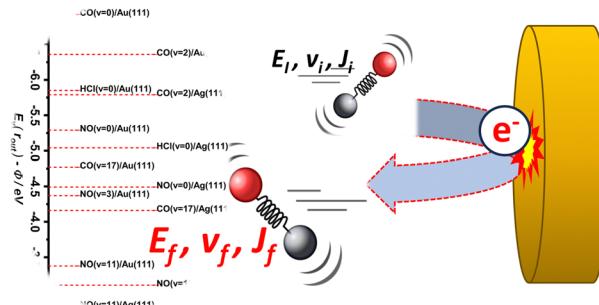


PERSPECTIVE

15090

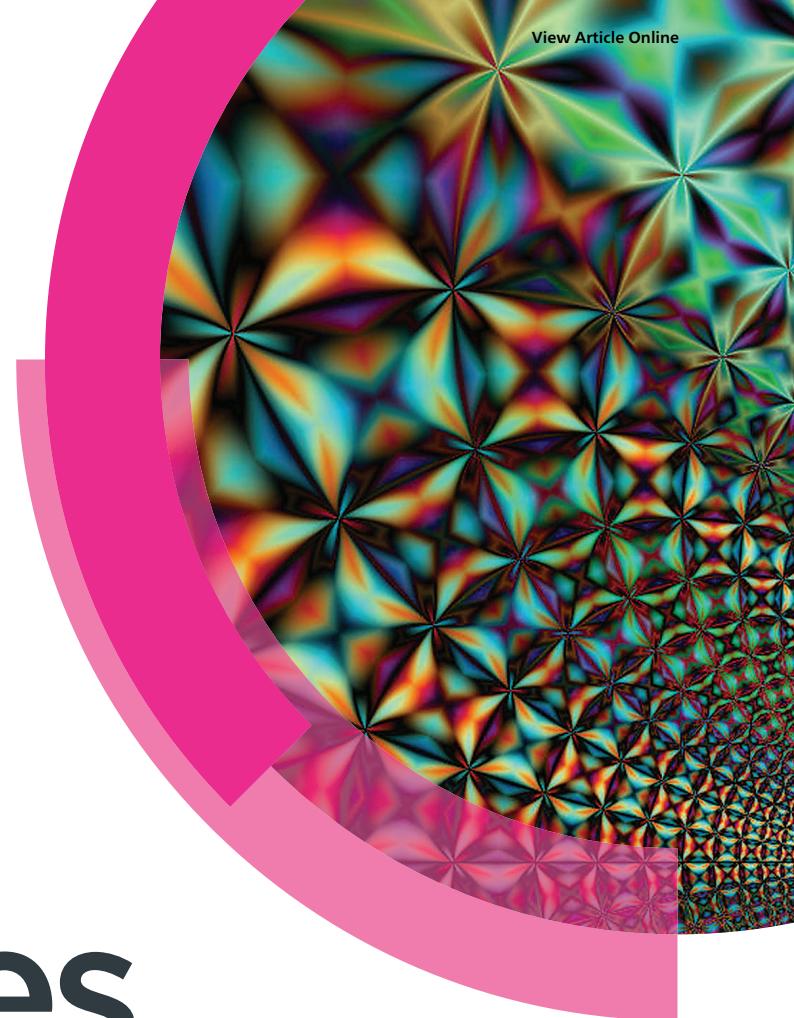
Vibrational energy transfer in collisions of molecules with metal surfaces

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





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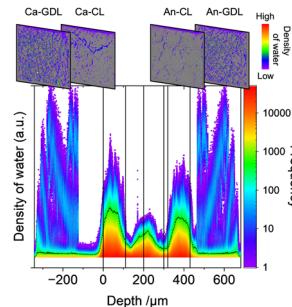
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COMMUNICATIONS

15115

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

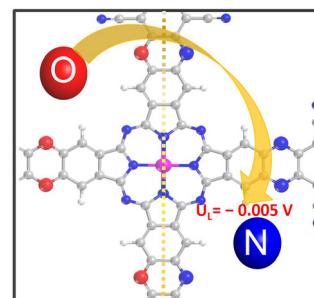
Hirosuke Matsui,* Tomoro Ohta, Takahiro Nakamura, Tomoya Uruga and Mizuki Tada*



15120

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

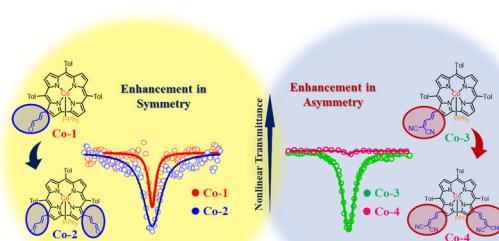
Jing Yu, Yu Wang* and Yafei Li*



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*

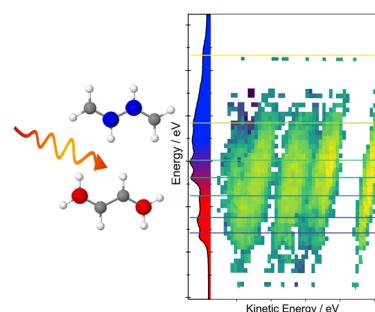


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15130

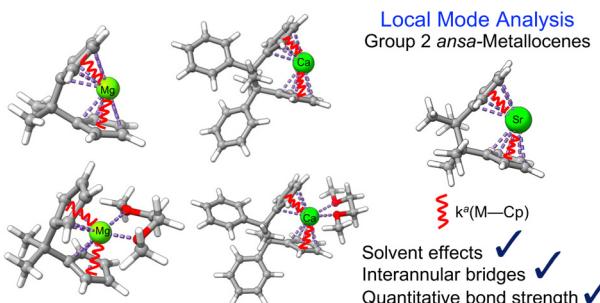
Deconvolution of the X-ray absorption spectrum of *trans*-1,3-butadiene with resonant Auger spectroscopy

