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Cover

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Inside cover

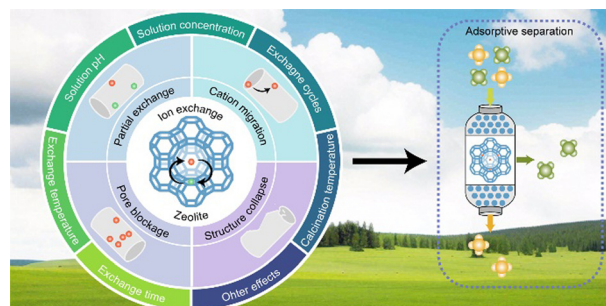
See Kazuteru Shinozaki *et al.*, pp. 15850–15857. Image reproduced by permission of Kazuteru Shinozaki from *Phys. Chem. Chem. Phys.*, 2025, 27, 15850.

TUTORIAL REVIEW

15819

Ion exchange: an essential piece in the fabrication of zeolite adsorbents

Chenxin Li, Tiesen Li,* Qingyan Cui, Tinghai Wang, Chan Wang, Jiao Yang, Jie Shi, Xiaojun Bao and Yuanyuan Yue*

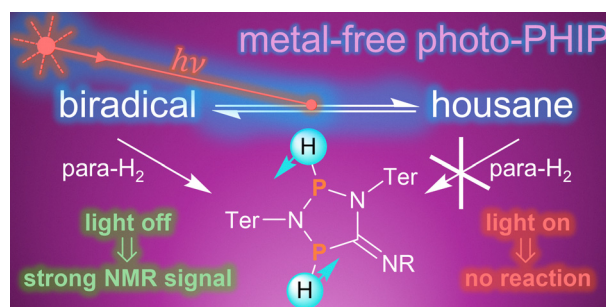


COMMUNICATIONS

15835

Photoswitchable, metal-free parahydrogen-induced polarization enabled by a phosphorus biradicaloid

Vladimir V. Zhivonitko,* Karolina Konsewicz, Jonas Bresien and Axel Schulz



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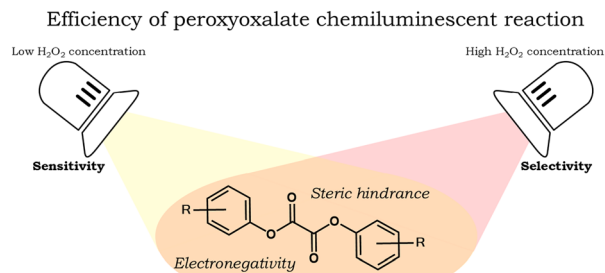
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COMMUNICATIONS

15840

Factors underlying sensitivity of aromatic oxalates in peroxyoxalate chemiluminescent reaction in aqueous-organic media

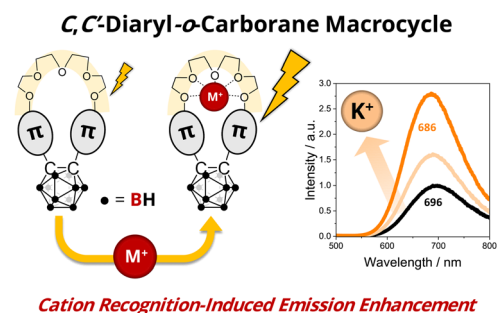
Evgenii O. Fomin, Nikolai P. Iakimov, Ekaterina M. Budynina, Irina D. Grozdova and Nikolay S. Melik-Nubarov*



15845

Macrocyclic C,C'-diaryl-o-carborane derivatives containing pseudo-crown ether: emission enhancement upon cation recognition

