

## IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 26(21) 15047–15786 (2024)



### Cover

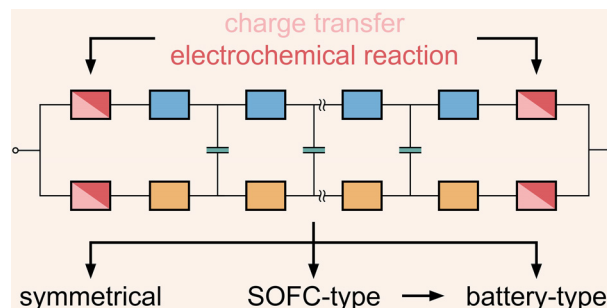
See Eva Muchová, Rebecca A. Ingle *et al.*, pp. 15130–15142. Image reproduced by permission of Rebecca Ingle and Jiri Suchan from *Phys. Chem. Chem. Phys.*, 2024, 26, 15130.

## TUTORIAL REVIEW

15068

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

Andreas E. Bumberger, Andreas Nening and Juergen Fleig\*

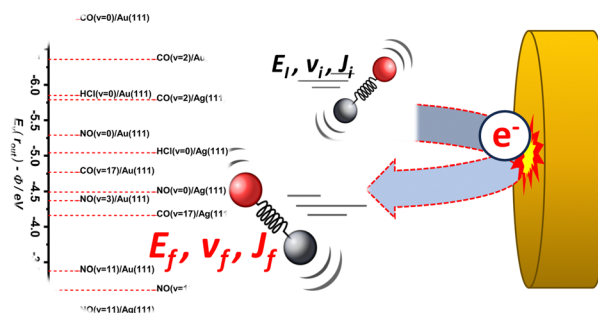


## PERSPECTIVE

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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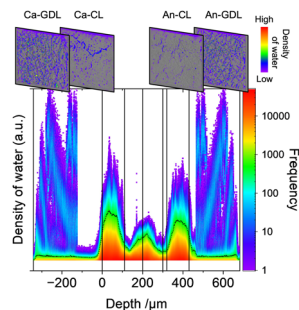


## COMMUNICATIONS

15115

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

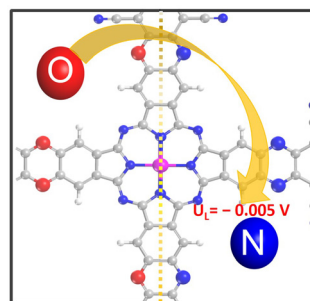
Hirosuke Matsui,\* Tomoro Ohta, Takahiro Nakamura, Tomoya Uruga and Mizuki Tada\*



15120

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

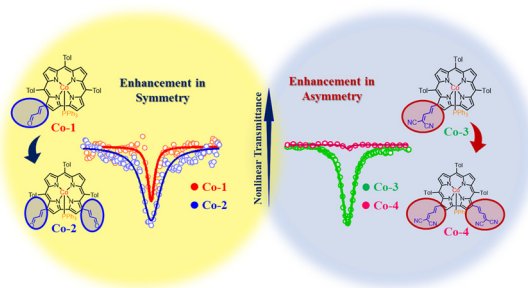
Jing Yu, Yu Wang\* and Yafei Li\*



15125

**Structurally influenced optical nonlinearities and ultrafast dynamics in  $\beta$ -acrolein- and  $\beta$ -dicyanobutadienyl-appended cobalt corroles**

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

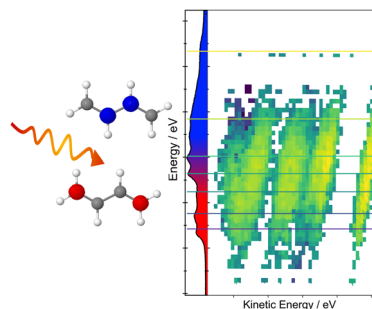


## RESEARCH PAPERS

15130

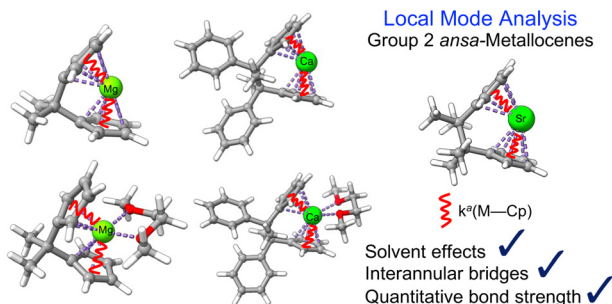
**Deconvolution of the X-ray absorption spectrum of *trans*-1,3-butadiene with resonant Auger spectroscopy**