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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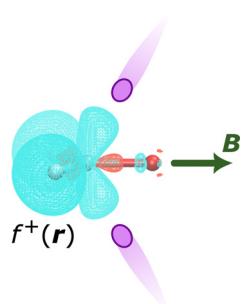
15143



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

Juliana J. Antonio and Elfi Kraka*

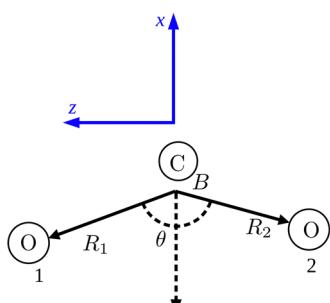
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Symmetry and reactivity of π -systems in electric and magnetic fields: a perspective from conceptual DFT

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

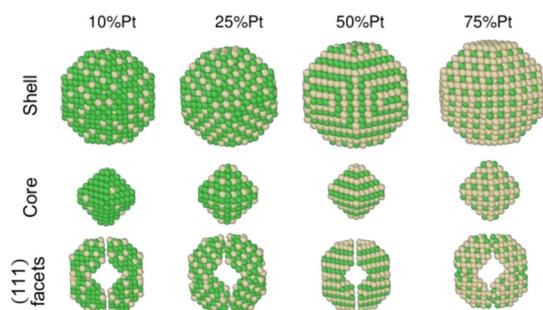
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A two-step quadrature-based variational calculation of ro-vibrational levels and wavefunctions of CO_2 using a bisector-x molecule-fixed frame

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

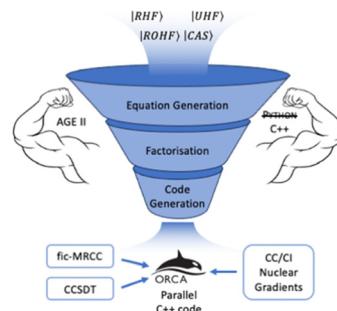


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Code generation in ORCA: progress, efficiency and tight integration

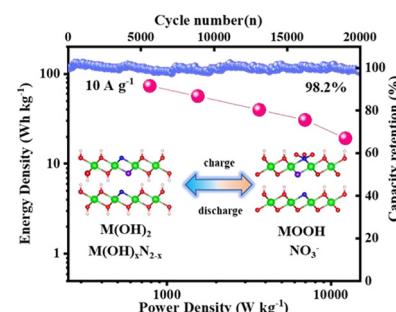
Marvin H. Lechner,* Anastasios Papadopoulos,* Kantharuban Sivalingam, Alexander A. Auer, Axel Koslowski, Ute Becker, Frank Wennmohs and Frank Neese*



15221

Achieving high-capacity aqueous supercapacitors via anion-doped construction of dual redox centers in $\text{Ni}_x\text{Co}_{1-x}\text{SeO}_3$

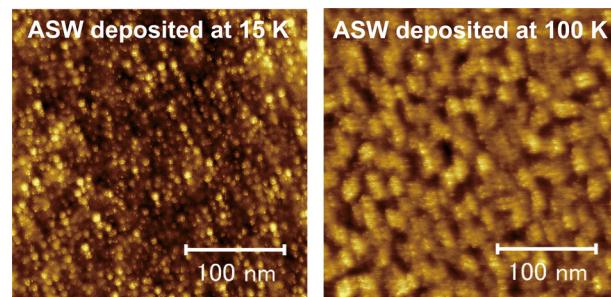
Tao Li, Jinyue Song, Hongguang Fan, Yanpeng Wang, Yusheng Luo, Chenchen Shao, Qingping Li and Wei Liu*



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

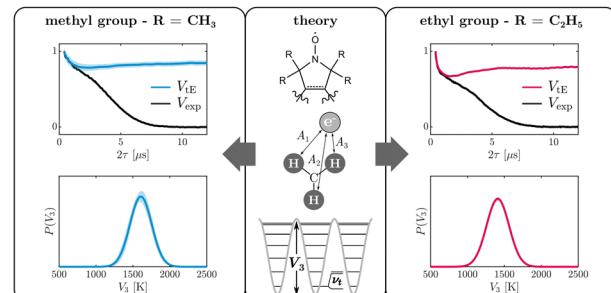
Takuto Tomaru, Hiroshi Hidaka,* Akira Kouchi and Naoki Watanabe



15240

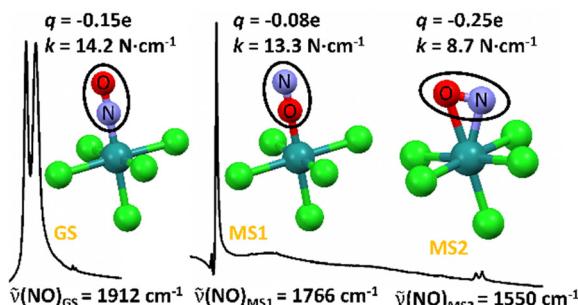
Exploring tunneling ESEEM beyond methyl groups in nitroxides at low temperatures