Mei Tokutomi, Kazuhiro Yuhara and Kazuo Tanaka*

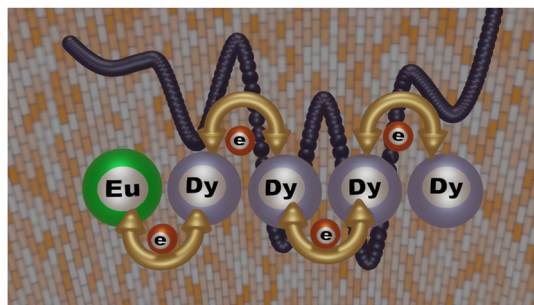


RESEARCH PAPERS

15850

Visualization of trap distribution in $\text{SrAl}_2\text{O}_4:\text{Eu}^{2+}, \text{Dy}^{3+}$ revealed by simulations of luminescence changes in charging and emission of persistent luminescence and thermoluminescence based on a random walk model

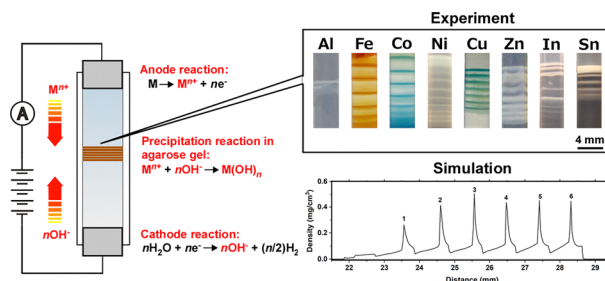
Ryusuke Koizumi, Ryoya Takahashi, Shigeki Yamada, Shingo Hattori and Kazuteru Shinozaki*



15858

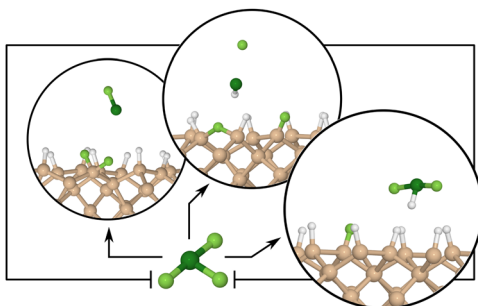
Periodic precipitation banding of metal hydroxides in agarose gels via cyclic-voltage-driven reaction–transport–reaction process

Hisashi Hayashi,* Rina Arifuku, Kaho Yamada, Misato Nampo, Kana Ogitani and Toyohiko Aiki



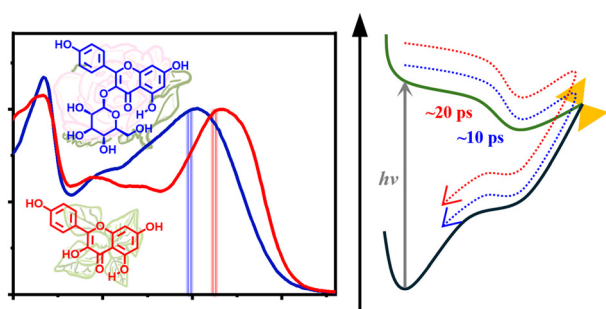
RESEARCH PAPERS

15872

**Mechanistic diversity in the reactive adsorption of chlorine trifluoride on monohydrogenated silicon**

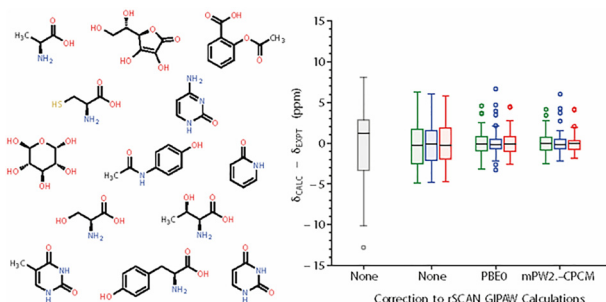
Henry Thake and Stephen J. Jenkins*

15895

**Excited state deactivation in phytochemical flavonoids: astragalin and kaempferol**

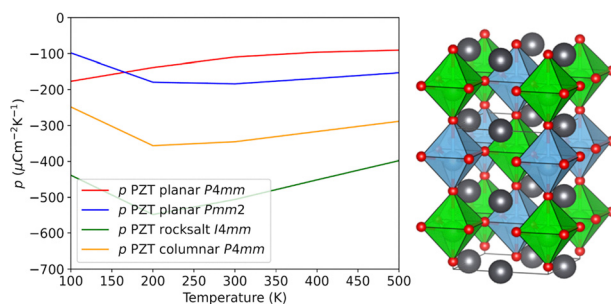
Michael Hymas, Jacob Eller, Mohammad Salehi, Reza Omidyan,* Stéphane Poigny* and Vasilios G. Stavros*

