

Dalton Transactions

An international journal of inorganic chemistry incorporating Acta Chemica Scandinavica
rsc.li/dalton

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

ISSN 1477-9226 CODEN DTARAF 53(34) 14119–14506 (2024)



Cover
See Feng Li *et al.*,
pp. 14144–14152.

Image reproduced by
permission of Feng Li from
Dalton Trans., 2024, **53**,
14144.

Acknowledgment:
Background by zoom-zoom
via iStock



Inside cover
See Yu Xiao *et al.*,
pp. 14153–14162.

Image reproduced by
permission of Yu Xiao from
Dalton Trans., 2024, **53**,
14153.

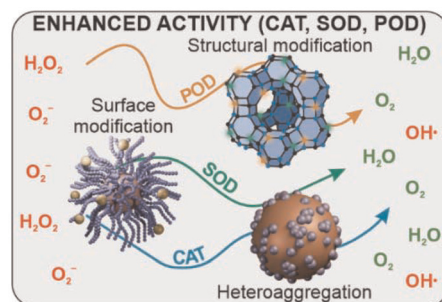
Acknowledgment: Created in
part with iStock AI image
generator

FRONTIER

14132

Engineering inorganic nanozyme architectures for decomposition of reactive oxygen species

Tibor G. Halmagyi, Laila Noureen, Adél Szerlauth and Istvan Szilagyí*

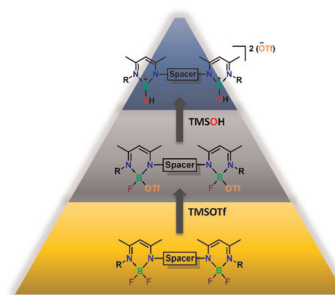


COMMUNICATION

14139

Bis(diiminato)-based boron difluoro complexes: effective synthon for bis(borenium) cations

Darakshan Parveen, Rahul Kumar Yadav, Bijan Mondal, Marie Dallon, Yann Sarazin and Dipak Kumar Roy*



**GOLD
OPEN
ACCESS**

EES Batteries

**Exceptional research on
batteries and energy storage**

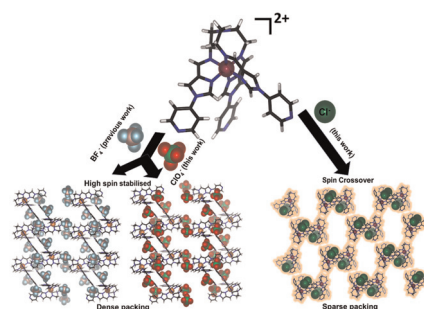
Part of the EES family

**Join
in** | Publish with us
rsc.li/EESBatteries

14144

Spin crossover of a Fe(II) mononuclear complex induced by intermolecular factors involving chloride and solvent ordering

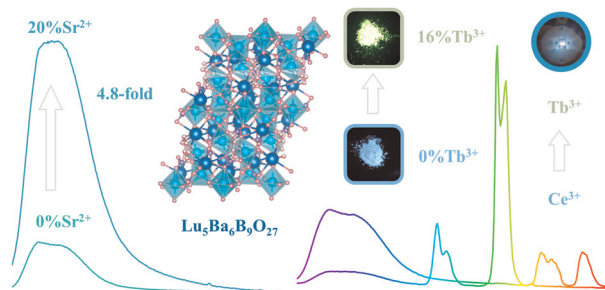
Kenneth Zhang, Matthew J. Wallis, Alexander R. Craze, Shinya Hayami, Hyunsung Min, Daniel J. Fanna, Mohan M. Bhadbhade, Ruoming Tian, Christopher E. Marjo, Leonard F. Lindoy and Feng Li*



14153

A novel borate phosphor $\text{Lu}_5\text{Ba}_6\text{B}_9\text{O}_{27}:\text{Ce}^{3+}$ codoped with $\text{Sr}^{2+}/\text{Tb}^{3+}$ for NUV-white light emitting diode application