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



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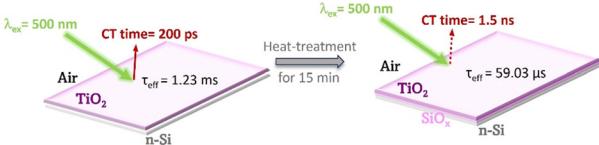
15255



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*

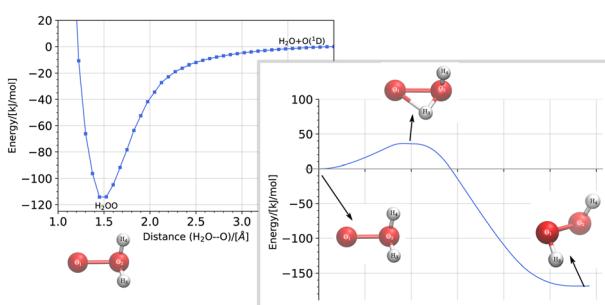
15268



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

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

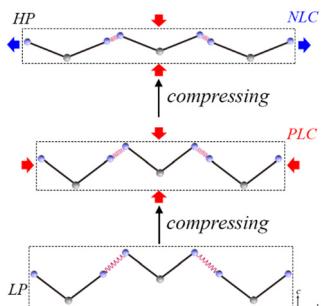
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Unraveling the interaction between singlet state atomic oxygen O^1D and water: toward the formation of oxywater and hydrogen peroxide

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*

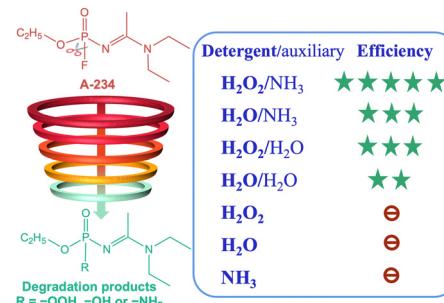


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Elucidating the degradation mechanism of the nerve agent A-234 using various detergents: a theoretical investigation

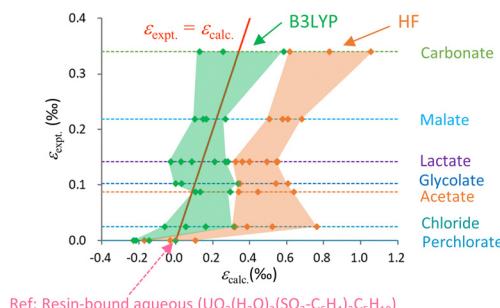
Rongxin Shi, Lin Zhang, Denghui Ma and Zexing Cao*



15301

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

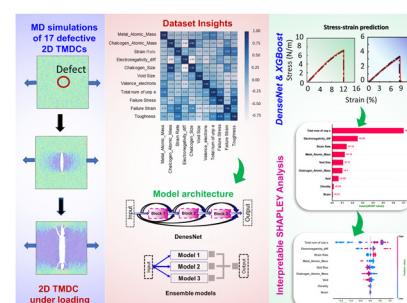
Ataru Sato, Masahiko Hada and Minori Abe*



15316

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

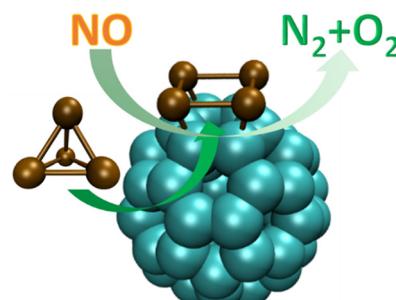
Ankit Anuragi, Ankit Das, Akash Baski, Vinay Maithani and Sankha Mukherjee*



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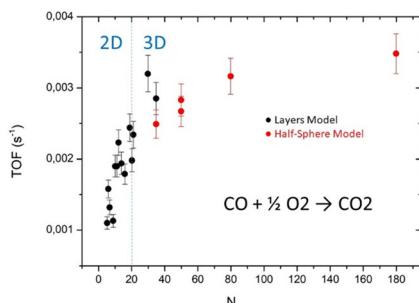
Direct reduction of NO into N₂ catalyzed by fullerene-supported rhodium clusters

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



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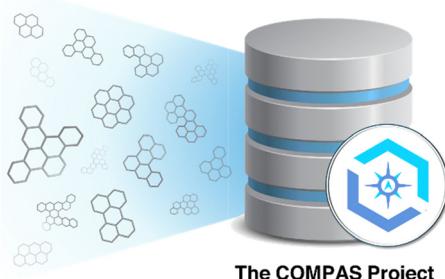
15338



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

Georges Sitja* and Claude R. Henry*

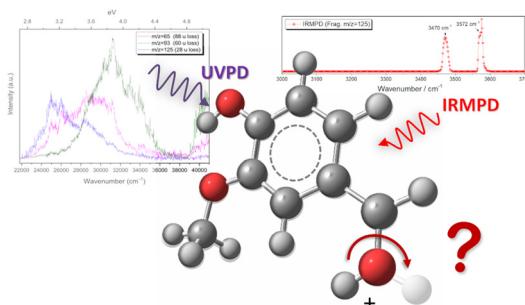
15344



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

Alexandra Wahab and Renana Gershoni-Poranne*

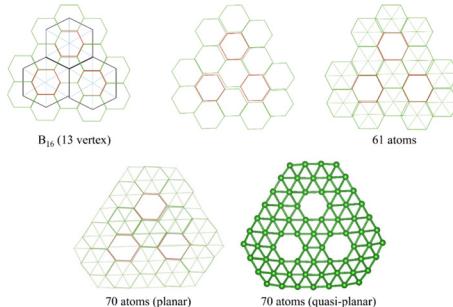
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Vibrational and electronic spectra of protonated vanillin: exploring protonation sites and isomerisation