15906

**Combining double-hybrid functionals with rSCAN yields solid-state ^{13}C chemical shifts with sub-ppm accuracy**

Harry Brough, Chris W. Cook, John M. Griffin and Michael J. G. Peach*

15920

**Pyroelectric properties of $\text{Pb}[\text{Zr}_{0.5}\text{Ti}_{0.5}]\text{O}_3$ studied with a hybrid density functional method**

Kim Eklund and Antti J. Karttunen*

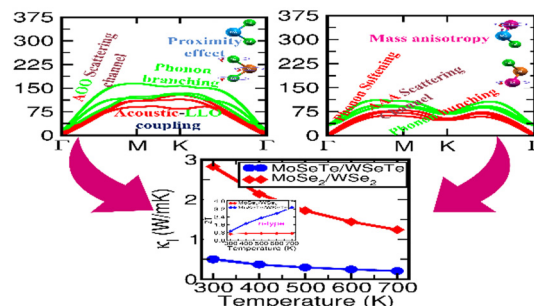


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Ultra-low lattice thermal conductivity and high thermoelectric performance in chiral phonon-protected heterostructures

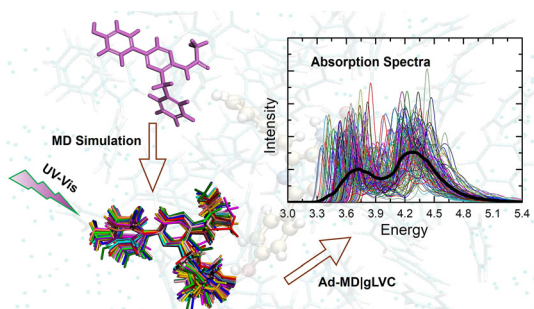
Jipin Peter, Tanu Choudhary and Raju K. Biswas*



15946

Modelling the role of internal flexibility and inter-state couplings modulated by an explicit environment in the absorption spectrum of coelenteramide

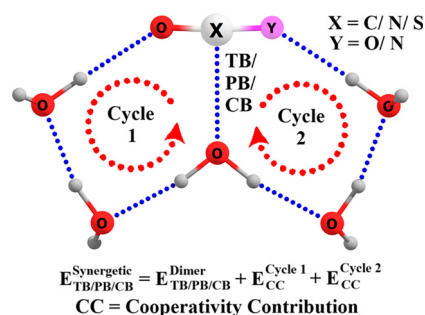
Mohammad Aarabi, Samira Gholami,* Samuele Giannini, Marco Garavelli, Giacomo Prampolini and Fabrizio Santoro*



15960

Synergistic cyclic cooperativity governs the strength of chalcogen, pnictogen and tetrel bonds in microhydrated clusters

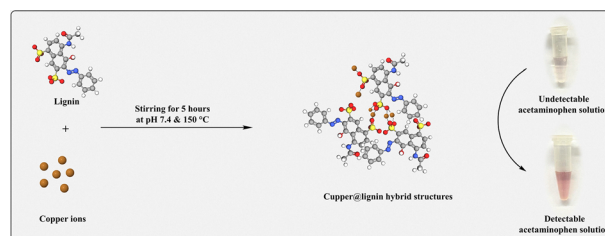
Ayush Shivhare, Chandan Kumar Lenka, Bharti Dehariya and Milind M. Deshmukh*



15975

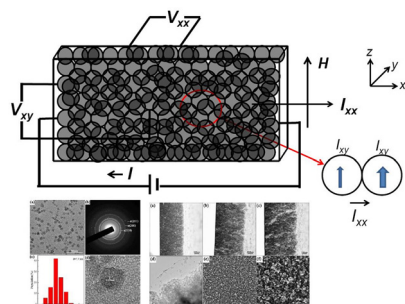
Synthesis and characterization of lignin–copper nanohybrids for colorimetric acetaminophen detection: a combined physical chemistry and machine learning study