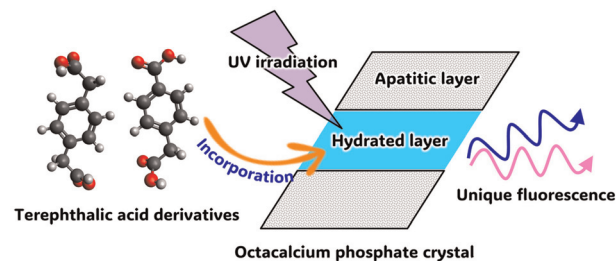
Chenggang Ma, Hailiang Chen, Min Luo, Fuyun Duan, Yun Ding, Yihang Han, Tianxiang Zheng, Xun Yang and Yu Xiao*



14163

Octacalcium phosphate with incorporated terephthalate ion derivatives: novel guest molecules and unique fluorescence properties

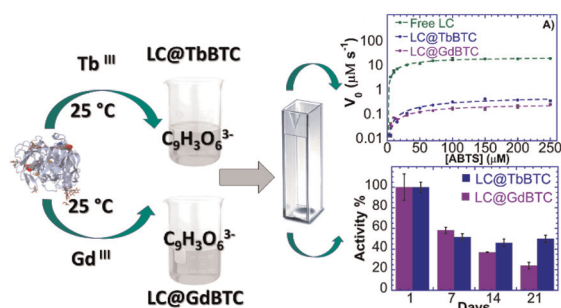
Taishi Yokoi,* Masahiro Watanabe and Masakazu Kawashita



14171

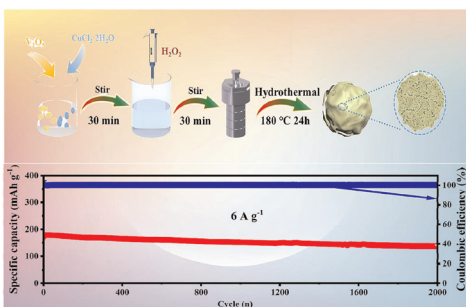
A green approach to encapsulate proteins and enzymes within crystalline lanthanide-based Tb and Gd MOFs

Davide Tocco, Madhura Joshi, Rosangela Mastrangelo, Emiliano Fratini, Andrea Salis* and Martin Hartmann



PAPERS

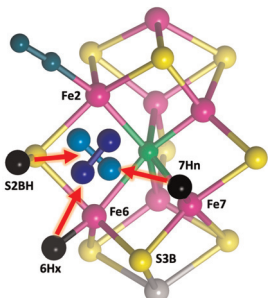
14182



Engineering VO_x structure by integrating oxygen vacancies for improved zinc-ion storage based on cation-doping regulation with electric density

Juan Xu,* Nengneng Han, Sihao Chen, Yahui Zhang, Yuezhou Jing, Pibin Bing and Zhongyang Li*

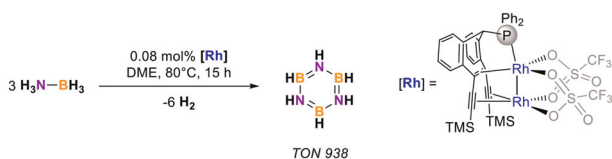
14193



The activating capture of N₂ at the active site of Mo–nitrogenase

Ian Dance

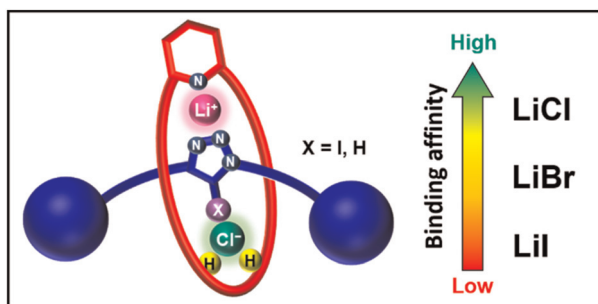
14212



Selective dehydrogenation of ammonia borane to borazine and derivatives by rhodium olefin complexes

Pascal Jurt, Juan José Gamboa-Carballo, Clara Schweinzer, Daniel Himmelbauer, Debora Thöny, Thomas L. Gianetti,* Monica Trincado* and Hansjörg Grützmacher*

14219



Lithium chloride selective ion-pair recognition by heteroditopic [2]rotaxanes

Vihanga K. Munasinghe, Hui Min Tay, Dilhan Manawadu, Jessica Pancholi, Zongyao Zhang and Paul D. Beer*