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

15369



A topological path to the formation of a quasi-planar B₇₀ boron cluster and its dianion

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

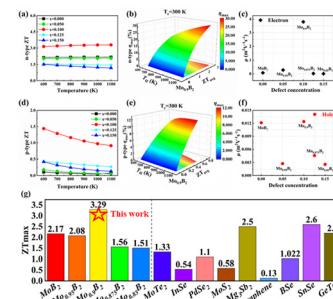


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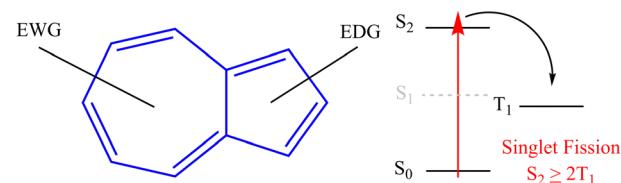
Two-dimensional $\text{Mo}_{1-x}\text{B}_2$ with ordered metal vacancies obtained for advanced thermoelectric applications based on first-principles calculations

Jie Pu, Ziyu Hu* and Xiaohong Shao*



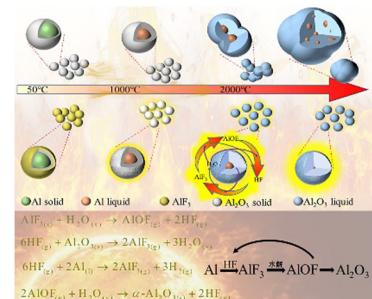
15386

Designing potentially singlet fission materials with an anti-Kasha behaviour

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

15393

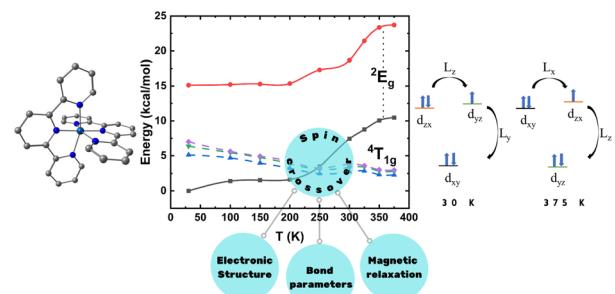
Enhancing the combustion of nAl with AlF_3 coating: gas–solid reaction mechanism for reducing combustion agglomeration of Al powder

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

15405

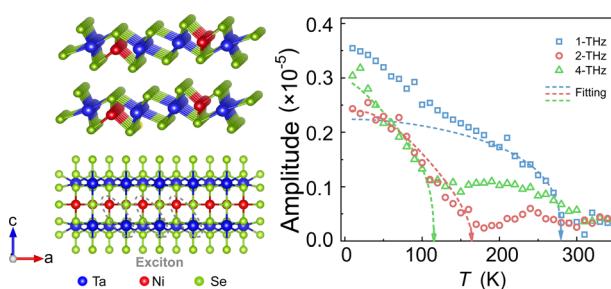
***Ab initio* calculation of magnetic anisotropy and thermal spin transition in the variable temperature crystal conformations of $[\text{Co}(\text{terpy})_2]^{2+}$**

Moromi Nath, Shalini Joshi and Sabyashachi Mishra*



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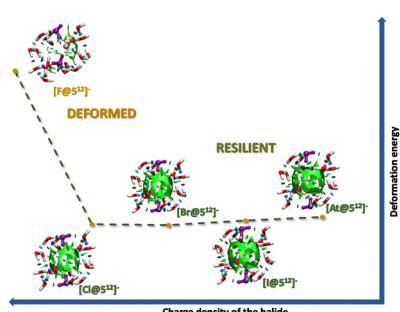
15417



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

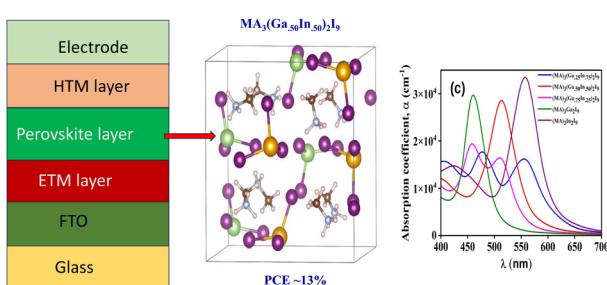
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Encapsulation of charged halogens by the 5^{12} water cage

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

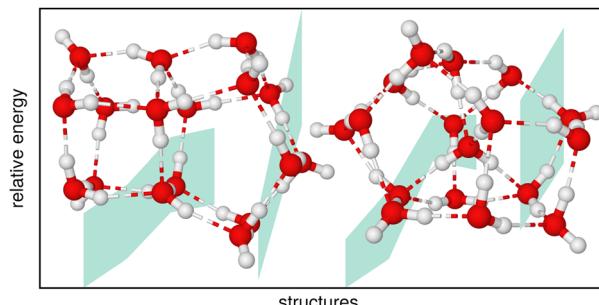
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Ga and In-based hybrid halide perovskites as an alternative to Pb: a first principles study

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

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On the brink of self-hydration: the water heptadecamer