Fatemeh Parad, Soroush Mohaddes, Fahimeh Ghasemi, Mohammad Ali Faramarzi* and Somayeh Mojtavavi*



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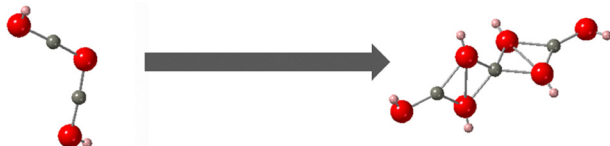
15993



Enhancement of the anomalous Hall effect *via* interfacial scattering in thick Fe nanocluster-assembled thin films

Junbao Wang,* Lanju Liang, Ju Gao, Jianquan Li and Xiaozhong Tian

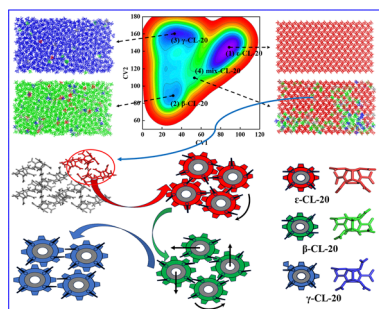
16003



Inorganic chemistry, cluster formation and solvent stability of PIM-1/ZnO_xH_y hybrid membranes synthesized *via* vapor phase infiltration

Benjamin C. Jean, Yi Ren, Ethan Read, Dong-Chan Lee, Faisal Alamgir, Ryan P. Lively and Mark D. Losego*

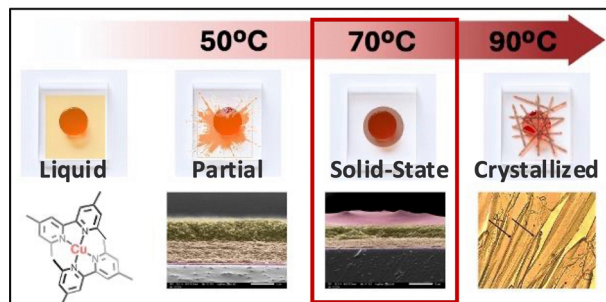
16012



Solid–solid polymorphic transition of 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (CL-20) at high temperature by metadynamics simulations

Chaoyu Wang, Yuchuan Shi, Chaoyang Zhang,* Bo You and Xianggui Xue*

16022



Temperature-guided solidification of copper coordination complexes as hole transport materials

Timo Keller, Iacopo Benesperi, Jakob Thyr, Tomas Edvinsson, Elizabeth A. Gibson and Marina Freitag*

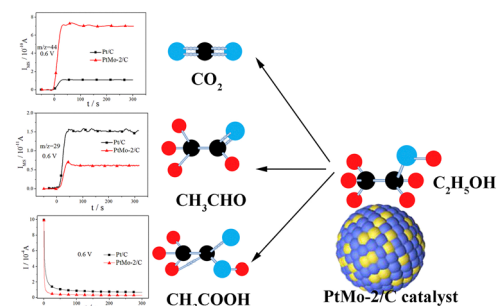


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Ethanol electro-oxidation on a carbon-supported Pt–Mo electrocatalyst: a study by pinhole on-line differential electrochemical mass spectrometry

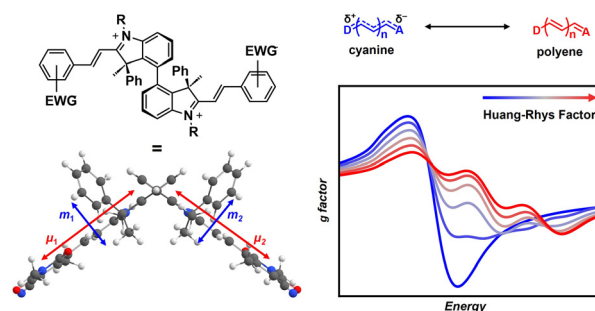
Kyong–Mi Kim, Kyong–Sik Ju* and Sung–Nam Pak



