

# Dalton Transactions

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## IN THIS ISSUE

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### Cover

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

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### Inside cover

See Yu Xiao et al.,  
pp. 14153–14162.

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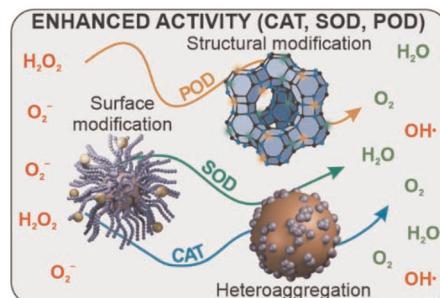
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## FRONTIER

14132

### Engineering inorganic nanzyme architectures for decomposition of reactive oxygen species

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

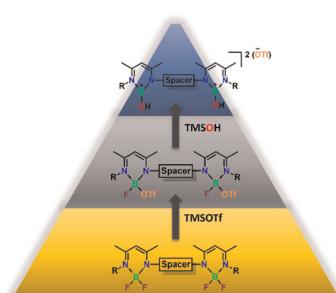


## COMMUNICATION

14139

### Bis(diiminate)-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\*



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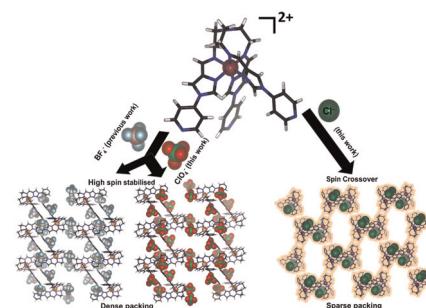
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## PAPERS

14144

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

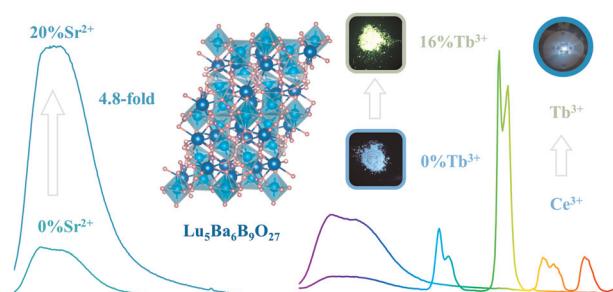
Kenneth Zhang, Matthew J. Wallis, Alexander R. Craze, Shinya Hayami, Hyunsung Min, Daniel J. Fanna, Mohan M. Bhadbhade, Ruoming Tian, Christopher E. Marjo, Leonard F. Lindoy and Feng Li\*



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**

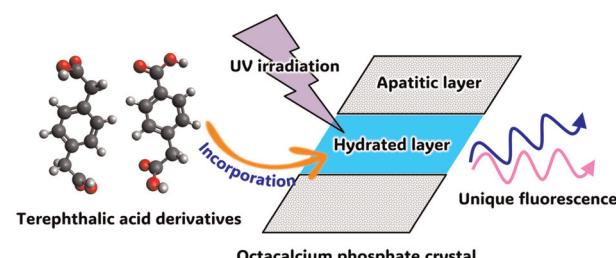
Chenggang Ma, Hailiang Chen, Min Luo, Fuyun Duan, Yun Ding, Yihang Han, Tianxiang Zheng, Xun Yang and Yu Xiao\*



14163

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

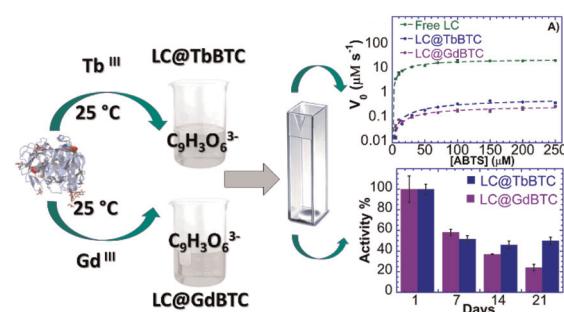
Taishi Yokoi,\* Masahiro Watanabe and Masakazu Kawashita