Bernd Hartke

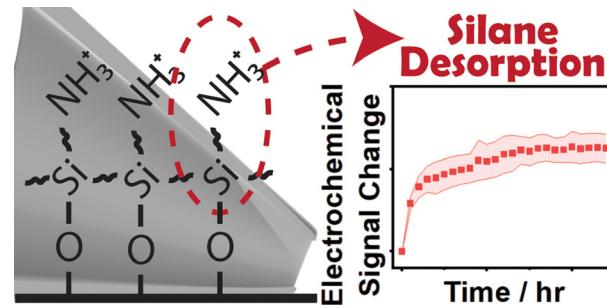


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Reproducibility and stability of silane layers in nanoconfined electrochemical systems

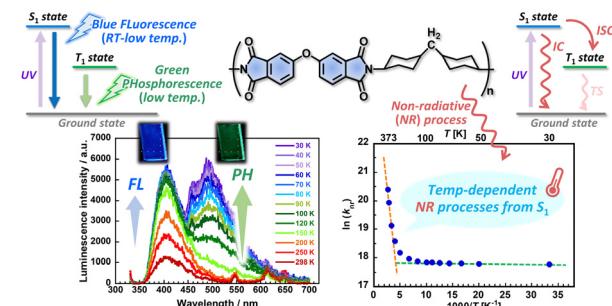
Dominik Duleba, Shekemi Denuga and Robert P. Johnson*



15461

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

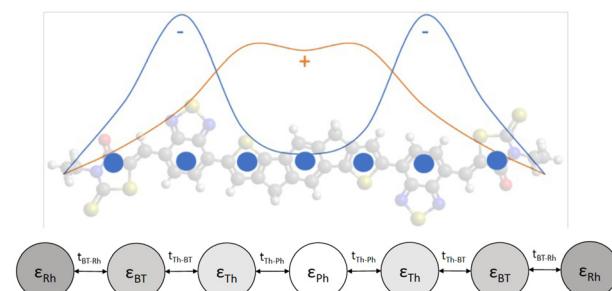
Mayuko Nara, Eisuke Fujiwara, Aurimas Vyšniauskas, Vidmantas Gulbinas* and Shinji Ando*



15472

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

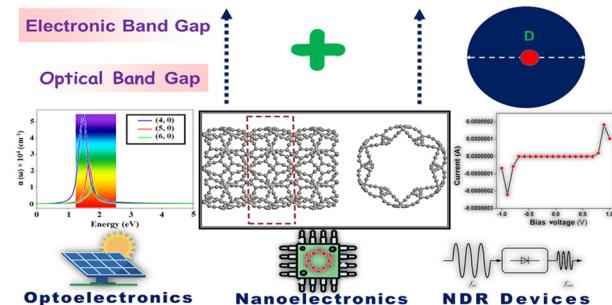
Vishal Jindal, Mohammed K. R. Aldahdooh, Enrique D. Gomez, Michael J. Janik and Scott T. Milner*



15484

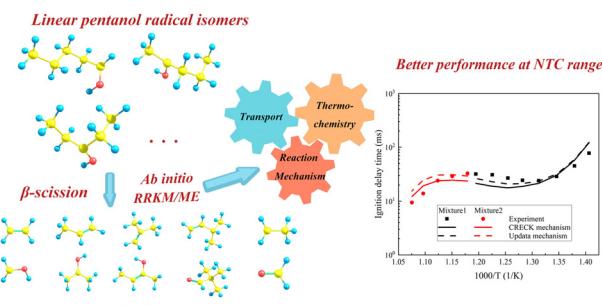
Density functional theory study of the electronic and optical properties of pentagraphyne nanotubes

Jyotirmoy Deb, N. Bedamani Singh and Utpal Sarkar*



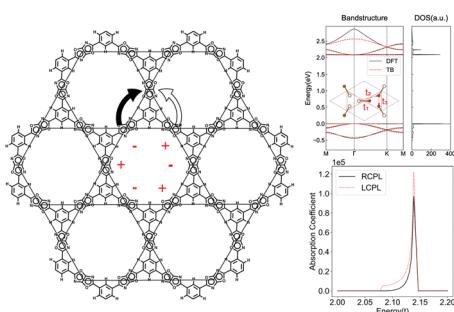
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15494

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

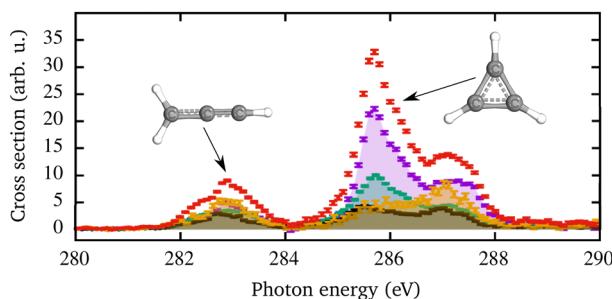
Yueying Liang, Yuxiang Zhu, Jintao Chen, Xingcai Lu* and Chong-Wen Zhou*

15511

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

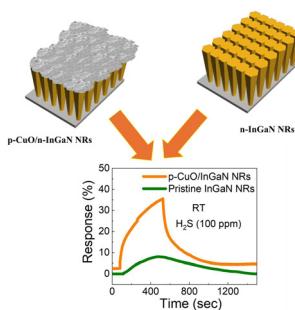
Quan Gao, Lei Yang, Zhikuan Wang, Dongmei Li, Bin Cui* and Desheng Liu*