16039

Chiroptical properties of axially chiral indolenine merocyanine dimers: role of the Huang–Rhys factor and interchromophore mixing of electric and magnetic transition dipole moments

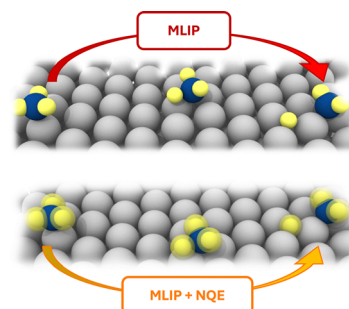
Emely Freytag, Michael Hofer, Michael Kopp, Marco Holzapfel, Matthias Stolte, Frank Würthner, Thomas Renger* and Christoph Lambert*



16051

Nuclear quantum effects of metal surface-mediated C–H activation

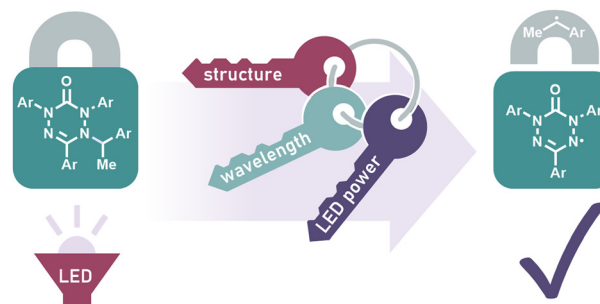
Rhys J. Bunting, Sam Shepherd, Nikhil Rampal, Sneha Akhade, David M. Wilkins* and Tuan Anh Pham*



16057

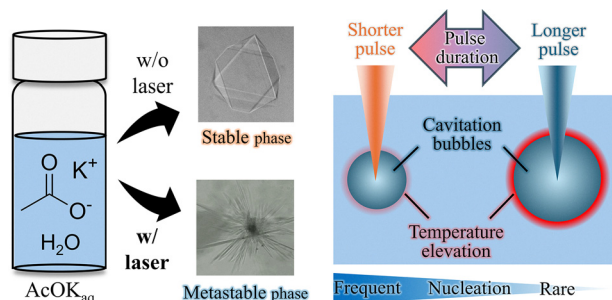
Photolysis of labile bonds towards radical generation: case study of alkyl verdazyls

Ekaterina S. Kovalskaya, Alexander E. Kurtsevich, Darya E. Votkina, Rashid R. Valiev,* Pavel S. Postnikov* and Pavel V. Petunin*



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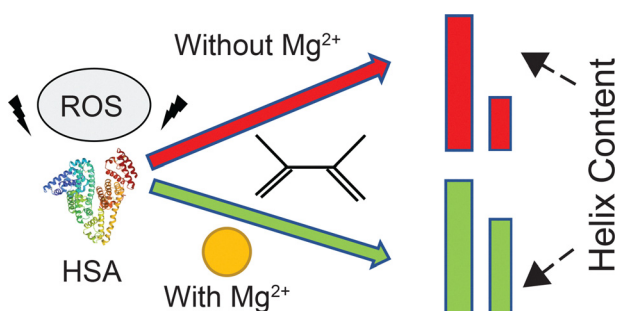
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Metastable-phase crystallization of potassium acetate triggered by focused irradiation with ultrashort laser pulses

Hozumi Takahashi* and Hiroshi Y. Yoshikawa*

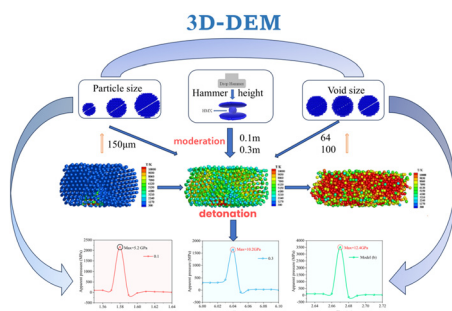
16077



Effect of magnesium(II) on the glycation-induced oxidative stress of human serum albumin: a spectroscopic investigation