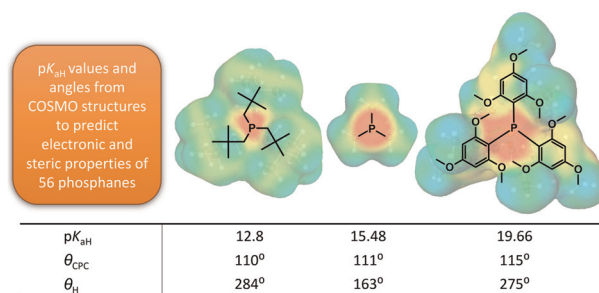


PAPERS

14226

 pK_{aH} values and θ_H angles of phosphanes to predict their electronic and steric parameters

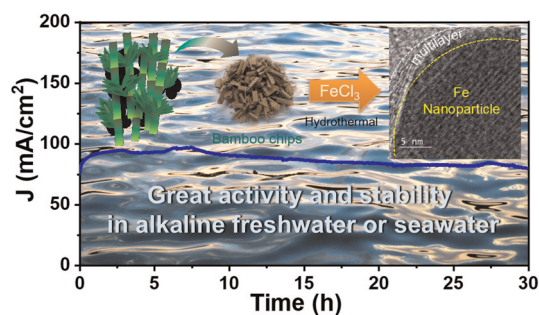
Marta-Lisette Pikma, Sofja Tshepelevitsh, Sigrid Selberg, Ivri Kaljurand, Ivo Leito and Agnes Kütt*



14237

Iron-impregnated cellulosic carbon as an effective electrocatalyst for seawater oxidation

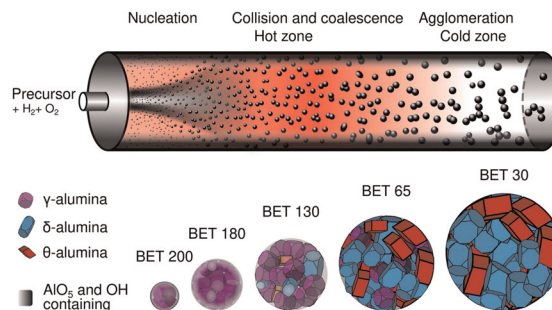
Sakila Khatun, Chandni Das and Poulomi Roy*



14246

Structure and phase changes of alumina produced by flame hydrolysis

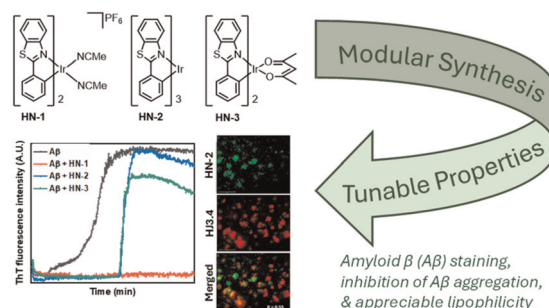
Jamal Nasir, Franz Schmidt, Frank Menzel and Jörn Schmedt auf der Günne*



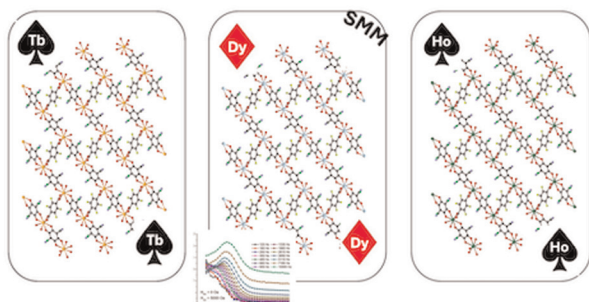
14258

2-Phenylbenzothiazolyl iridium complexes as inhibitors and probes of amyloid β aggregation

Karna Terpstra, Yiran Huang, Hanah Na, Liang Sun, Citlali Gutierrez, Zhengxin Yu and Liviu M. Mirica*