15519

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

Simon Reinhardt, 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*

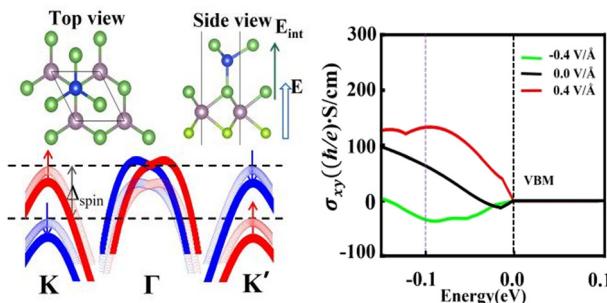


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Spin Hall effect modulated by an electric field in asymmetric two-dimensional MoSiAs₂Se

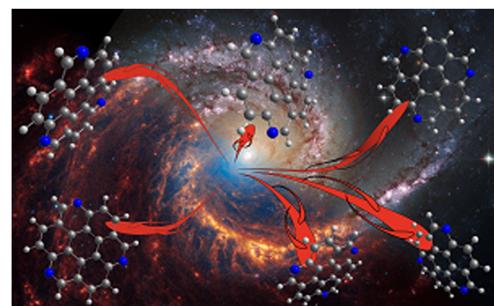
Jinhui Xing, Chao Wu, Shiqi Li, Yuanping Chen, Lizhi Zhang, Yuee Xie,* Jiaren Yuan* and Lichuan Zhang*



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

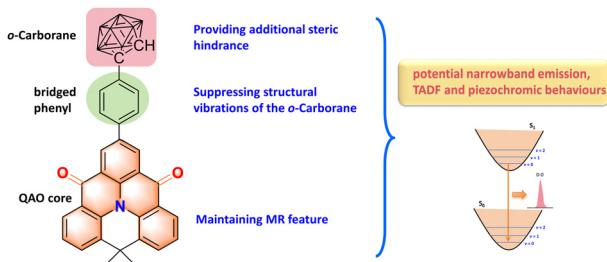
Domenik Schleier,* Jerry Kamer, Andy Jiao, Grégory F. Schneider, Harold Linnartz and Jordy Bouwman*



15559

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

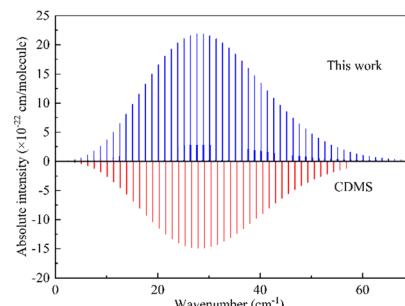
Qing Zhang, Tao Liu, Yuhua Guo, Yujian Zhang, Chunyan Lv,* Yue Zhang* and Zexing Cao*



15569

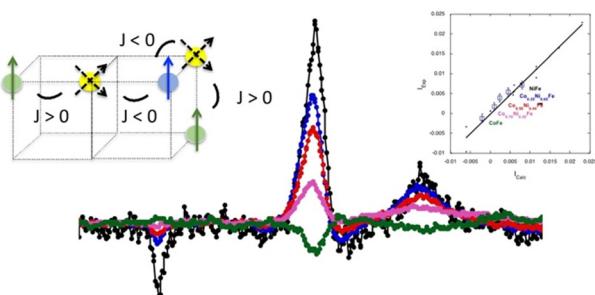
High-temperature rotation–vibration spectrum of iminosilylene (HNSi)

Ximing Li, Zhi Qin and Linhua Liu*



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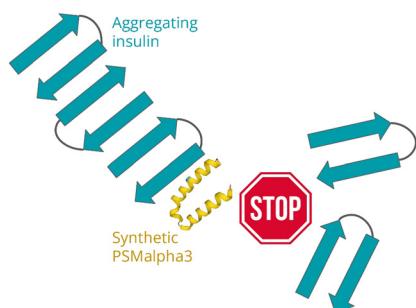
15576



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*

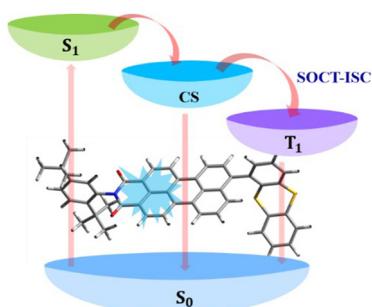
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Cytotoxic *Staphylococcus aureus* PSM α 3 inhibits the aggregation of human insulin *in vitro*

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

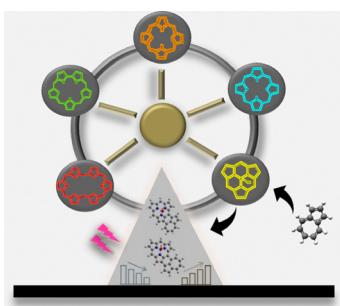
15600



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*

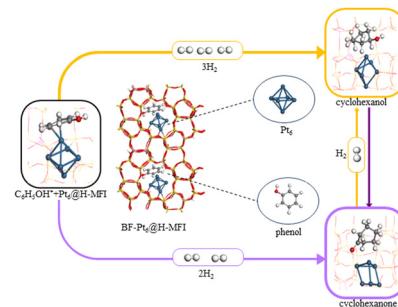


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Phenol hydrogenation over H-MFI zeolite encapsulated platinum nanocluster catalyst

