

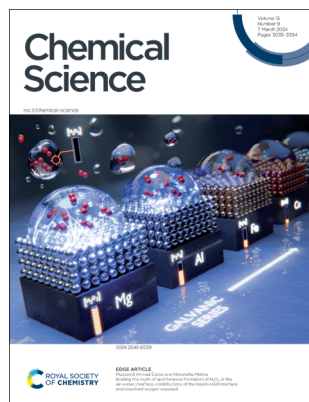
# Chemical Science

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## IN THIS ISSUE

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**Cover**  
See Muzzamil Ahmad Eatoo and Himanshu Mishra, pp. 3093–3103. Image reproduced by permission of KAUST from *Chem. Sci.*, 2024, 15, 3093.



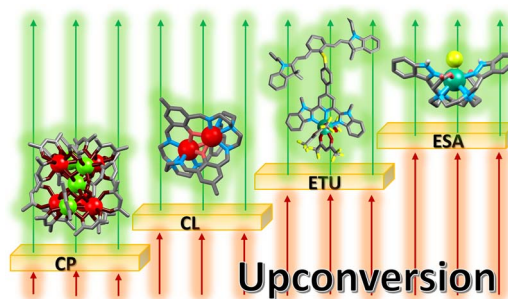
**Inside cover**  
See Vera Krewald, Mark J. Muldoon, Ulrich Hintermair *et al.*, pp. 3104–3115. Image reproduced by permission of Qun Cao, Mark Muldoon, Martin Diefenbach, Vera Krewald and Ulrich Hintermair from *Chem. Sci.*, 2024, 15, 3104.

## PERSPECTIVES

3048

### Upconverting photons at the molecular scale with lanthanide complexes

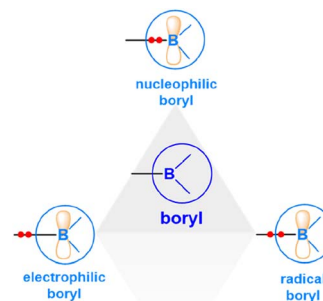
Loïc J. Charbonnière,\* Aline M. Nonat, Richard C. Knighton and Léna Godec



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### Boryls, their compounds and reactivity: a structure and bonding perspective

Xueying Guo and Zhenyang Lin\*



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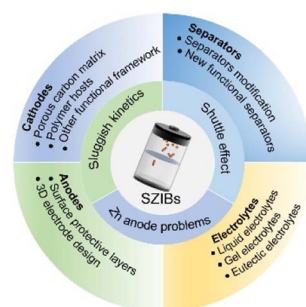
Fundamental questions  
Elemental answers

## REVIEW

3071

### Advancements in aqueous zinc–iodine batteries: a review

Zhongchao Bai, Gulian Wang, Hongmin Liu, Yitao Lou, Nana Wang,\* HuaKun Liu and Shixue Dou\*

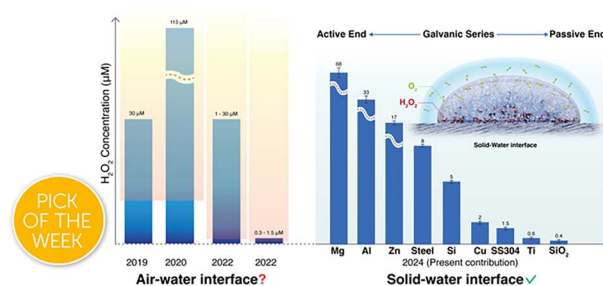


## EDGE ARTICLES

3093

### Busting the myth of spontaneous formation of H<sub>2</sub>O<sub>2</sub> at the air–water interface: contributions of the liquid–solid interface and dissolved oxygen exposed

