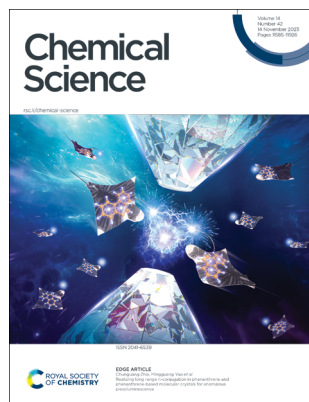
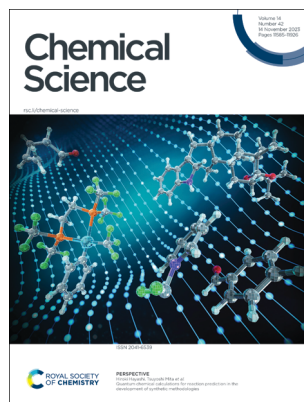


## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 14(42) 11585–11926 (2023)



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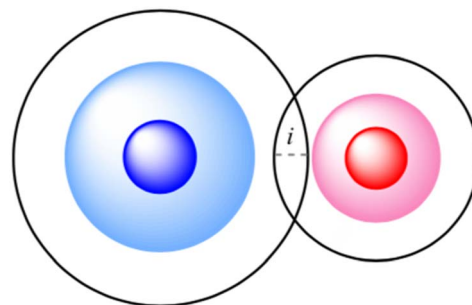
**Inside cover**  
See Hiroki Hayashi, Tsuyoshi Mita *et al.*, pp. 11601–11616. Image reproduced by permission of Hiroki Hayashi, Satoshi Maeda and Tsuyoshi Mita from *Chem. Sci.*, 2023, **14**, 11601.

## COMMENTARY

11597

### A focus on penetration index – a new descriptor of chemical bonding

Wojciech Grochala

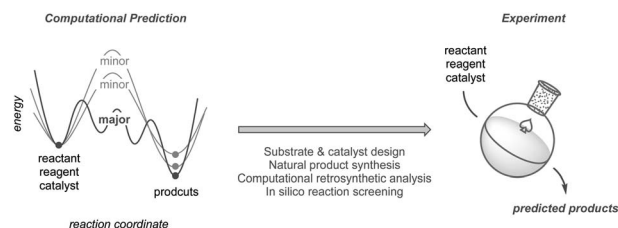


## PERSPECTIVES

11601

### Quantum chemical calculations for reaction prediction in the development of synthetic methodologies

Hiroki Hayashi,\* Satoshi Maeda and Tsuyoshi Mita\*



# Chemical Science

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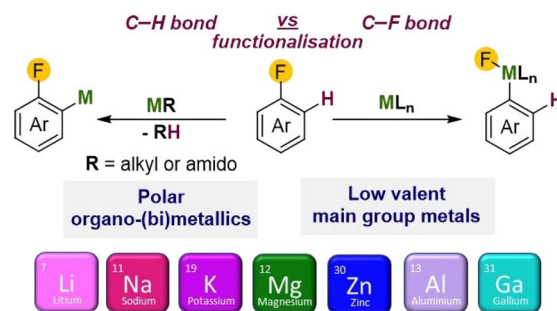


## PERSPECTIVES

11617

## Main group metal-mediated strategies for C–H and C–F bond activation and functionalisation of fluoroarenes

Neil R. Judge, Alessandra Logallo and Eva Hevia\*

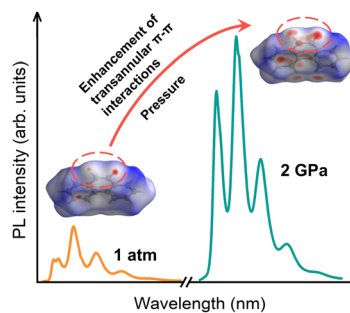


## EDGE ARTICLES

11629

Realizing long range  $\pi$ -conjugation in phenanthrene and phenanthrene-based molecular crystals for anomalous piezoluminescence