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\*



## RESEARCH PAPERS

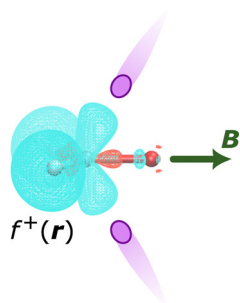
15143



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

Juliana J. Antonio and Elfi Kraka\*

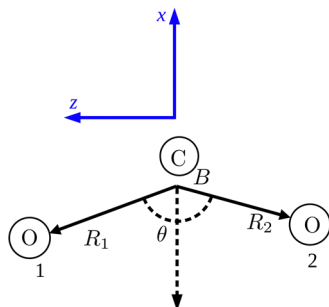
15156



### Symmetry and reactivity of $\pi$ -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\*

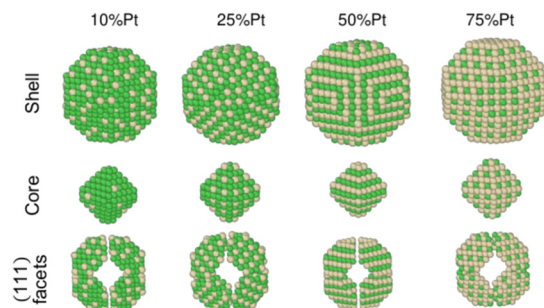
15181



### A two-step quadrature-based variational calculation of ro-vibrational levels and wavefunctions of $\text{CO}_2$ 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

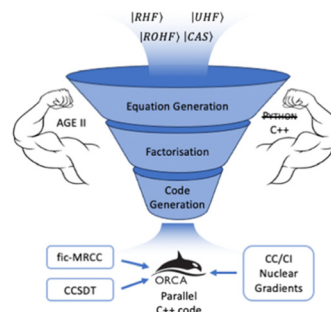
Pamela Camilos,\* Céline Varvenne and Christine Mottet



15205

## Code generation in ORCA: progress, efficiency and tight integration

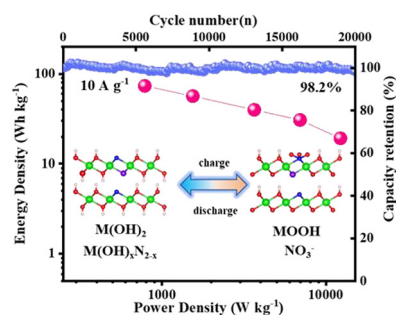
Marvin H. Lechner,\* Anastasios Papadopoulos,\* Kantharuban Sivalingam, Alexander A. Auer, Axel Koslowski, Ute Becker, Frank Wennmohs and Frank Neese\*



15221

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

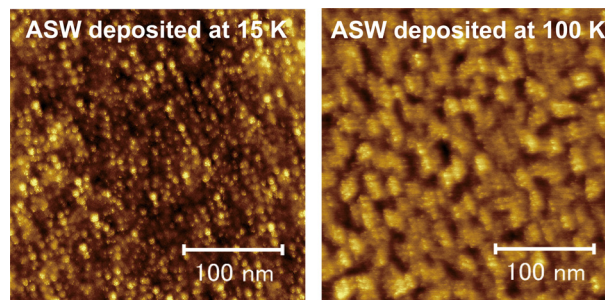
Tao Li, Jinyue Song, Hongguang Fan, Yanpeng Wang, Yusheng Luo, Chenchen Shao, Qingping Li and Wei Liu\*



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

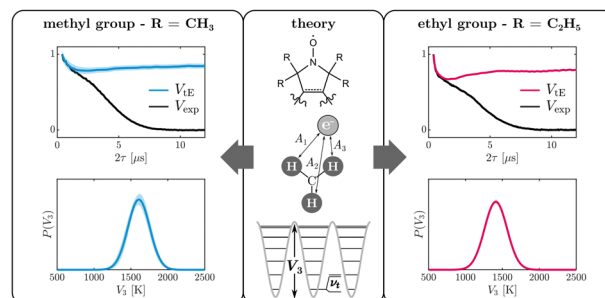
Takuto Tomaru, Hiroshi Hidaka,\* Akira Kouchi and Naoki Watanabe



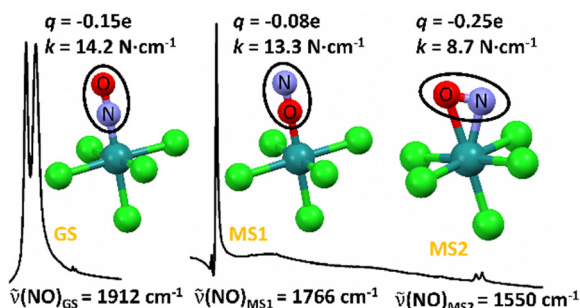
15240

## Exploring tunneling ESEEM beyond methyl groups in nitroxides at low temperatures

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



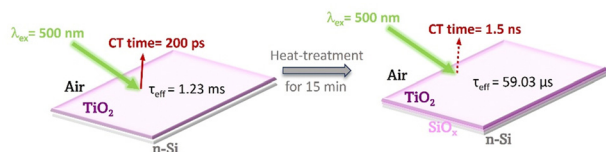
15255



### 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\*

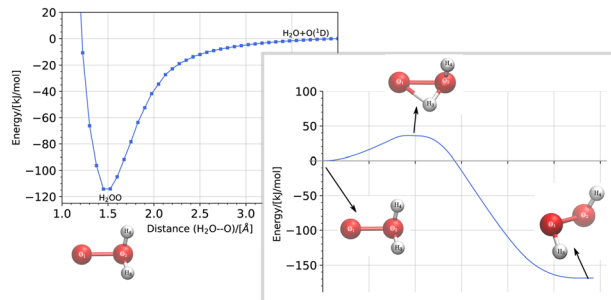
15268



### Contactless analysis of surface passivation and charge transfer at the TiO<sub>2</sub>–Si interface

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

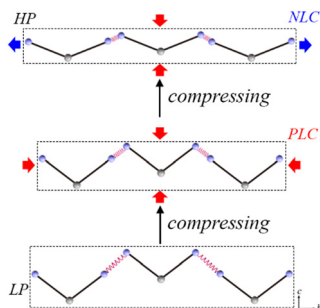
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### Unraveling the interaction between singlet state atomic oxygen O(<sup>1</sup>D) and water: toward the formation of oxywater and hydrogen peroxide