Debdip Brahma, Utkarsh Sinha and Amar Nath Gupta*

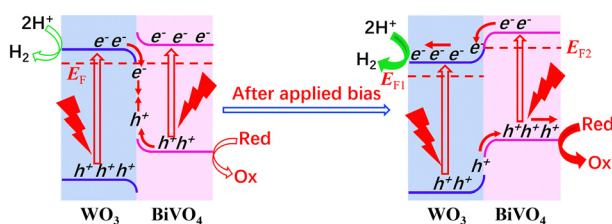
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A 3D-DEM study on influencing factors of ignition, combustion, and detonation of single HMX particles with voids

Jing Liu, Zhi-Xin Bai,* Fu-Sheng Liu and Qi-Jun Liu*

16103



Efficient photoelectrocatalytic performances using a $\text{WO}_3/\text{BiVO}_4$ heterojunction photoanode: applied bias-promoted photoinduced charge transfer and separation

Yunni Liu, Yuna Kang, Zhenyi Zhang and Jun Lin*

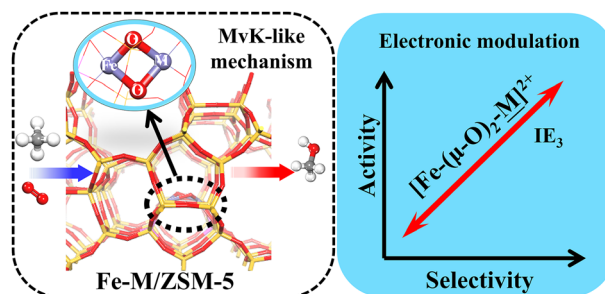


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16113

Mechanistic insights into electronic modulation of binuclear iron-based zeolites for selective oxidation of methane to methanol

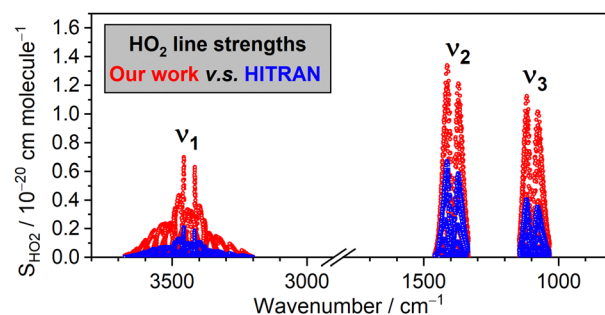
Lu Cheng and Xiao-Ming Cao*



16123

Precision measurements of absolute line strengths of the HO₂ radical in the ν_1 and ν_2 vibrational bands

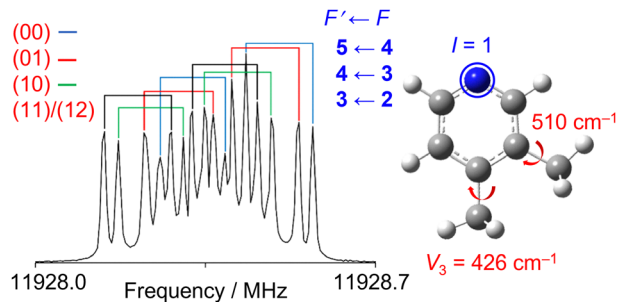
I-Yun Chen, Che-Wei Chang, Qian-Rui Huang, Jer-Lai Kuo and Pei-Ling Luo*



16135

Complex hyperfine-fine structure overlapping in the microwave spectrum of 3,4-lutidine

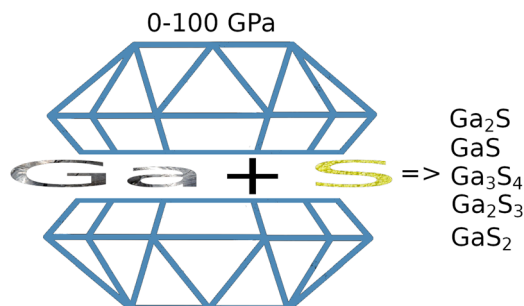
Eléonore Antonelli and Ha Vinh Lam Nguyen*