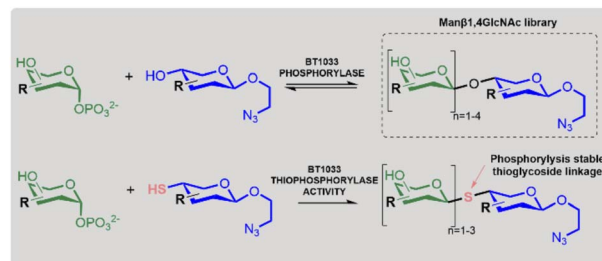
Tongge Xu, Xiu Yin, Chunguang Zhai,\* Desi Chen, Xiaoying Yang, Shuhe Hu, Kuo Hu, Yuchen Shang, Jiajun Dong, Zhen Yao, Quanjun Li, Peng Wang, Ran Liu, Mingguang Yao\* and Bingbing Liu



11638

Reverse thiophosphorylase activity of a glycoside phosphorylase in the synthesis of an unnatural Man $\beta$ 1,4GlcNAc library

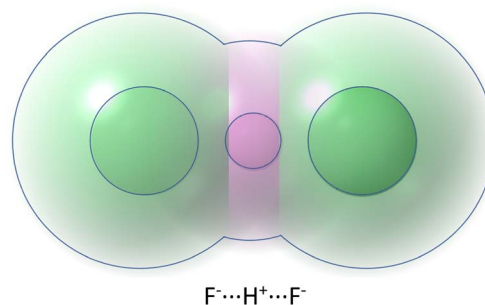
Tessa Keenan, Natasha E. Hatton, Jack Porter, Jean-Baptiste Vendeville, David E. Wheatley, Mattia Ghirardello, Alice J. C. Wahart, Sanaz Ahmadipour, Julia Walton, M. Carmen Galan, Bruno Linclau, Gavin J. Miller\* and Martin A. Fascione\*



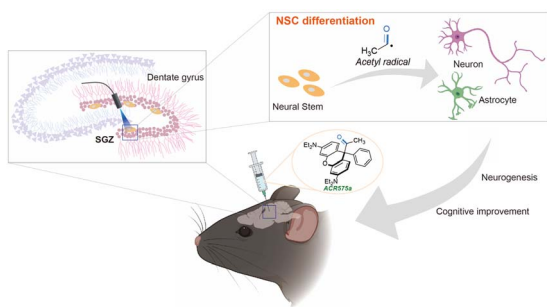
11647

## The borderless world of chemical bonding across the van der Waals crust and the valence region

Jorge Echeverría and Santiago Alvarez



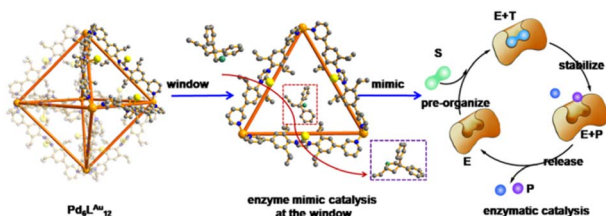
11689



### Acyl-caged rhodamines: photo-controlled and self-calibrated generation of acetyl radicals for neural function recovery in early AD mice

Xiao Luo,\* Zhonghui Zhang, Jie Wang, Xueli Wang, Yan Zhang, Jinqian Chen, Guangbo Ge, Wen Yang,\* Xuhong Qian,\* Yang Tian\* and Youjun Yang\*

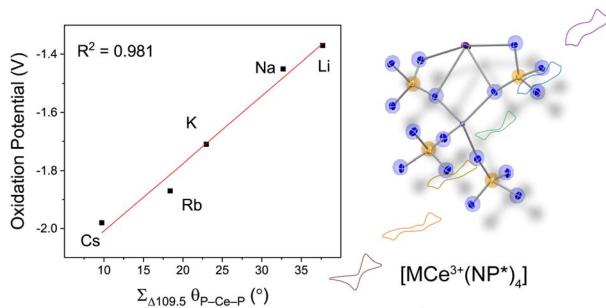
11699



### Broadening the catalytic region from the cavity to windows by $M_6L_{12}$ nanospheres in cyclizations

Meiling Xu, Bin Sun, David A. Poole, III, Eduard O. Bobylev, Xu Jing,\* Jinguo Wu, Cheng He, Chunying Duan\* and Joost N. H. Reek\*