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\*

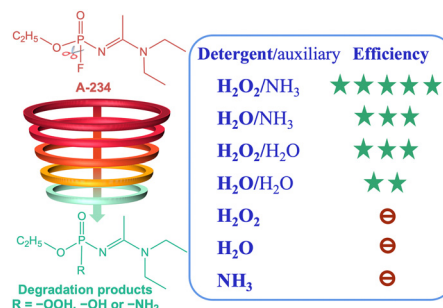


## RESEARCH PAPERS

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

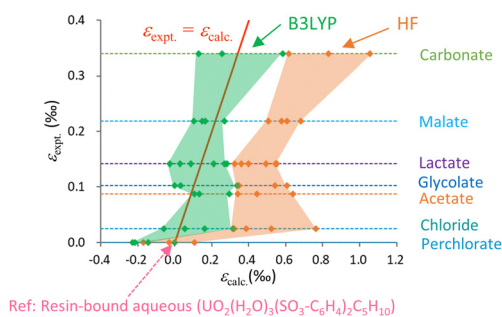
Rongxin Shi, Lin Zhang, Denghui Ma and Zexing Cao\*



15301

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

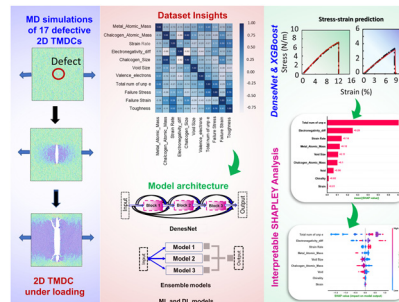
Ataru Sato, Masahiko Hada and Minori Abe\*



15316

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

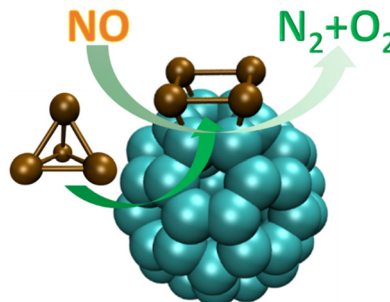
Ankit Anuragi, Ankit Das, Akash Baski, Vinay Maithani and Sankha Mukherjee\*



15332

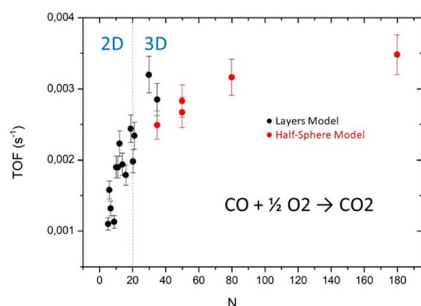
### Direct reduction of NO into N<sub>2</sub> catalyzed by fullerene-supported rhodium clusters