14171

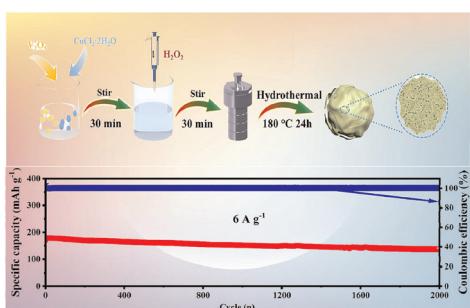
**A green approach to encapsulate proteins and enzymes within crystalline lanthanide-based Tb and Gd MOFs**

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



## PAPERS

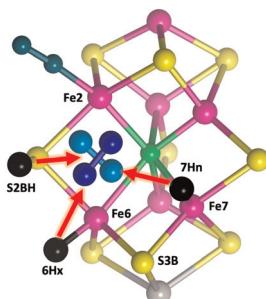
14182



# Engineering VO<sub>x</sub> 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\*

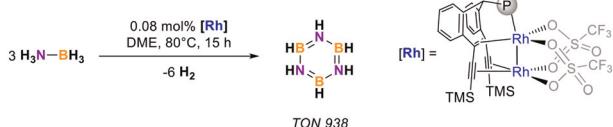
14193



## The activating capture of N<sub>2</sub> at the active site of Mo-nitrogenase

Ian Dance

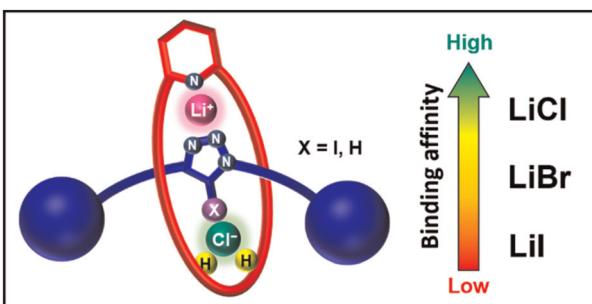
14212



## 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, Zongvao Zhang and Paul D. Beer\*

**14124** | *Dalton Trans.*, 2024, **53**, 14121–14131

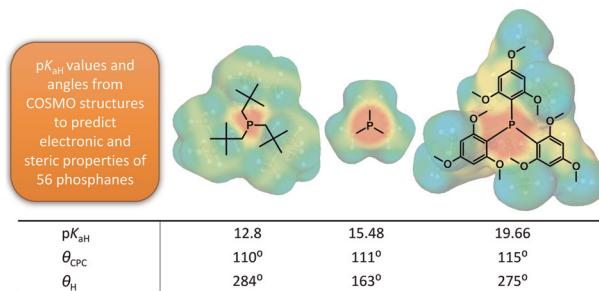
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## PAPERS

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 **$pK_{\text{aH}}$  values and  $\theta_{\text{H}}$  angles of phosphanes to predict their electronic and steric parameters**

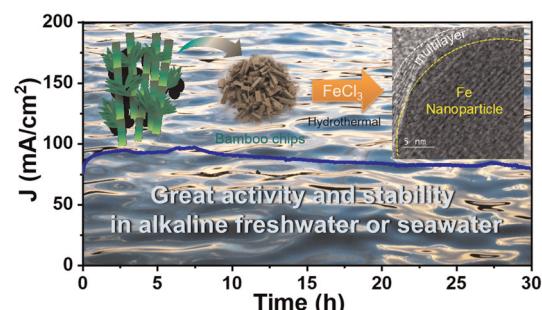
Marta-Lisette Pikma, Sofja Tshepelevitsh, Sigrid Selberg, Ivari Kaljurand, Ivo Leito and Agnes Kütt\*



14237

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

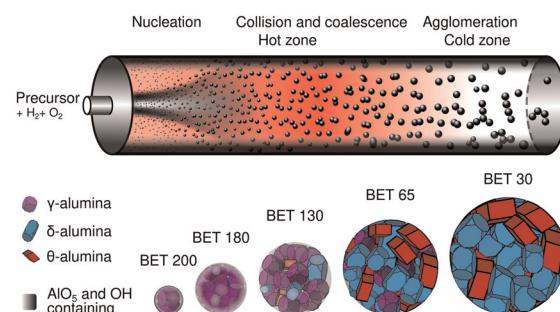
Sakila Khatun, Chandni Das and Poulomi Roy\*