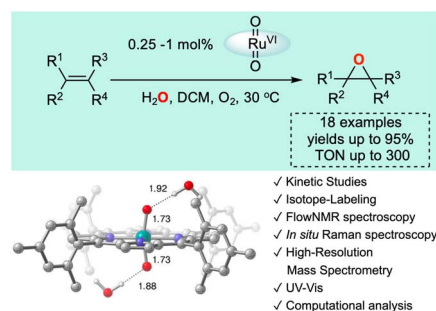
Muzzamil Ahmad Eatoo and Himanshu Mishra\*



3104

### Water co-catalysis in aerobic olefin epoxidation mediated by ruthenium oxo complexes

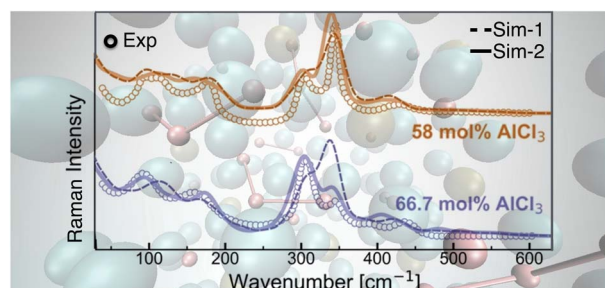
Qun Cao, Martin Diefenbach, Calum Maguire, Vera Krewald,\* Mark J. Muldoon\* and Ulrich Hintermair\*



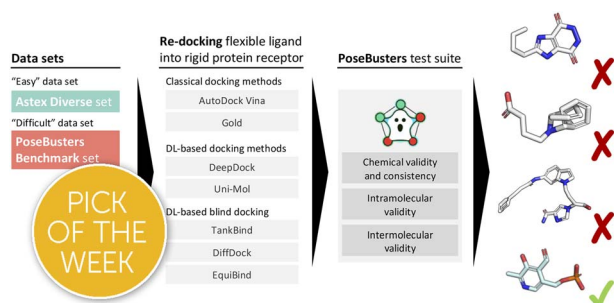
3116

### Tracing mechanistic pathways and reaction kinetics toward equilibrium in reactive molten salts

Luke D. Gibson, Santanu Roy,\* Rabi Khanal, Rajni Chahal, Ada Sedova and Vyacheslav S. Bryantsev\*



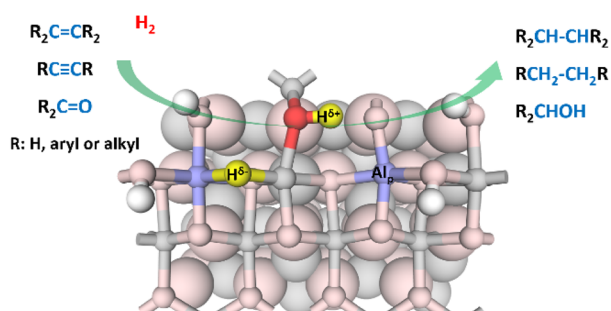
3130



### PoseBusters: AI-based docking methods fail to generate physically valid poses or generalise to novel sequences

Martin Butterschoen, Garrett M. Morris and Charlotte M. Deane\*

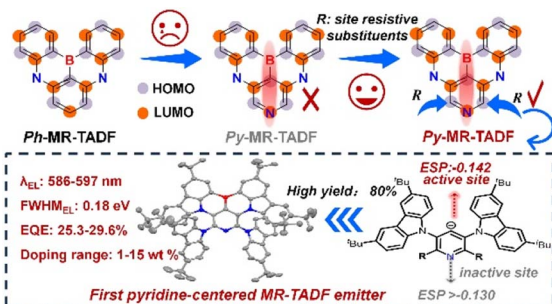
3140



### Frustrated Lewis pairs on pentacoordinated $Al^{3+}$ -enriched $Al_2O_3$ promote heterolytic hydrogen activation and hydrogenation

Qingyuan Wu, Ruixuan Qin, Mengsi Zhu, Hui Shen, Shenshui Yu, Yuanyuan Zhong, Gang Fu, Xiaodong Yi\* and Nanfeng Zheng\*