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



## RESEARCH PAPERS

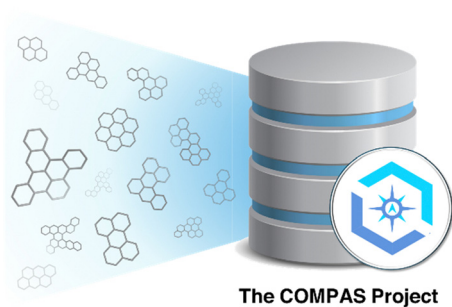
15338



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

Georges Sitja\* and Claude R. Henry\*

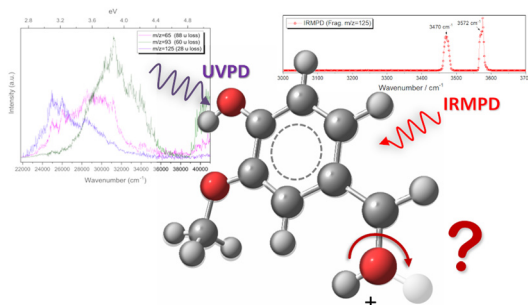
15344



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

Alexandra Wahab and Renana Gershoni-Poranne\*

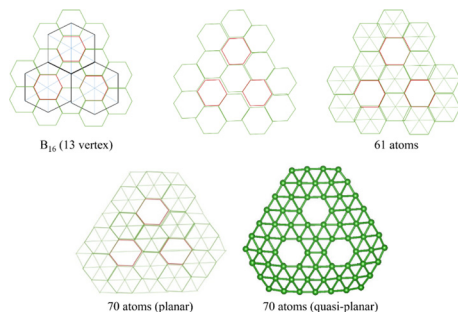
15358



### 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<sub>70</sub> boron cluster and its dianion

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

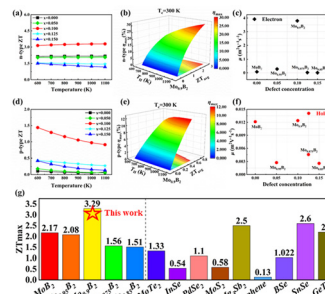


## RESEARCH PAPERS

15376

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

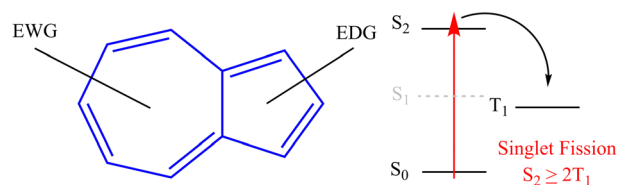
Jie Pu, Ziyu Hu\* and Xiaohong Shao\*



15386

## Designing potentially singlet fission materials with an anti-Kasha behaviour

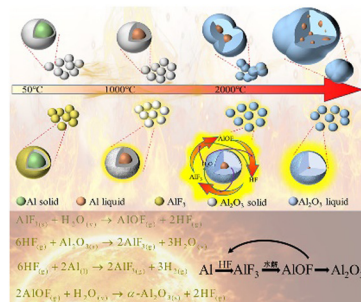
Ricardo Pino-Rios,\* Rodrigo Báez-Grez, Dariusz W. Szczepanik and Miquel Solà\*



15393

Enhancing the combustion of nAl with  $\text{AlF}_3$  coating: gas–solid reaction mechanism for reducing combustion agglomeration of Al powder

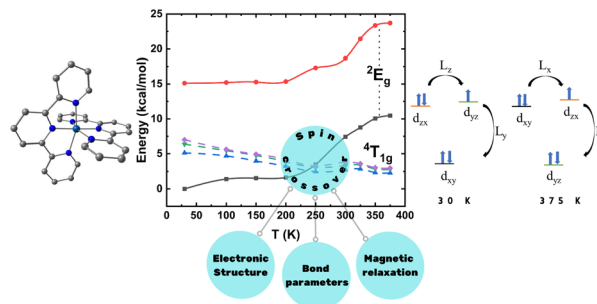
Chen Shen, Shi Yan,\* Jie Yao, Hui Ren, Xueyong Guo, Jianxin Nie, Yapeng Ou, Qingjie Jiao and Yunjun Luo



15405

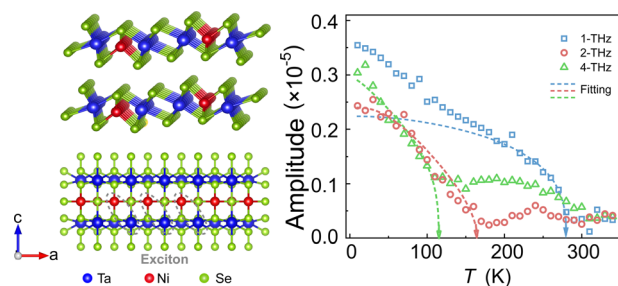
*Ab initio* calculation of magnetic anisotropy and thermal spin transition in the variable temperature crystal conformations of  $[\text{Co}(\text{terpy})_2]^{2+}$ 

Moromi Nath, Shalini Joshi and Sabyashachi Mishra\*



## RESEARCH PAPERS

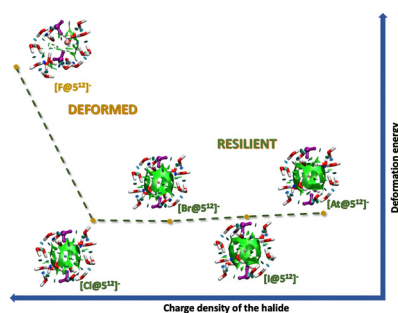
15417



### Multiple coherent amplitude modes and exciton–phonon coupling in quasi-one-dimensional excitonic insulator $\text{Ta}_2\text{NiSe}_5$

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

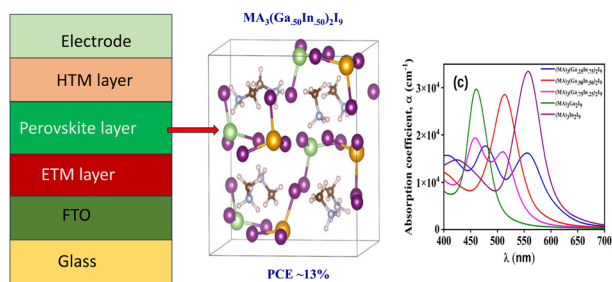
15426



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

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

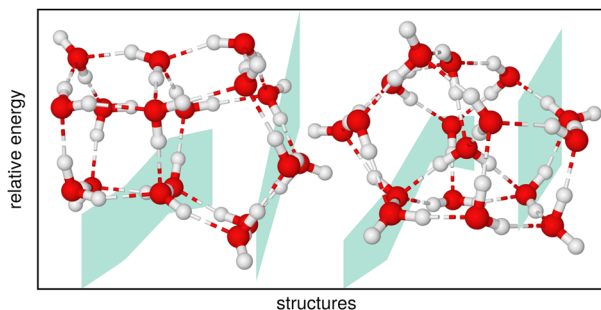
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### Ga and In-based hybrid halide perovskites as an alternative to Pb: a first principles study