14246

**Structure and phase changes of alumina produced by flame hydrolysis**

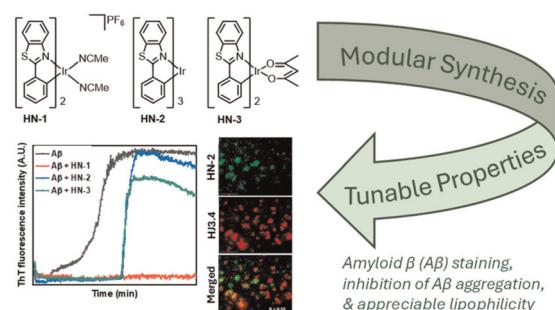
Jamal Nasir, Franz Schmidt, Frank Menzel and Jörn Schmedt auf der Günne\*



14258

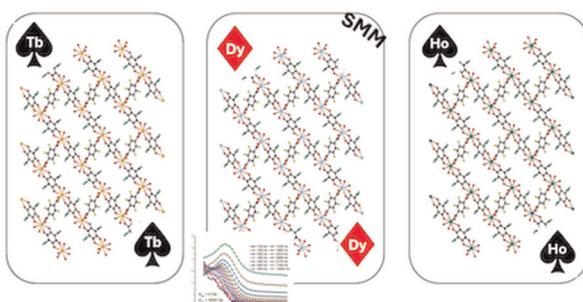
**2-Phenylbenzothiazolyl iridium complexes as inhibitors and probes of amyloid β aggregation**

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



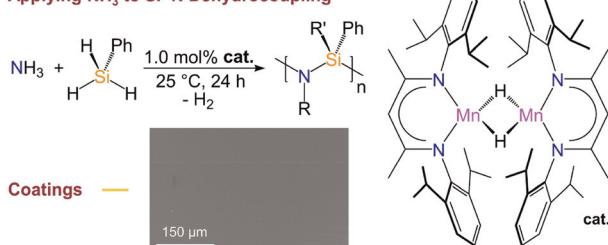
## PAPERS

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**Slow magnetic relaxation in a heteroleptic anilate-based Dy<sup>III</sup> metal–organic framework**

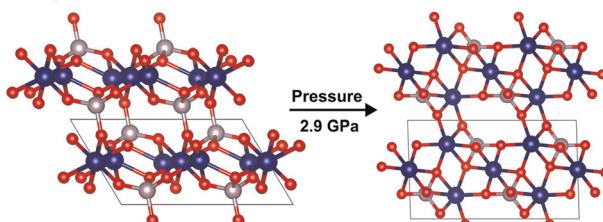
Mariangela Oggianu, Federica Bertolotti, Fabio Manna, Francesco Congiu, Antonio Cappai, Claudio Melis, Giorgio Concias, Narcis Avarvari, Norberto Masciocchi and Maria Laura Mercuri\*

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**Applying NH<sub>3</sub> to Si–N Dehydrocoupling****Manganese catalysed dehydrocoupling of silanes and siloxanes with ammonia to prepare oligosilazanes and polysiloxazanes**

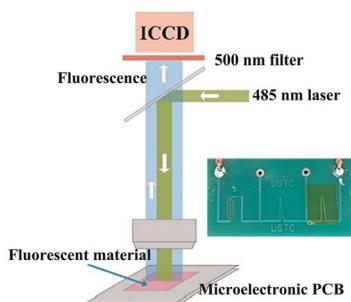
Gautam K. Mehta, Thao T. Nguyen, Marco Flores and Ryan J. Trovitch\*

14278

**High-pressure polymorph of Co<sub>3</sub>P<sub>2</sub>O<sub>8</sub>: 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 SrB<sub>4</sub>O<sub>7</sub>:Tm<sup>2+</sup> 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\*