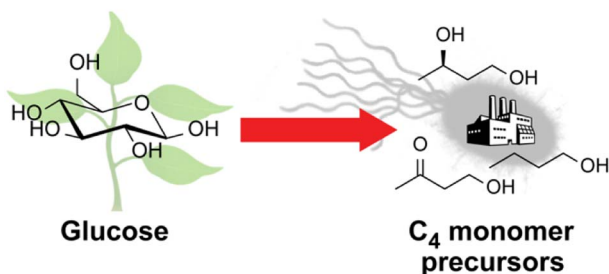
11708



### Structural distortion by alkali metal cations modulates the redox and electronic properties of $Ce^{3+}$ imidophosphorane complexes

Andrew C. Boggiano, Chad M. Studvick, Alexander Steiner, John Bacsá, Ivan A. Popov\* and Henry S. La Pierre\*

11718



### A cellular platform for production of $C_4$ monomers

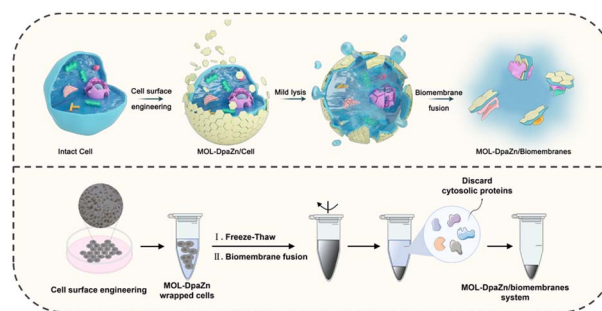
Matthew A. Davis, Vivian Yaci Yu, Beverly Fu, Miao Wen, Edward J. Koleski, Joshua Silverman, Charles A. Berdan, Daniel K. Nomura and Michelle C. Y. Chang\*



11727

### Metal organic layers enabled cell surface engineering coupling biomembrane fusion for dynamic membrane proteome profiling

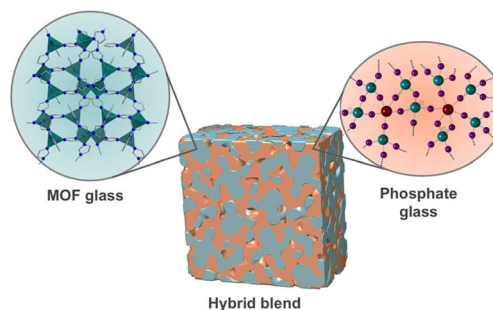
Qianqian Jiang, He Wang, Zichun Qiao, Yutong Hou, Zhigang Sui, Baofeng Zhao, Zhen Liang, Bo Jiang,\* Yukui Zhang and Lihua Zhang\*



11737

### Structural insights into hybrid immiscible blends of metal–organic framework and sodium ultraphosphate glasses

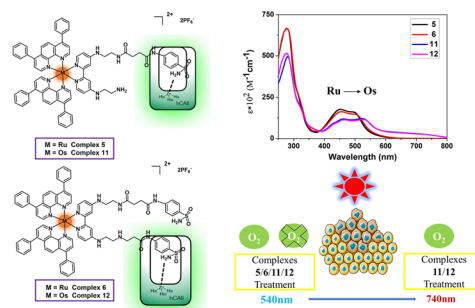
Ashleigh M. Chester, Celia Castillo-Blas, Roman Sajzew, Bruno P. Rodrigues, Ruben Mas-Balleste, Alicia Moya, Jessica E. Snelson, Sean M. Collins, Adam F. Sapnik, Georgina P. Robertson, Daniel J. M. Irving, Lothar Wondraczek, David A. Keen and Thomas D. Bennett\*



11749

### Ru(II)/Os(II)-based carbonic anhydrase inhibitors as photodynamic therapy photosensitizers for the treatment of hypoxic tumours

Youchao Wang, Pierre Mesdom, Kallol Purkait, Bruno Saubaméa, Pierre Burckel, Philippe Arnoux, Céline Frochot, Kevin Cariou,\* Thibaud Rossel\* and Gilles Gasser\*



11761

### Palladium nanoparticles on gallium nitride as a Mott–Schottky catalyst for efficient and durable photoactivation of unactivated alkanes

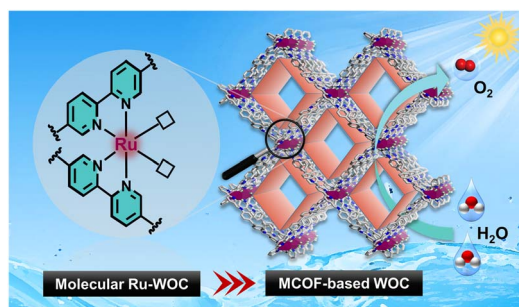
Lida Tan, Xianghua Kong, Mingxin Liu, Hui Su, Hong Guo\* and Chao-Jun Li\*