Tridip Chutia, Tanmoy Kalita, Uddipana Saikia and Dhruva Jyoti Kalita\*

15445



### On the brink of self-hydration: the water heptadecamer

Bernd Hartke

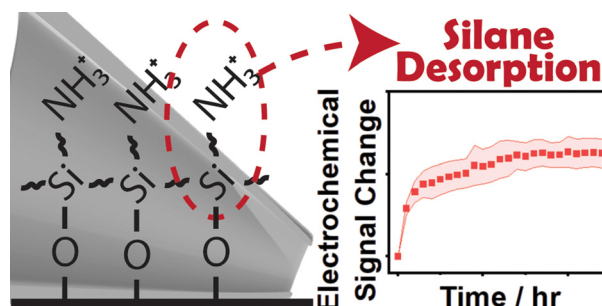


## RESEARCH PAPERS

15452

**Reproducibility and stability of silane layers in nanoconfined electrochemical systems**

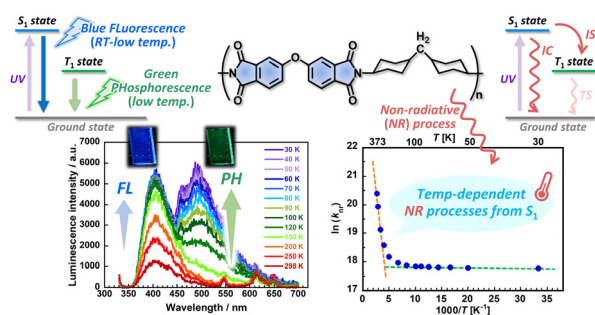
Dominik Duleba, Shekemi Denuga and Robert P. Johnson\*



15461

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

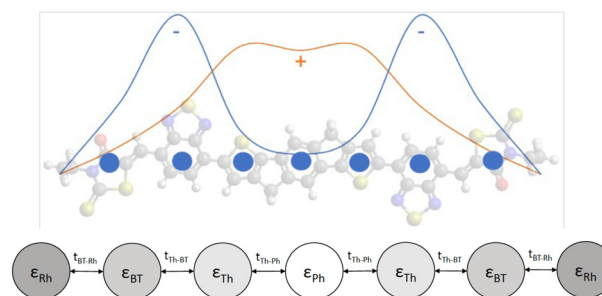
Mayuko Nara, Eisuke Fujiwara, Aurimas Vyšniauskas, Vidmantas Gulbinas\* and Shinji Ando\*



15472

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

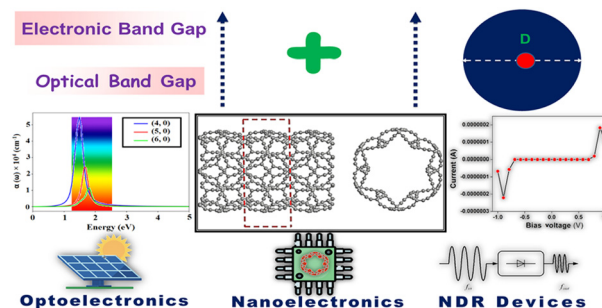
Vishal Jindal, Mohammed K. R. Aldahdooh, Enrique D. Gomez, Michael J. Janik and Scott T. Milner\*



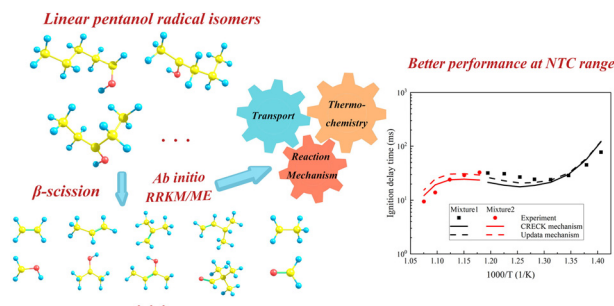
15484

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

Jyotirmoy Deb, N. Bedamani Singh and Utpal Sarkar\*



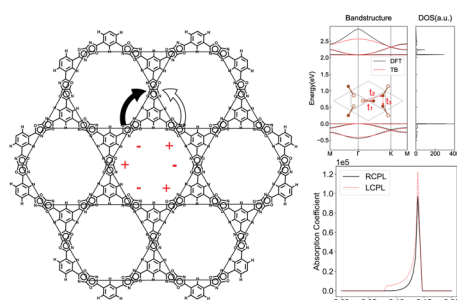
15494



## 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\*

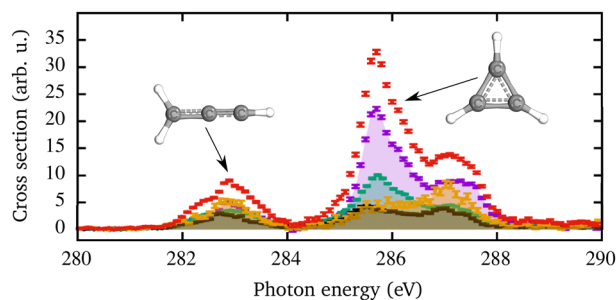
15511



## 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\*

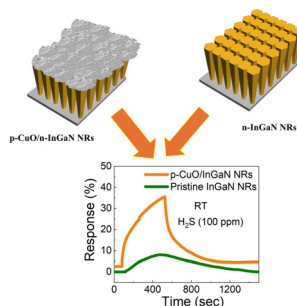
15519



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

Simon 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<sub>2</sub>S gas detection