16142

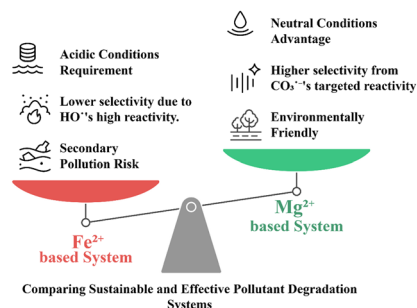
Prediction of novel gallium–sulfur compositions under pressure

Reza Shahsavari, Sylvain Pitié, Somayeh Faraji, Lewis J. Conway, Chris J. Pickard, S. Javad Hashemifar, Alireza Shahidi and Gilles Frapper*



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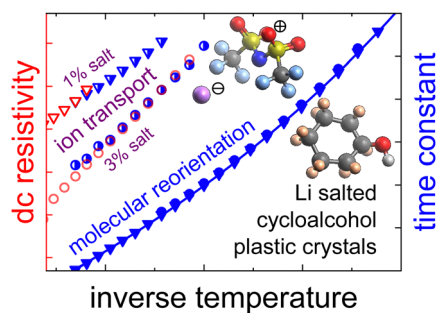
16153



Magnesium(II)-bicarbonate complexes catalyze the Fenton-like reaction under nearly neutral conditions: kinetics and mechanism

Anushka Lucas, Dalia Gitin, Tomer Zidki, Prashant H. Desai, Alexander I. Shames, Virender K. Sharma, Haya Kornweitz,* Yael Albo* and Dan Meyerstein*

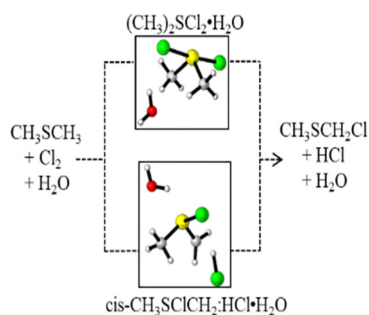
16161



Coupling and decoupling of molecular reorientation and charge transport in Li-salt-doped cycloalcohol ion conductors

Sofiane Lansab, Yannik Hinz, Bastian Grabe, Peter Lunkenheimer and Roland Böhmer

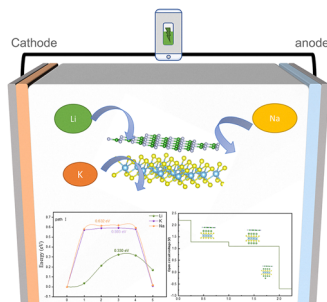
16172



A study of the atmospherically relevant reaction between dimethyl sulphide (DMS) and Cl₂ in the absence and presence of water using electronic structure methods

Lydia Rhyman,* Edmond P. F. Lee, Ponnadurai Ramasami* and John M. Dyke*

16182



Exploring the enhanced anode performance of BN/TiS₂ heterostructures for Li/Na/K-ion batteries via first-principles calculations

Qi Wang, Xing Wei, Mengya Li, Yan Zhang, Yun Yang, Jian Liu, Ye Tian, Ziyuan Li, Shijie Wei and Li Duan*

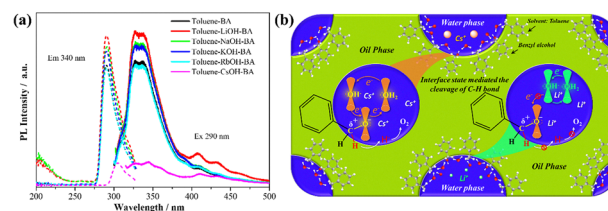


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16195

Alkali metal cation-anchored hydrated hydroxide complexes at the nanoscale interface as catalytic active sites for selective liquid-phase aerobic oxidation of benzyl alcohol to benzaldehyde