- ✓ Heterogeneous catalysis
- ✓ Photocatalytic C(sp<sup>3</sup>)-N bond formation
- ✓ Mild conditions
- ✓ Unactivated alkanes
- ✓ Long term stability



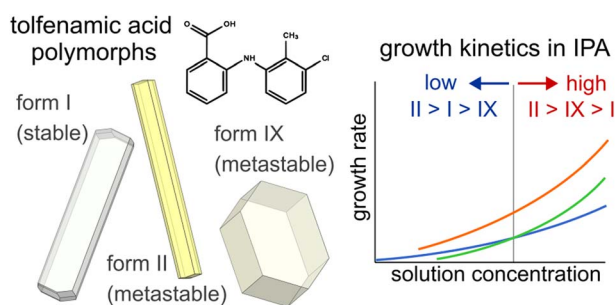
11768



### Engineering a molecular ruthenium catalyst into three-dimensional metal covalent organic frameworks for efficient water oxidation

Wang-Kang Han, Yong Liu, Jing-Dong Feng, Xiaodong Yan, Huan Pang and Zhi-Guo Gu\*

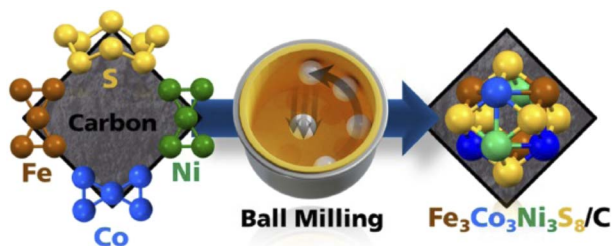
11775



### Do metastable polymorphs always grow faster? Measuring and comparing growth kinetics of three polymorphs of tolfenamic acid

Pietro Sacchi,\* Petros Neoptolemos, Roger J. Davey, Susan M. Reutzel-Edens and Aurora J. Cruz-Cabeza\*

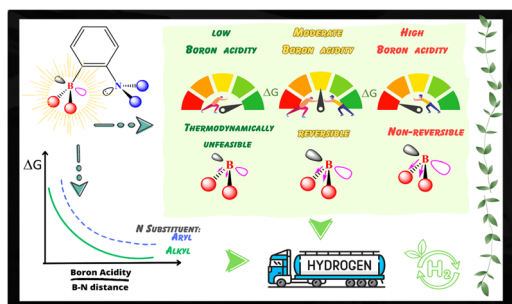
11790



### Mechanochemical one-pot synthesis of heterostructured pentlandite-carbon composites for the hydrogen evolution reaction

David Tetzlaff, Tilo Rensch, Leonard Messing, Petra Banke, Sven Grätz, Daniel Siegmund, Lars Borchardt\* and Ulf-Peter Apfel\*

11798



### New insights into H<sub>2</sub> activation by intramolecular frustrated Lewis pairs based on aminoboranes: the local electrophilicity index of boron as a suitable indicator to tune the reversibility of the process

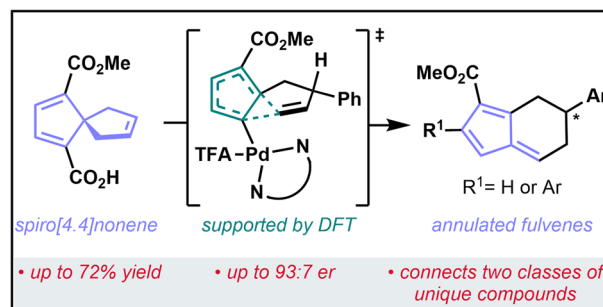
César Barrales-Martínez,\* Rocío Durán and Pablo Jaque



11809

### Rearrangement of a carboxy-substituted spiro[4.4]nonatriene to annulated fulvenes through a Pd(II)-mediated 1,5-vinyl shift