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

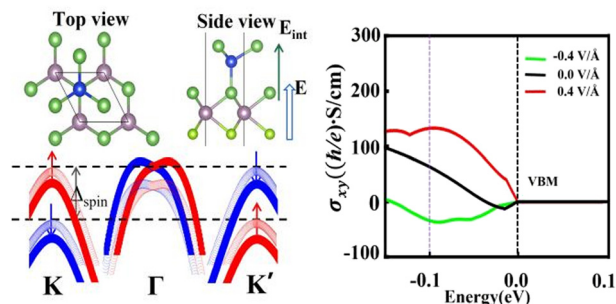


## RESEARCH PAPERS

15539

**Spin Hall effect modulated by an electric field in asymmetric two-dimensional MoSiAs<sub>2</sub>Se**

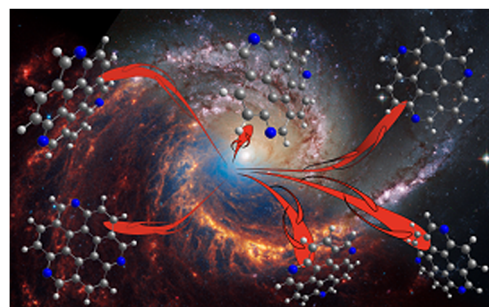
Jinhui Xing, Chao Wu, Shiqi Li, Yuanping Chen, Lizhi Zhang, Yuee Xie,\* Jiaren Yuan\* and Lichuan Zhang\*



15547

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

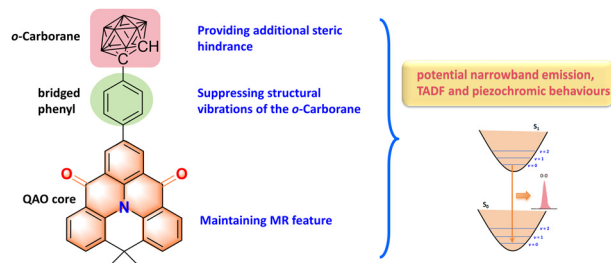
Domenik Schleier,\* Jerry Kamer, Andy Jiao, Grégory F. Schneider, Harold Linnartz and Jordy Bouwman\*



15559

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

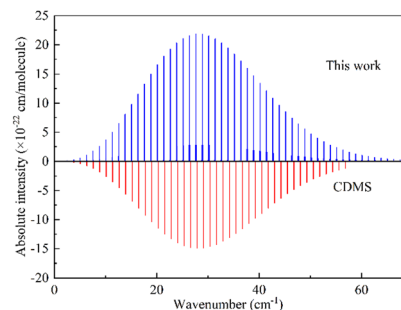
Qing Zhang, Tao Liu, Yuhua Guo, Yujian Zhang, Chunyan Lv,\* Yue Zhang\* and Zexing Cao\*



15569

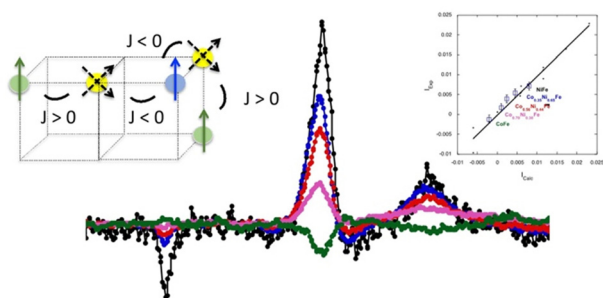
**High-temperature rotation–vibration spectrum of iminosilylene (HNSi)**