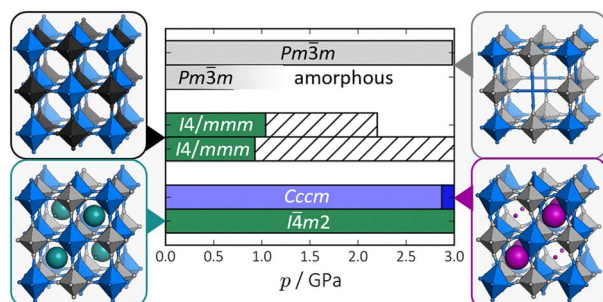
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### Stereo effects for efficient synthesis of orange-red multiple resonance emitters centered on a pyridine ring

Mingxu Du, Minqiang Mai, Dongdong Zhang, Lian Duan and Yuewei Zhang\*

3155



### The pressure response of Jahn–Teller-distorted Prussian blue analogues

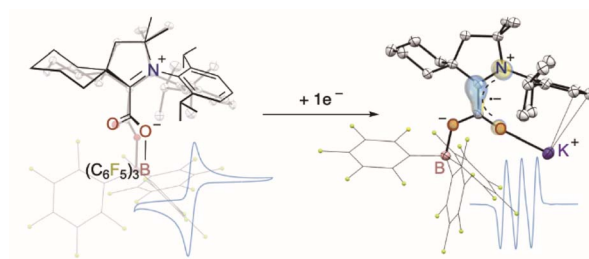
Hanna L. B. Boström,\* Andrew B. Cairns, Muzi Chen, Dominik Daisenberger, Christopher J. Ridley and Nicholas P. Funnell



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### Single electron reduction of NHC–CO<sub>2</sub>–borane compounds

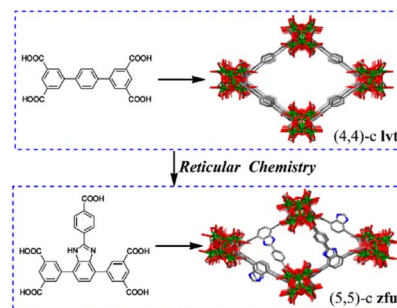
Agustín Morales, Caroline Gonçalves, Alix Sournia-Saquet, Laure Vendier, Agustí Lledós,\* Olivier Baslé\* and Sébastien Bontemps\*



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### Reticular chemistry guided precise construction of zirconium-pentacarboxylate frameworks with 5-connected Zr<sub>6</sub> clusters

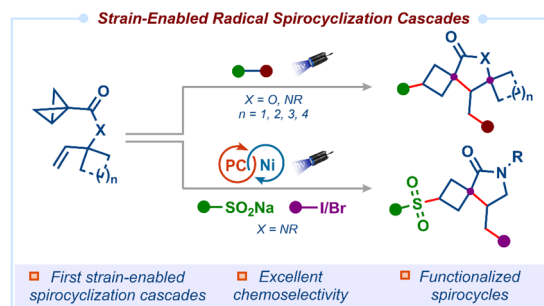
Tianyou Peng, Chao-Qin Han, Hai-Lun Xia, Kang Zhou, Jian Zhang, Jincheng Si, Lei Wang, Jiafeng Miao, Fu-An Guo, Hao Wang, Lu-Lu Qu, Guozhong Xu,\* Jing Li\* and Xiao-Yuan Liu\*



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### Strain-enabled radical spirocyclization cascades: rapid access to spirocyclobutyl lactones and – lactams

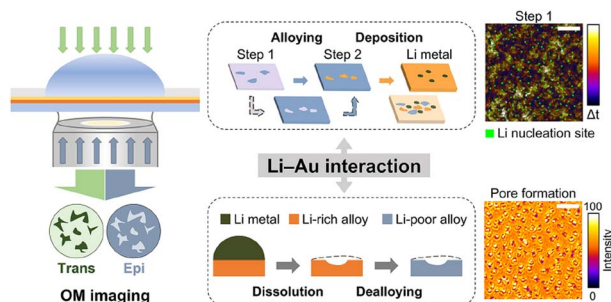
Kousik Das, Abhilash Pedada, Tushar Singha and Durga Prasad Hari\*