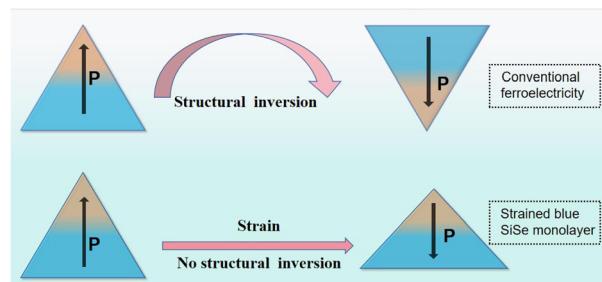
Kexin Wang, Weiwei Zhang* and Donghai Mei*



15629

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

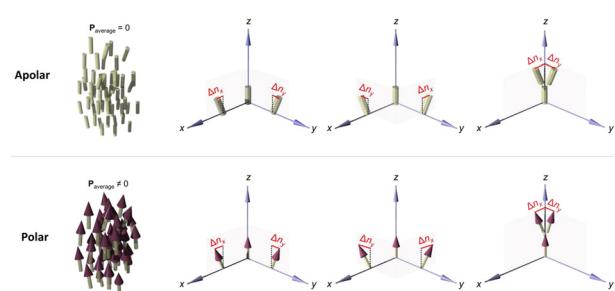
Yan-Dong Guo,* Rui-Jie Meng, Xue-Qin Hu, Li-Yan Lin, Yu-Rong Yang,* Ming-Yu Yang, Yun You, Lan-Qi Zhang, Yi-Long Xu and Xiao-Hong Yan



15637

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

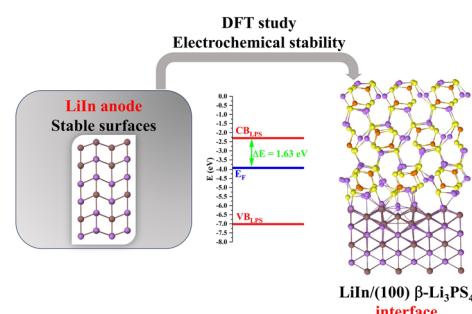
Yu Zou and Satoshi Aya*



15648

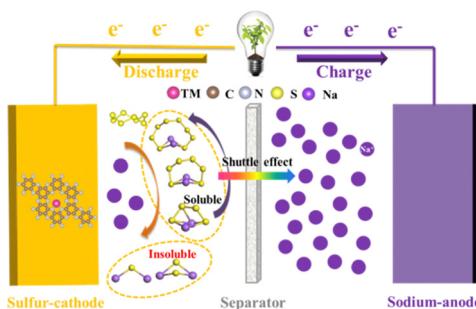
A computational study of the negative LiIn modified anode and its interaction with β -Li₃PS₄ solid-electrolyte for battery applications

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



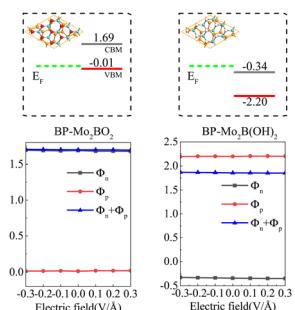
RESEARCH PAPERS

15657

**Single-atom catalysts based on C₂N for sulfur cathodes in Na-S batteries: a first-principles study**

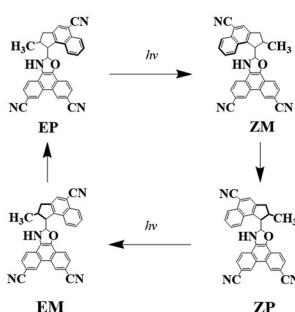
Wanlin Xu, Tengrui Feng, Jiezheng Xia, Rong Cao and Qi Wu*

15666

**Surface-engineered Mo₂B: a promising electrode material for constructing Ohmic contacts with blue phosphorene for electronic device applications**

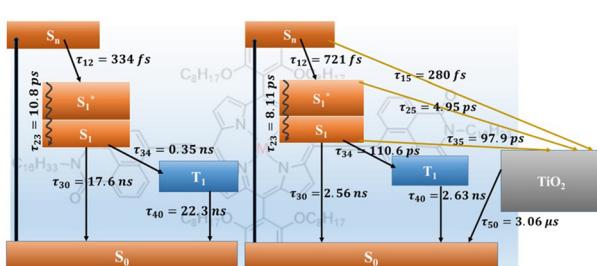
Jingying Yang, Xiang Liu, Xiaohui Deng, Zhenkun Tang and Liemao Cao*

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 metallated 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*

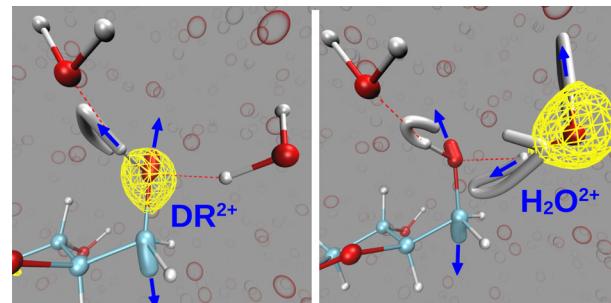


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15693

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

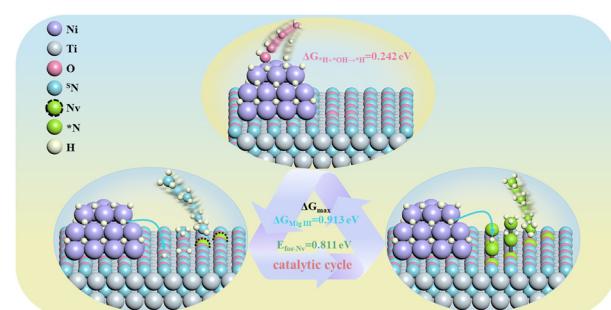
Marie-Anne Hervé du Penhoat,* Alexandre Souchaud, Aashini Rajpal, Rodolphe Vuilleumier, Marie-Pierre Gaigeot, Ivano Tavernelli, Kentaro Fujii, Akinari Yokoya, Sergio Diaz-Tendero and Marie-Françoise Politis