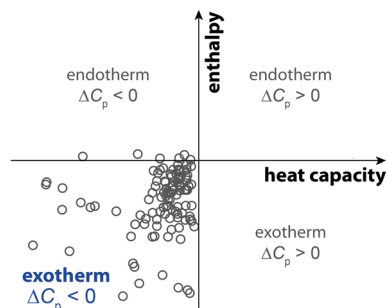
Karan Goyal, Garrett A. Kukier, Xiangyang Chen, Aneta Turlik, K. N. Houk\* and Richmond Sarpong\*



11818

### The temperature-dependence of host–guest binding thermodynamics: experimental and simulation studies

Laura M. Grimm,\* Jeffry Setiadi, Boryslav Tkachenko, Peter R. Schreiner, Michael K. Gilson\* and Frank Biedermann\*



11830

### Ion sieving membrane for direct seawater anti-precipitation hydrogen evolution reaction electrode

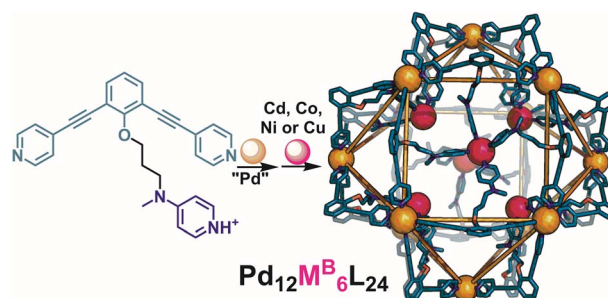
Qianfeng Liu, Zhao Yan, Jianxin Gao, Hefei Fan, Min Li and Erdong Wang\*



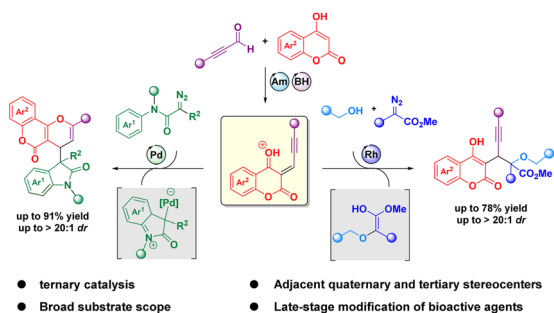
11840

### Pd<sub>12</sub>M<sub>n</sub>L<sub>24</sub> (for n = 6, 8, 12) nanospheres by post-assembly modification of Pd<sub>12</sub>L<sub>24</sub> spheres

Eduard O. Bobylev, Leonardo Passerini, Felix J. de Zwart, David A. Poole, III, Simon Mathew, Martina Huber, Bas de Bruin and Joost N. H. Reek\*



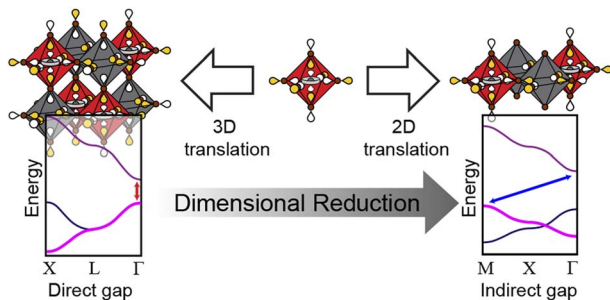
11850



### Construction of 4-hydroxycoumarin derivatives with adjacent quaternary and tertiary stereocenters via ternary catalysis

Mengchu Zhang, Tianyuan Zhang, Sifan Yu, Huang Qiu, Abdulla Yusuf, Xinfang Xu, Yu Qian\* and Wenhao Hu\*

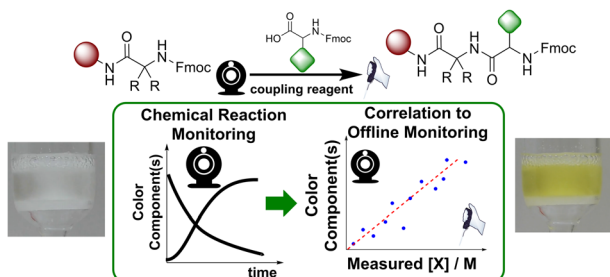
11858



### Understanding the evolution of double perovskite band structure upon dimensional reduction

Bridget A. Connor, Alexander C. Su, Adam H. Slavney, Linn Leppert\* and Hemamala I. Karunadasa\*