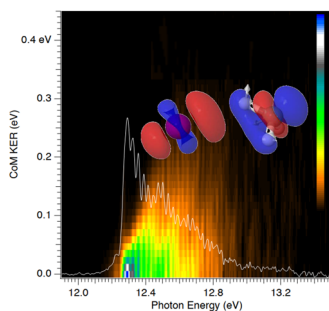
3192

### Direct imaging of dynamic heterogeneous lithium–gold interaction at the electrochemical interface during the charging/discharging processes

Jiaxin Mao, Guopeng Li, Dongwei Xu and Rui Hao\*



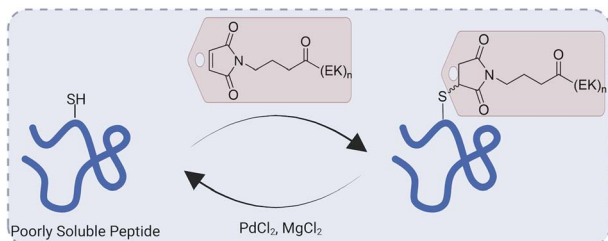
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### Evidencing an elusive conical intersection in the dissociative photoionization of methyl iodide

Jesús González-Vázquez, Gustavo A. García, David V. Chicharro, Luis Bañares and Sonia Marggi Poullain\*

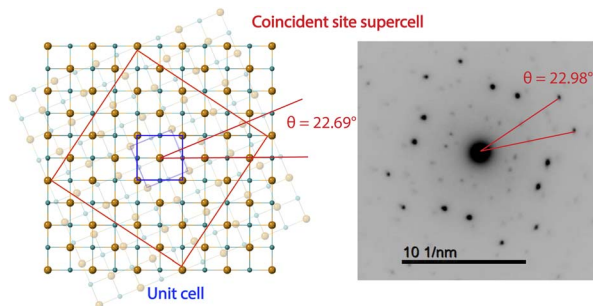
3214



### A cysteine-specific solubilizing tag strategy enables efficient chemical protein synthesis of difficult targets

Wenchao Li, Michael T. Jacobsen, Claire Park, Jae Un Jung, Nai-Pin Lin, Po-Ssu Huang, Rayhan A. Lal and Danny Hung-Chieh Chou\*

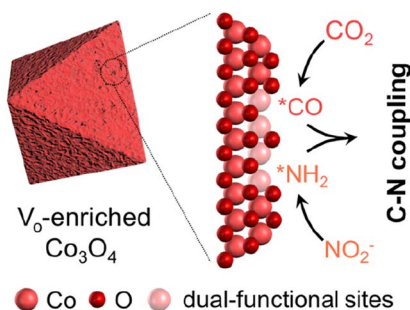
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### Twisting two-dimensional iron sulfide layers into coincident site superlattices via intercalation chemistry

Lahari Balisetty, Brandon Wilfong, Xiuquan Zhou, Huafei Zheng, Sz-Chian Liou and Efrain E. Rodriguez

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### Efficient C–N coupling for urea electrosynthesis on defective $\text{Co}_3\text{O}_4$ with dual-functional sites

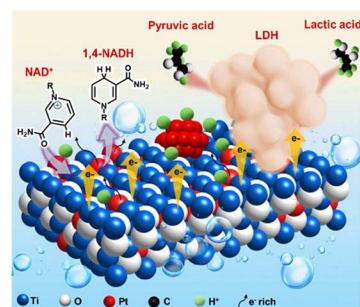
Pengsong Li, Qinggong Zhu,\* Jiyuan Liu, Tianbin Wu, Xinling Song, Qinglei Meng, Xinchun Kang, Xiaofu Sun and Buxing Han\*



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### *In situ* electrochemical regeneration of active 1,4-NADH for enzymatic lactic acid formation via concerted functions on Pt-modified TiO<sub>2</sub>/Ti