Ximing Li, Zhi Qin and Linhua Liu\*



## RESEARCH PAPERS

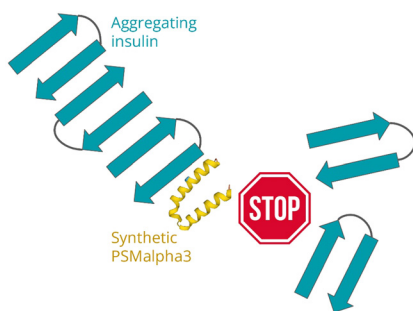
15576



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

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

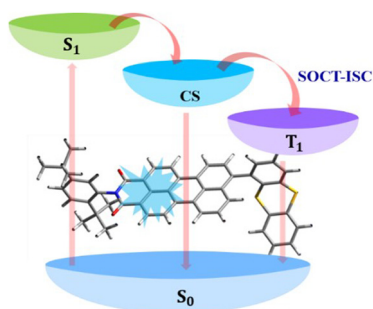
15587



**Cytotoxic *Staphylococcus aureus* PSM $\alpha$ 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\*

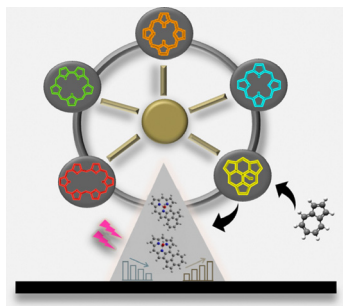
15600



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

Suman Dhama, 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\*

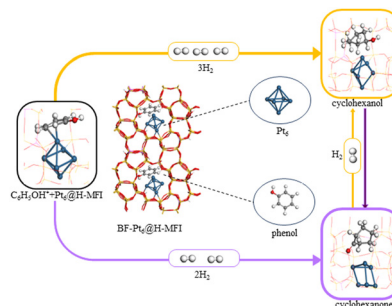


## RESEARCH PAPERS

15620

## Phenol hydrogenation over H-MFI zeolite encapsulated platinum nanocluster catalyst

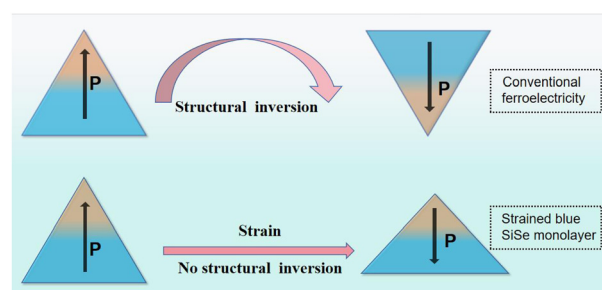
Kexin Wang, Weiwei Zhang\* and Donghai Mei\*



15629

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

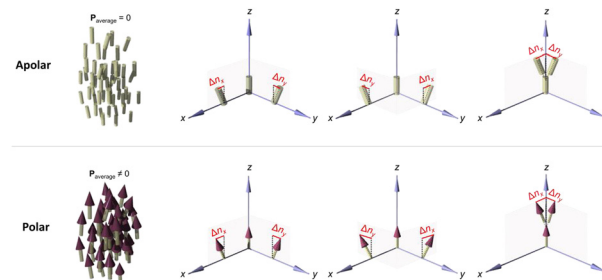
Yan-Dong Guo,\* Rui-Jie Meng, Xue-Qin Hu, Li-Yan Lin, Yu-Rong Yang,\* Ming-Yu Yang, Yun You, Lan-Qi Zhang, Yi-Long Xu and Xiao-Hong Yan



15637

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

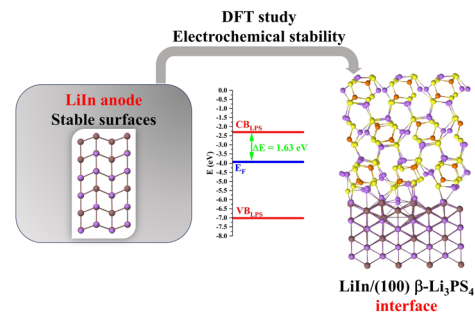
Yu Zou and Satoshi Aya\*



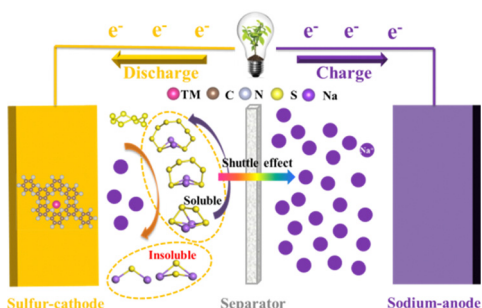
15648

A computational study of the negative LiIn modified anode and its interaction with  $\beta$ -Li<sub>3</sub>PS<sub>4</sub> solid–electrolyte for battery applications

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



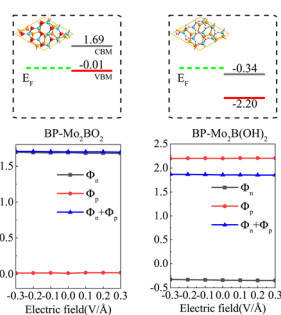
15657



### Single-atom catalysts based on C<sub>2</sub>N for sulfur cathodes in Na–S batteries: a first-principles study

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

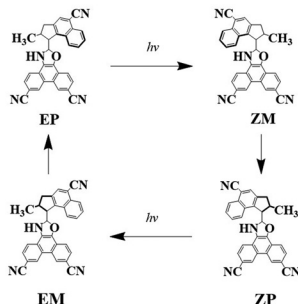
15666



### Surface-engineered Mo<sub>2</sub>B: 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\*

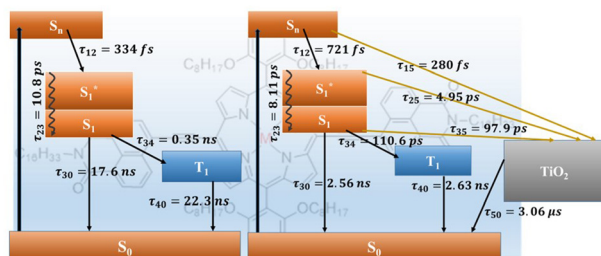
15672



### 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\*

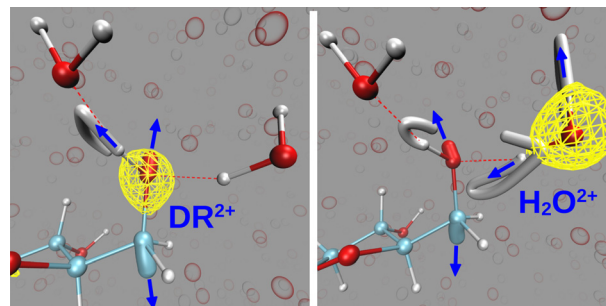


## RESEARCH PAPERS

15693

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

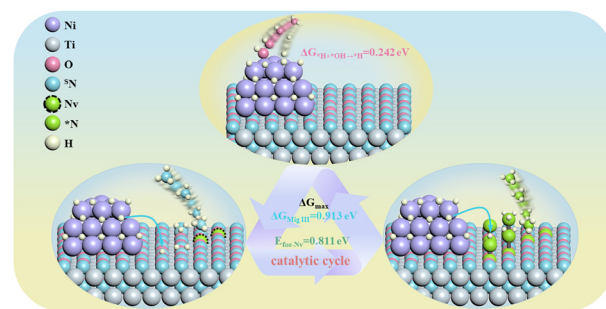
Marie-Anne Hervé du Penhoat,\* Alexandre Souchaud, Aashini Rajpal, Rodolphe Vuilleumier, Marie-Pierre Gaigeot, Ivano Tavernelli, Kentaro Fujii, Akinari Yokoya, Sergio Díaz-Tendero and Marie-Françoise Politis