14265

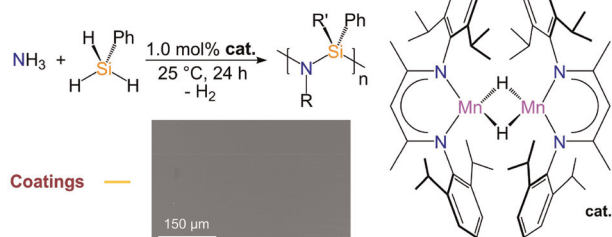


Slow magnetic relaxation in a heteroleptic anilate-based Dy^{III} metal–organic framework

Mariangela Oggianu, Federica Bertolotti, Fabio Manna, Francesco Congiu, Antonio Cappai, Claudio Melis, Giorgio Concas, Narcis Avarvari, Norberto Masciocchi and Maria Laura Mercuri*

14272

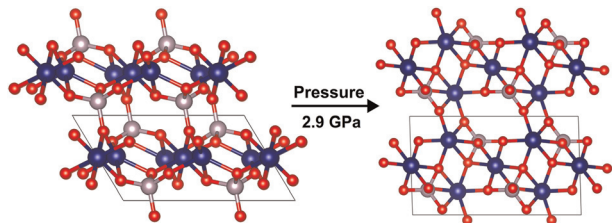
Applying NH₃ to Si–N Dehydrocoupling



Manganese catalysed dehydrocoupling of silanes and siloxanes with ammonia to prepare oligosilazanes and polysiloxazanes

Gautam K. Mehta, Thao T. Nguyen, Marco Flores and Ryan J. Trovitch*

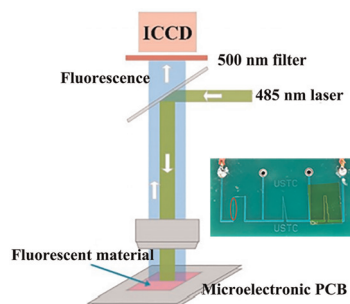
14278



High-pressure polymorph of Co₃P₂O₈: phase transition to an olivine-related structure

Robin Turnbull, Josu Sánchez Martín, Akun Liang, Daniel Díaz-Anichtchenko, Catalin Popescu, K. Sandeep Rao, S. Nagabhusan Achary, Alfonso Muñoz, Vinod Panchal and Daniel Errandonea*

14289



Investigation of SrB₄O₇:Tm²⁺ luminescence for temperature imaging with high sensitivity based on time-resolved luminescence

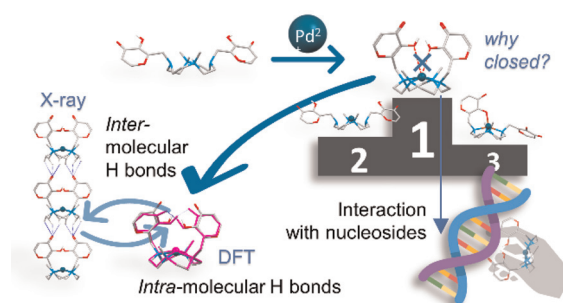
Qian Zhang, Zhicheng Liao, Liting Qiu, Xiantao Wei, Yonghu Chen* and Min Yin*



14300

A combined solid state, solution and DFT study of a dimethyl-cyclen-Pd(II) complex

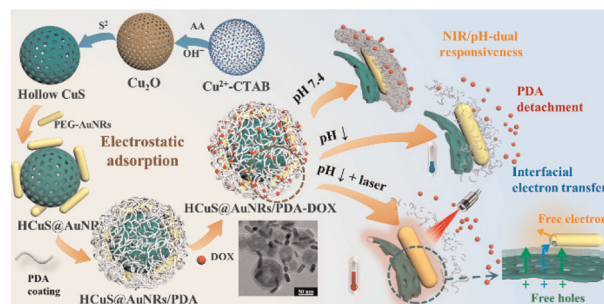
Daniele Paderni, Maria Voccia, Eleonora Macedi,*
Mauro Formica, Luca Giorgi, Lucia Caporaso and
Vieri Fusi*



14315

Self-assembled hollow CuS@AuNRs/PDA nanohybrids with synergistically enhanced photothermal efficiency

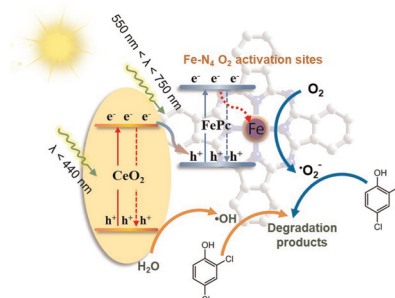
Chi Yin Zhang, Panping Yang, Jingguo Li, Shaokui Cao,
Yingliang Liu and Jun Shi*