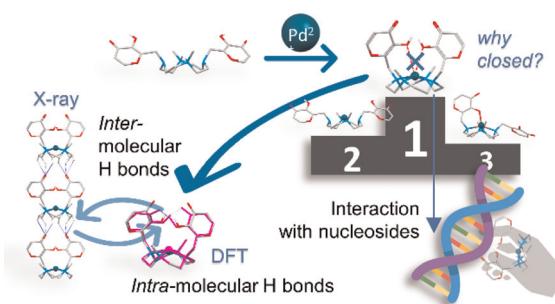


## PAPERS

14300

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

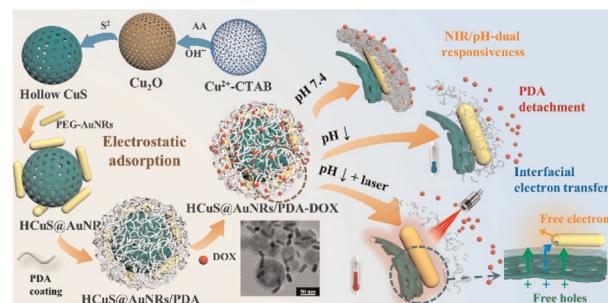
Daniele Paderni, Maria Voccia, Eleonora Macedi,\* Mauro Formica, Luca Giorgi, Lucia Caporaso and Vieri Fusi\*



14315

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

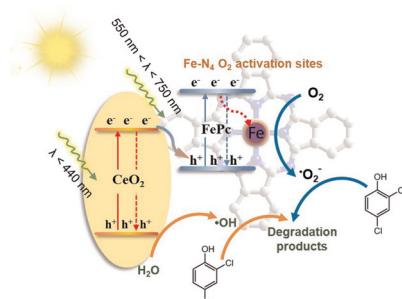
Chiyan Zhang, Panping Yang, Jingguo Li, Shaokui Cao, Yingliang Liu and Jun Shi\*



14325

**Synthesis of iron phthalocyanine/CeO<sub>2</sub> Z-scheme nanocomposites as efficient photocatalysts for degradation of 2,4-dichlorophenol**

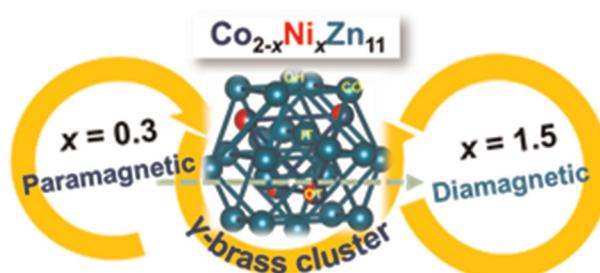
Xiaoyu Chu,\* Xinrui Wang, Shuo Tian, Yongkuo Zhao, Shikai Liu, Hong Yan\* and Yan Shang\*



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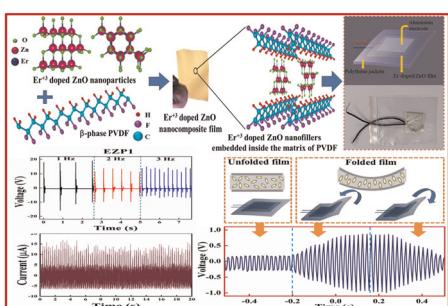
**Understanding of magnetic behavior of the pseudo-binary Co<sub>2-x</sub>Ni<sub>x</sub>Zn<sub>11</sub>: in the light of crystal and electronic structures**

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



## PAPERS

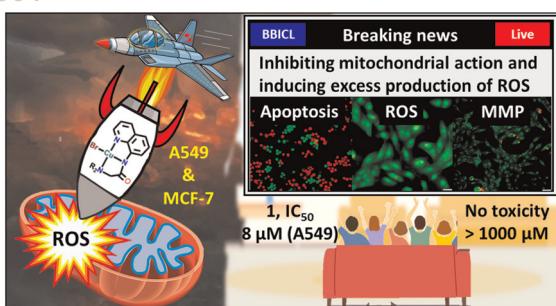
14347



## 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, Dhananjoy Mondal, Aliva Saha, Anup Kumar Pradhan, Chanchal Chakraborty, Sukhen Das\* and Soumyaditya Sutradhar\*