15705

**\*H migration-assisted MvK mechanism for efficient electrochemical NH<sub>3</sub> synthesis over TM–TiNO**

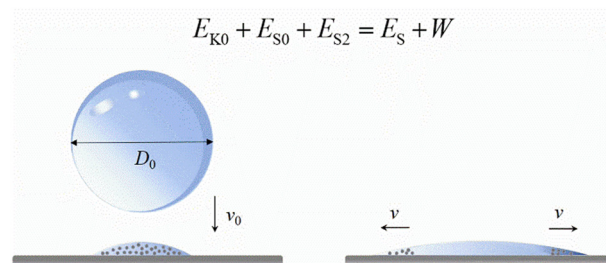
Luyao Cui, Zijun Sun, Yawen Wang, Xuan Jian, Houfen Li, Xiao Zhang, Xiaoming Gao, Rui Li\* and Jianxin Liu\*



15717

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

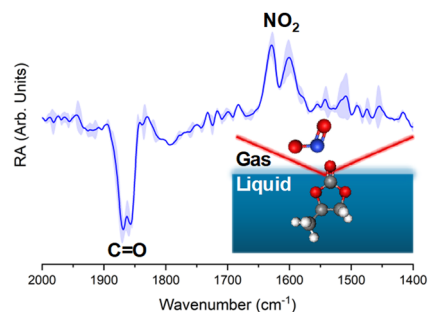
Jiale Wang, Lei Li, Xinlong Lu, Yu Zhou, Jiandong Zhou and Dengwei Jing\*



15733

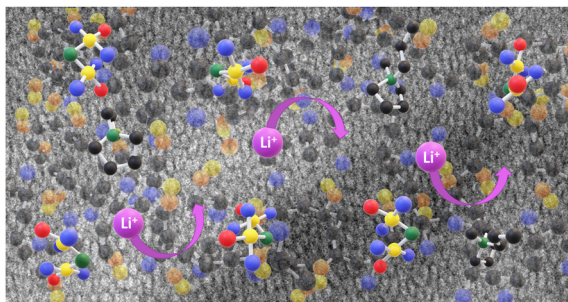
**Interfacial carbonyl groups of propylene carbonate facilitate the reversible binding of nitrogen dioxide**

Jessica B. Clark and Heather C. Allen\*



## RESEARCH PAPERS

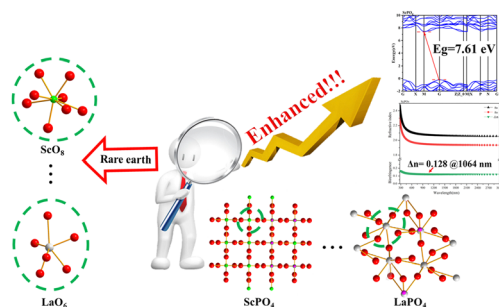
15742



### 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

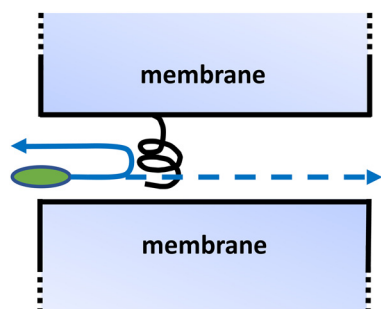
15751



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

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

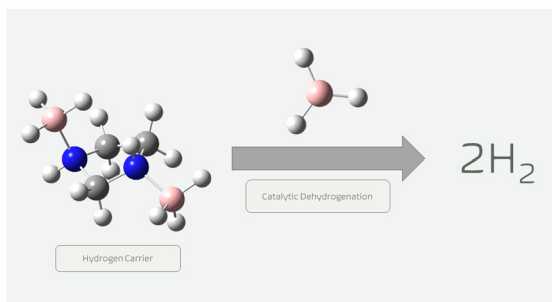
15758



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

Fathima Rifana Mohamed Irfan and Sarah L. Masters\*

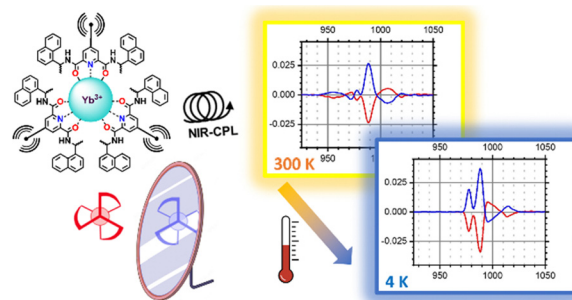


## RESEARCH PAPERS

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<sub>70</sub> boron cluster and its dianion**

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