14325

Synthesis of iron phthalocyanine/CeO₂ Z-scheme nanocomposites as efficient photocatalysts for degradation of 2,4-dichlorophenol

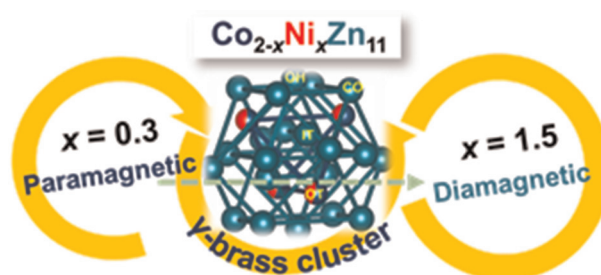
Xiaoyu Chu,* Xinrui Wang, Shuo Tian, Yongkuo Zhao,
Shikai Liu, Hong Yan* and Yan Shang*



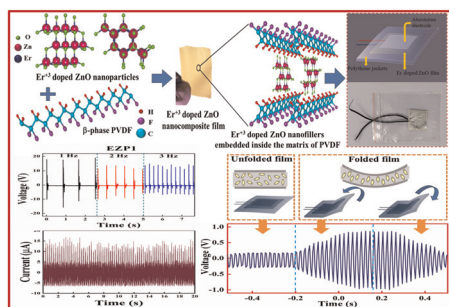
14333

Understanding of magnetic behavior of the pseudo-binary Co_{2-x}Ni_xZn₁₁: in the light of crystal and electronic structures

Amit Mondal, Sandip Kumar Kuila, Rahul Pan,
Shubham Patel, Krishnendu Buxi, Subhadip Saha,
Sivaprasad Ghanta, Maxim Avdeev and
Partha Pratim Jana*



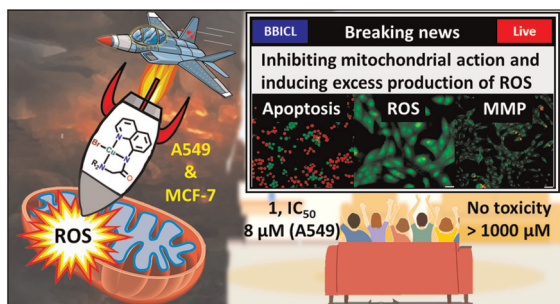
14347



Fabrication of rare earth-doped ZnO-PVDF flexible nanocomposite films for ferroelectric response and their application in piezo-responsive bending sensors

Subhojit Dutta, Tanmoy Chakraborty, Shivam Sharma, Dhananjay Mondal, Aliva Saha, Anup Kumar Pradhan, Chanchal Chakraborty, Sukhen Das* and Soumyaditya Sutradhar*

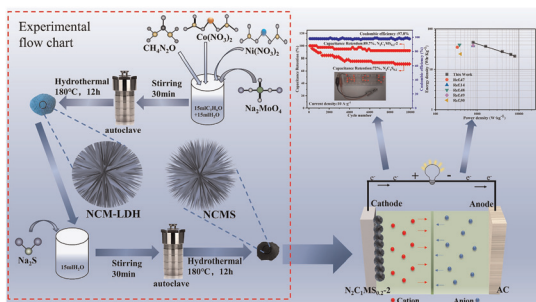
14364



Unravelling the mechanism of apoptosis induced by copper(II) complexes of NN₂-pincer ligands in lung cancer cells

Athulya Das and Muniyandi Sankaralingam*

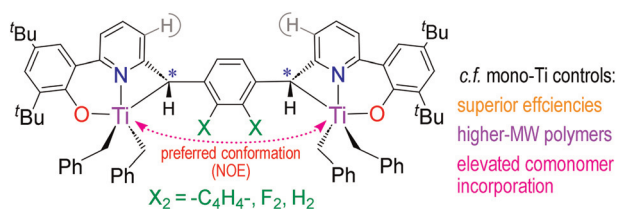
14378



Optimisation of Mo doping to form NiCoMo ternary sulphides for high performance charge storage