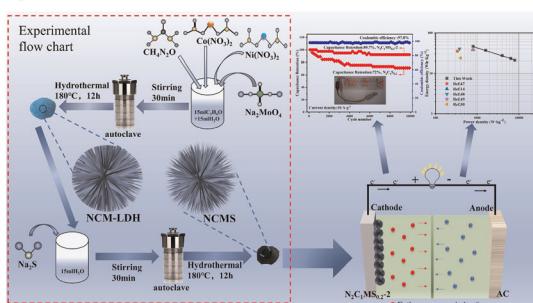
14364



## Unravelling the mechanism of apoptosis induced by copper(II) complexes of NN<sub>2</sub>-pincer ligands in lung cancer cells

Athulya Das and Muniyandi Sankaralingam\*

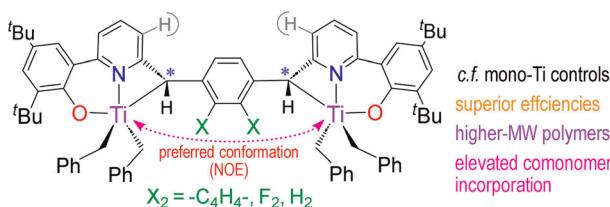
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## Optimisation of Mo doping to form NiCoMo ternary sulphides for high performance charge storage

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

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## Bis-[C(sp<sup>3</sup>)-chelating] Ti<sub>2</sub> catalysts supported by arylene-1,4-diyl-2,3-X<sub>2</sub> bridges for olefin copolymerisation: X substituents impose conformational cooperative effects

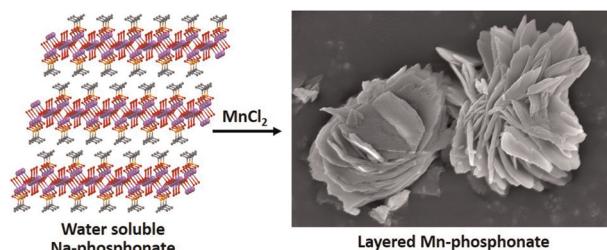
Yufang Li, Junhui Bao, Qian Liu, Man-Kit Tse and Michael C. W. Chan\*



## PAPERS

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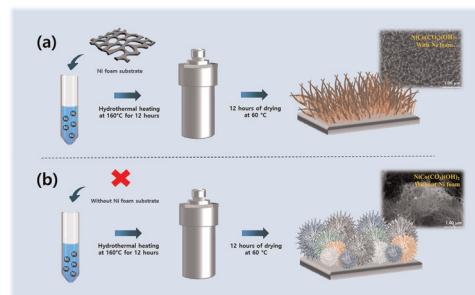
**Facile room-temperature synthesis of layered transition metal phosphonates *via* hitherto unknown alkali metal *tert*-butyl phosphonates**  
Anuj Kumar, Aheli Ghatak and Ramaswamy Murugavel\*



14411

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

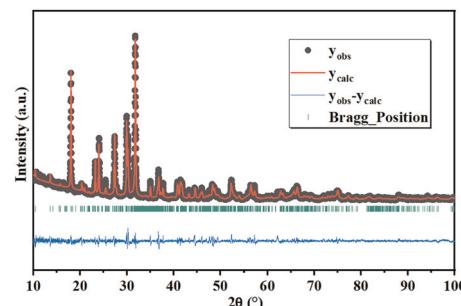
Damin Lee,\* Jong Wook Roh, Dong Hwan Kim and Jeongmin Kim\*



14422

**Optical and theoretical study of NaCr(P<sub>2</sub>O<sub>7</sub>): a look through the Neuhauser model and Racah theory**