15705

***H migration-assisted MvK mechanism for efficient electrochemical NH₃ synthesis over TM–TiNO**

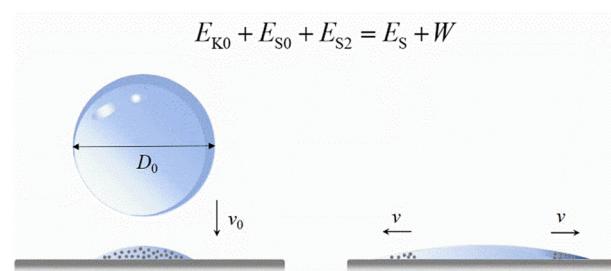
Luyao Cui, Zijun Sun, Yawen Wang, Xuan Jian, Houfen Li, Xiao Zhang, Xiaoming Gao, Rui Li* and Jianxin Liu*



15717

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

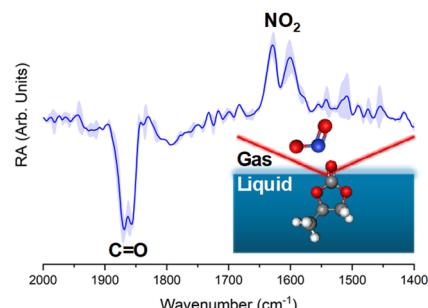
Jiale Wang, Lei Li, Xinlong Lu, Yu Zhou, Jiandong Zhou and Dengwei Jing*



15733

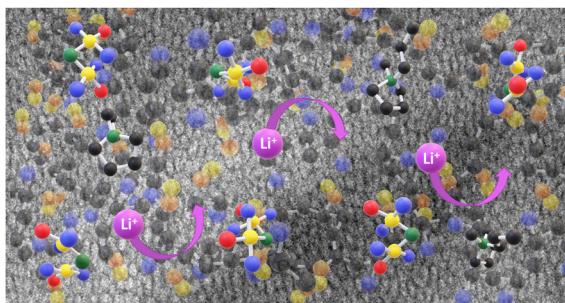
Interfacial carbonyl groups of propylene carbonate facilitate the reversible binding of nitrogen dioxide

Jessica B. Clark and Heather C. Allen*



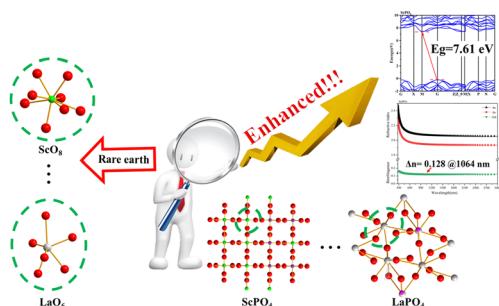
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15742

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

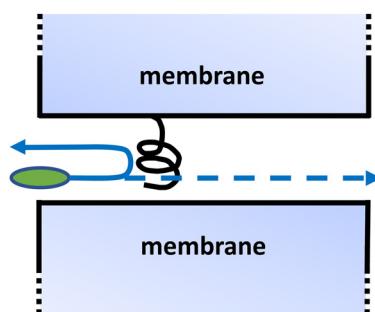
Greg Rollo-Walker,* Meisam Hasanpoor, Nino Malic, Faezeh Makhlooghi Azad, Luke O'Dell, Jacinta White, John Chiefari and Maria Forsyth

15751

**The enhanced bandgap and birefringence of rare-earth phosphates $X\text{PO}_4$ ($X = \text{Sc, Y, La, and Lu}$): a first-principles investigation**

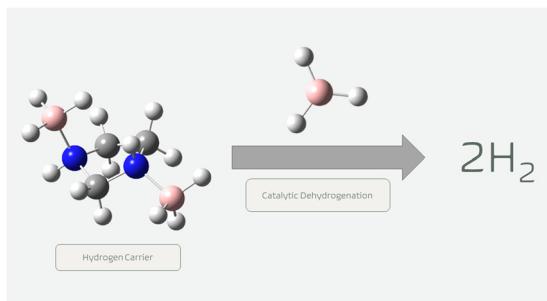
Nuerbiye Tuerhong, Hongheng Chen, Mei Hu, Xiuhua Cui, Haiming Duan, Qun Jing* and Zhaohui Chen*

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)- $1\lambda^4,3\lambda^4$ -imidazolidine adduct for chemical hydrogen storage**

Fathima Rifana Mohamed Irfan and Sarah L. Masters*

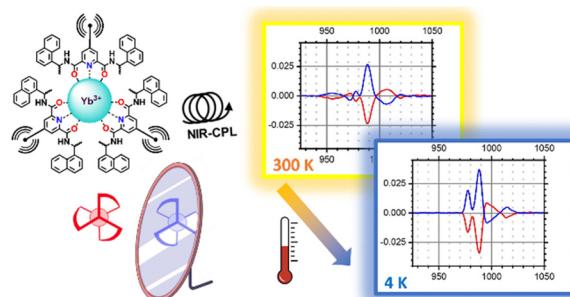


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15776

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 B₇₀ boron cluster and its dianion

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