Qiang Long, Chenhan Xiong, Jingbo Li, Zhihong Yang, Guoping Du and Nan Chen*

14391



Bis-[C(sp³)-chelating] Ti₂ catalysts supported by arylene-1,4-diyl-2,3-X₂ bridges for olefin copolymerisation: X substituents impose conformational cooperative effects

Yufang Li, Junhui Bao, Qian Liu, Man-Kit Tse and Michael C. W. Chan*

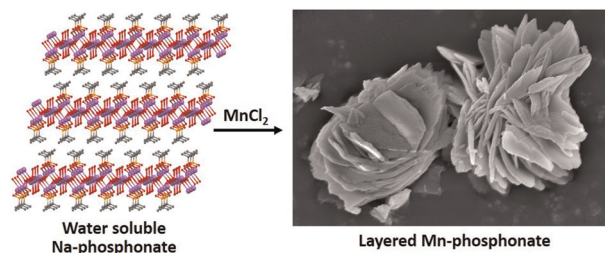


PAPERS

14399

Facile room-temperature synthesis of layered transition metal phosphonates *via* hitherto unknown alkali metal *tert*-butyl phosphonates

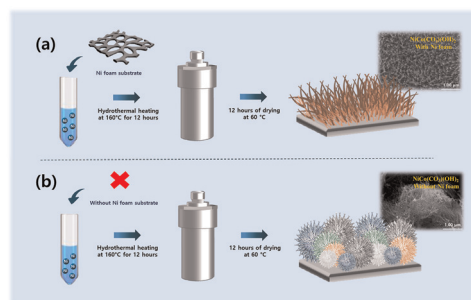
Anuj Kumar, Aheli Ghatak and Ramaswamy Murugavel*



14411

Development of 3D compound structures and highly wettable carbonate hydroxide electrodes for high-performance supercapacitors

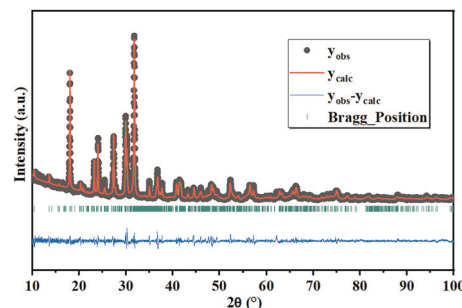
Damin Lee,* Jong Wook Roh, Dong Hwan Kim and Jeongmin Kim*



14422

Optical and theoretical study of NaCr(P₂O₇): a look through the Neuhauser model and Racah theory

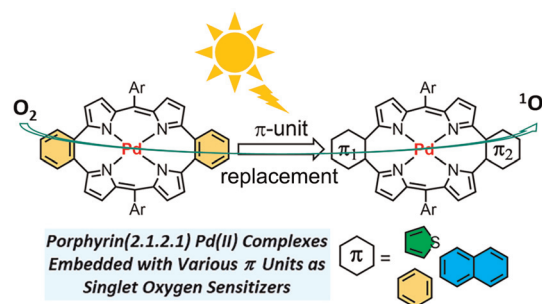
H. Souissi,* S. Kammoun, E. Dhahri and E. López-Lago



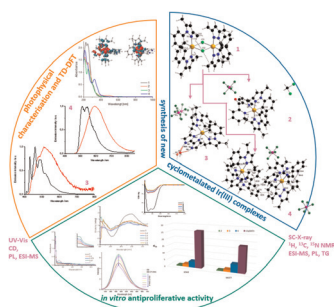
14433

Synthesis of porphyrin(2.1.2.1) Pd(II) complexes embedded with various π units and their singlet oxygen generation capacity

Xiaojuan Lv, Feng Chen,* Mingbo Zhou, Tao Zhang, Fengxian Qiu and Songlin Xue*



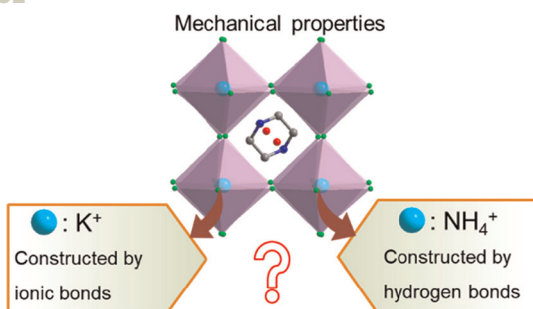
14438



Synthesis, photophysical characterisation, quantum-chemical study and *in vitro* antiproliferative activity of cyclometalated Ir(III) complexes based on 3,5-dimethyl-1-phenyl-1*H*-pyrazole and N,N-donor ligands