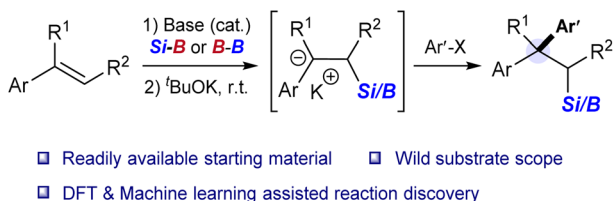
11872



### Computer vision as a new paradigm for monitoring of solution and solid phase peptide synthesis

Chunhui Yan, Calum Fyfe, Laura Minty, Henry Barrington, Craig Jamieson\* and Marc Reid\*

11881



### Base-mediated C–B bond activation of benzylic boronate for the rapid construction of $\beta$ -silyl/boryl functionalized 1,1-diaryllalkanes from aromatic alkenes

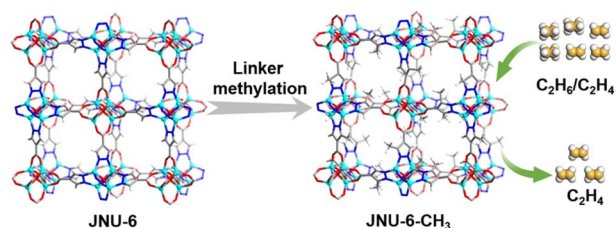
Liuzhou Gao, Xinyi Liang, Linke He, Guoao Li, Shengda Chen, Jia Cao, Jing Ma, Guoqiang Wang\* and Shuhua Li\*



11890

### Surface engineering on a microporous metal–organic framework to boost ethane/ethylene separation under humid conditions

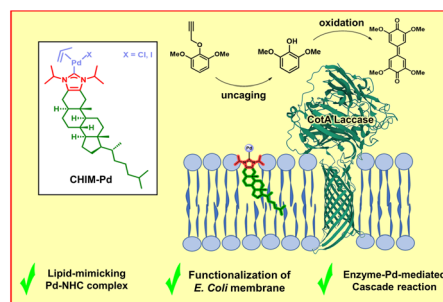
Xiao-Jing Xie, Ying Wang, Qi-Yun Cao, Rajamani Krishna, Heng Zeng,\* Weigang Lu\* and Dan Li



11896

### Combining lipid-mimicking-enabled transition metal and enzyme-mediated catalysis at the cell surface of *E. coli*

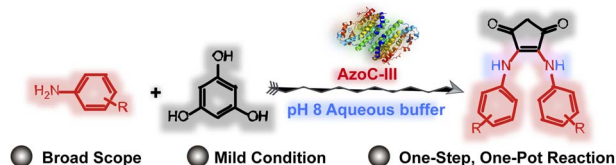
Tristan Wegner, Alexander Dombovski, Katrin Gesing, Alexander Köhrer, Matthias Elinkmann, Uwe Karst, Frank Glorius\* and Joachim Jose\*



11907

### Unlocking mild-condition benzene ring contraction using nonheme diiron *N*-oxygenase

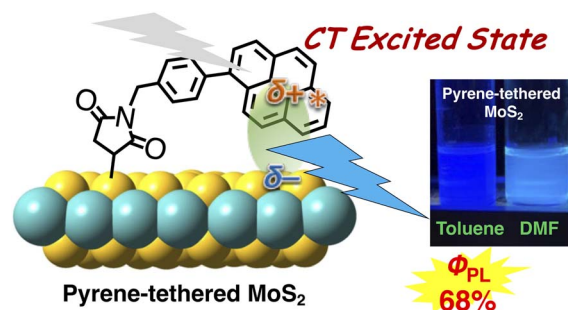
Yuan-Yang Guo,\* Ze-Hua Tian, ChunHua Ma, Yu-Chen Han, DaChang Bai and ZhiYong Jiang



11914

### An emissive charge-transfer excited-state at the well-defined hetero-nanostructure interface of an organic conjugated molecule and two-dimensional inorganic nanosheet

Tomokazu Umeyama,\* Daizu Mizutani, Yuki Ikeda, W. Ryan Osterloh, Futa Yamamoto, Kosaku Kato, Akira Yamakata,\* Masahiro Higashi,\* Takumi Urakami, Hirofumi Sato and Hiroshi Imahori\*



## CORRECTION

11924

**Correction: Evidence for and evaluation of fluorine–tellurium chalcogen bonding**

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