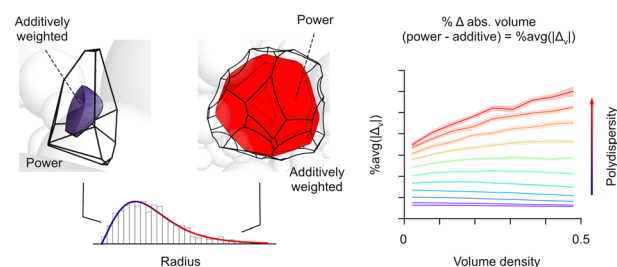
Bo Peng, Weiyu Zhou, Jiayu Dong, Changjiu Xia,*
Peng Wu and Kun Zhang*



16204

Evaluation of weighted Voronoi decompositions of physicochemical ensembles

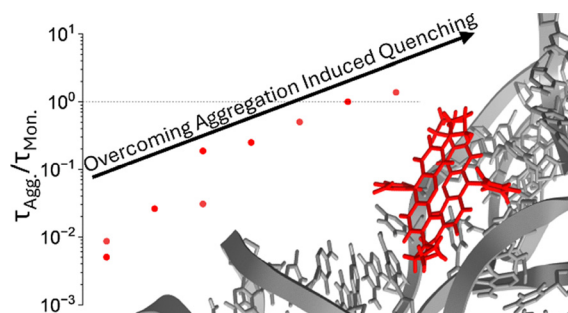
John M. Ericson, Nicola Wolpert* and
Gregory M. K. Poon*



16219

Overcoming aggregation-induced quenching in DNA-assembled rhodamine dimers

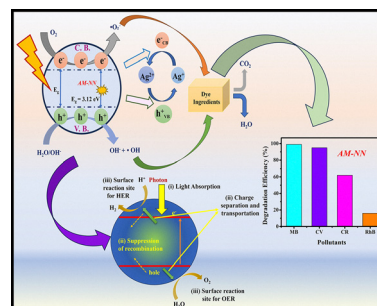
Paul Cavanaugh, Simon K. Roy, Austin Biaggne,
Maia Ketteridge, Matthew S. Barclay, Ryan Rau,
Jeunghoon Lee, Paul H. Davis, William B. Knowlton,
Bernard Yurke, Jacob C. Dean, Lan Li, Daniel B. Turner
and Ryan D. Pensack*



16236

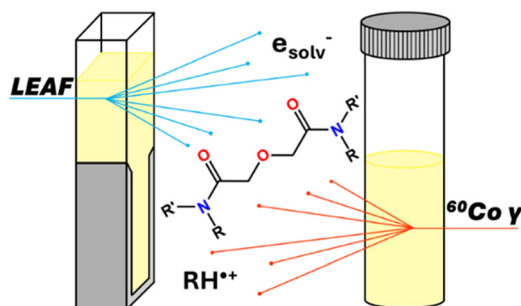
Oxygen vacancies assisted photocatalytic dye degradation and photoelectrochemical water splitting performance in Ag and Mg-modified NaNbO₃

Arpita Singha, Mohit Kumar, Phyu Phyu Cho,
Sireesha Lavadiya, Sai Santosh Kumar Raavi,
Challapalli Subrahmanyam and Saket Asthana*



RESEARCH PAPERS

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Impacts of molecular architecture on the radiation-induced degradation and reaction kinetics of hydrophobic diglycolamides with the solvated electron and the dodecane radical cation

Michaela R. Bronstetter,* Gregory P. Horne,* Andrew R. Cook, Stephen P. Mezyk, Joseph R. Wilbanks, Bobby Layne, Alyssa Gaiser and Jacy K. Conrad*

CORRECTIONS

16264

Correction: Superconductivity and high hardness in scandium-borides under pressure

Xiangru Tao, Aiqin Yang, Yundi Quan* and Peng Zhang*

16265

Correction: Exciton dynamics from the mapping approach to surface hopping: comparison with Förster and Redfield theories

Johan E. Runeson,* Thomas P. Fay and David E. Manolopoulos

16266

Correction: Influence of pseudo-Jahn–Teller activity on the singlet–triplet gap of azaphenalenenes

Atreyee Majumdar, Komal Jindal, Surajit Das and Raghunathan Ramakrishnan*