Joanna Masternak,* Karol Okła, Adam Kubas, Jiří Voller, Karolína Kozlanská, Małgorzata Zienkiewicz-Machnik, Agnieszka Gilewska, Jerzy Sitkowski, Anna Kamecka, Katarzyna Kazmierczuk and Barbara Barszcz

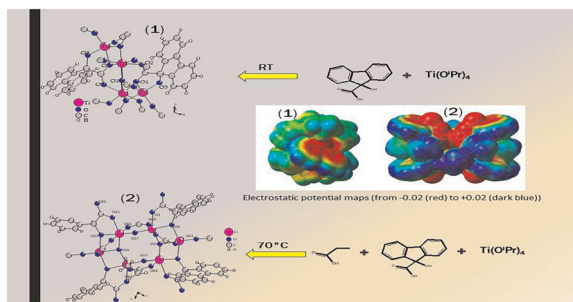
14451



B-site substitution effects on the mechanical properties of halide perovskites [C₄H₁₂N₂][BCl₃]₂·H₂O (B = NH₄⁺; K⁺)

Kai Li,* Zhi-Gang Li, Yong-Qiang Chen* and Wei Li

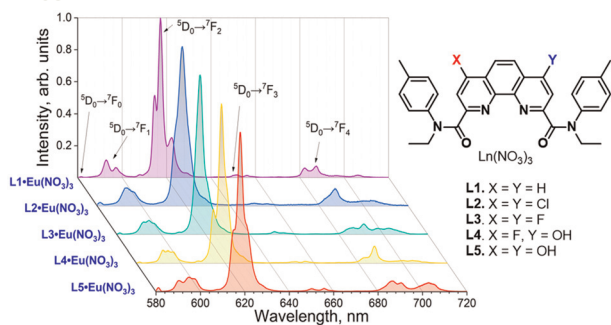
14457



Investigation of titanium(IV)-oxo complexes stabilized with α -hydroxy carboxylate ligands: structural analysis and DFT studies

Barbara Kubiak,* Tadeusz Muzioł, Mirosław Jabłoński, Aleksandra Radtke and Piotr Piszczek*

14469



4,7-Substituted 1,10-phenanthroline-2,9-dicarboxamides: photophysics of ligands and their complexes with the Eu–Gd–Tb triad

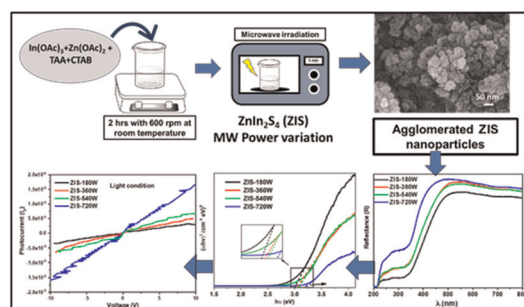
Nane A. Avagyan, Pavel S. Lempert, Trofim A. Polikovskiy, Alisia V. Tsorieva, Mikhail T. Metlin, Ilya V. Taydakov, Roman V. Zonov, Konstantin A. Lyssenko, Mikhail F. Vokuev, Igor A. Rodin, Boris N. Tarasevich, Yuri A. Ustynyuk and Valentine G. Nenajdenko*



14481

Microwave assisted synthesis of ZnIn_2S_4 nanoparticles: effect of power variation for photoresponse and optoelectronic applications

Priyanka Priyadarshini,* Swasti Padma Panda, Abinash Parida and Ramakanta Naik*



14496

Structural diversity and solvent-induced transformations of a copper-based metal–organic framework with highly aromatic ligands

Abigail Edwards, Landon J. Elkins, Carla Slebodnick, Jinglei Wang, Qiang Zhang and Tegan A. Makal*