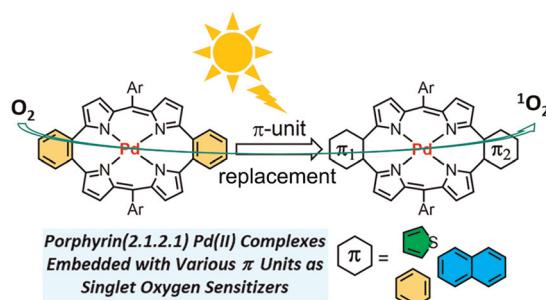
H. Souissi,\* S. Kammoun, E. Dahri and E. López-Lago



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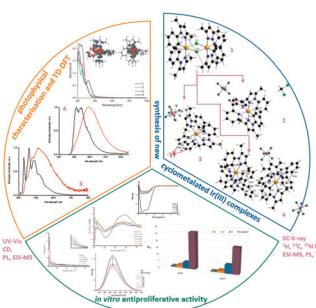
**Synthesis of porphyrin(2.1.2.1) Pd(II) complexes embedded with various π units and their singlet oxygen generation capacity**

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



## PAPERS

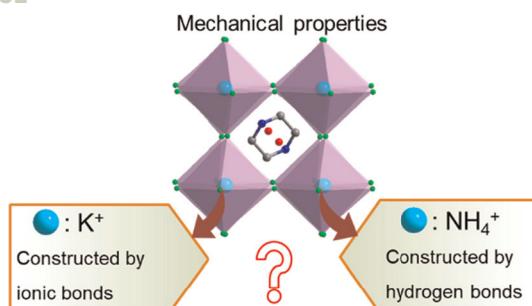
14438



**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 Okla, Adam Kubas, Jiří Voller, Karolína Kozlanská, Małgorzata Zienkiewicz-Machnik, Agnieszka Gilewska, Jerzy Sitkowski, Anna Kamecka, Katarzyna Kazimierczuk and Barbara Barszcz

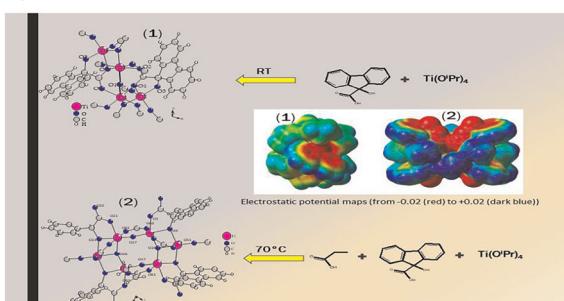
14451



**B-site substitution effects on the mechanical properties of halide perovskites  $[C_4H_{12}N_2][BCl_3] \cdot H_2O$  ( $B = NH_4^+$ ;  $K^+$ )**

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

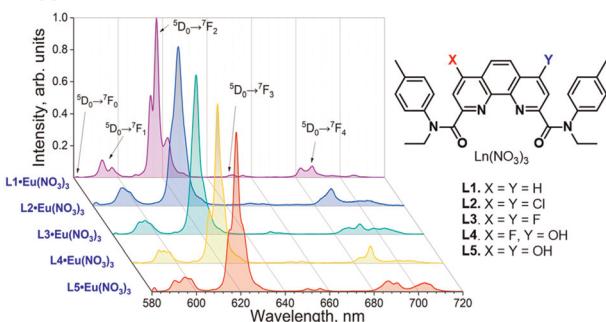
14457



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

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

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**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. Lemport, 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. Ustyryuk and Valentine G. Nenajdenko\*

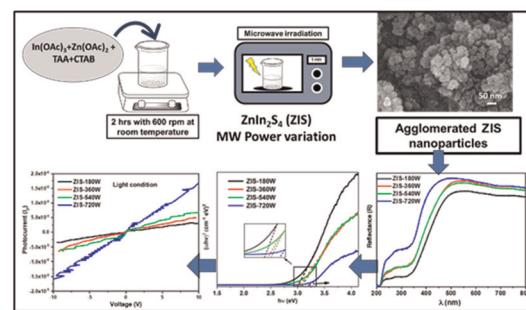


## PAPERS

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## Microwave assisted synthesis of $\text{ZnIn}_2\text{S}_4$ nanoparticles: effect of power variation for photoresponse and optoelectronic applications

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



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

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