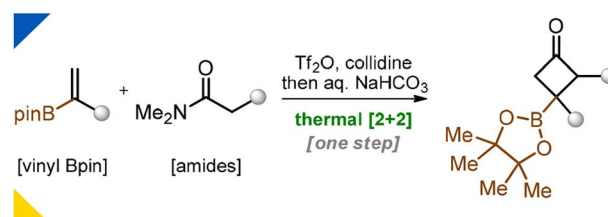
Nada H. A. Besisa, Ki-Seok Yoon and M. Yamauchi\*



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### Borylated cyclobutanes via thermal [2 + 2]-cycloaddition

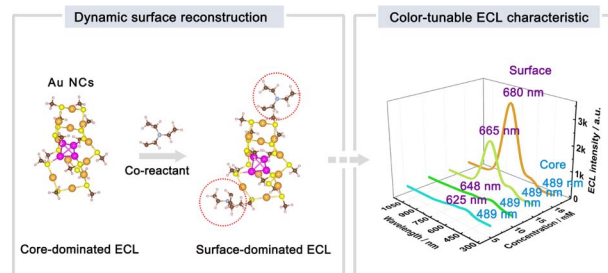
Kateryna Prysiashniuk, Oleksandr Polishchuk, Stanislav Shulha, Kyrylo Gudzikeych, Oleksandr P. Datsenko, Vladimir Kubyskhin and Pavel K. Mykhailiuk\*



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### Dynamic surface reconstruction of individual gold nanoclusters by using a co-reactant enables color-tunable electrochemiluminescence

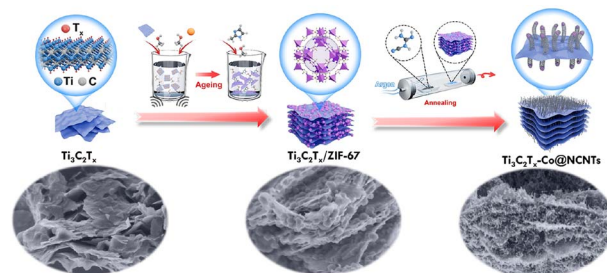
Yan-Mei Lei, Di Wu, Mei-Chen Pan, Xiu-Li Tao, Wei-Jia Zeng, Li-Yong Gan, Ya-Qin Chai, Ruo Yuan and Ying Zhuo\*



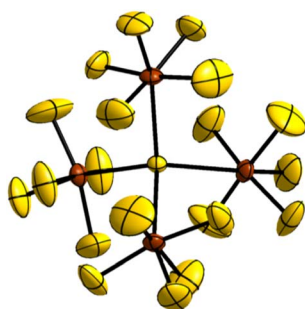
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### Elastic MXene conductive layers and electrolyte engineering enable robust potassium storage

Xinyue Xu, Qingqing Jiang,\* Chenyu Yang, Jinxi Ruan, Weifang Zhao, Houyu Wang, Xinxin Lu, Zhe Li, Yuanzhen Chen, Chaofeng Zhang,\* Juncheng Hu\* and Tengfei Zhou\*



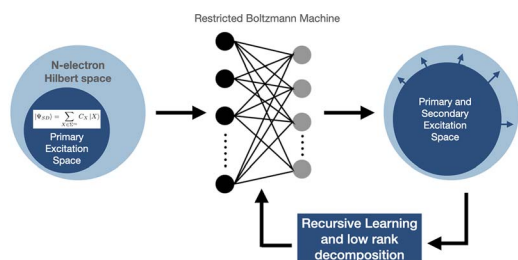
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### [Br<sub>4</sub>F<sub>21</sub>]<sup>-</sup> – a unique molecular tetrahedral interhalogen ion containing a μ<sub>4</sub>-bridging fluorine atom surrounded by BrF<sub>5</sub> molecules

Martin Möbs, Tim Graubner, Antti J. Karttunen and Florian Kraus\*

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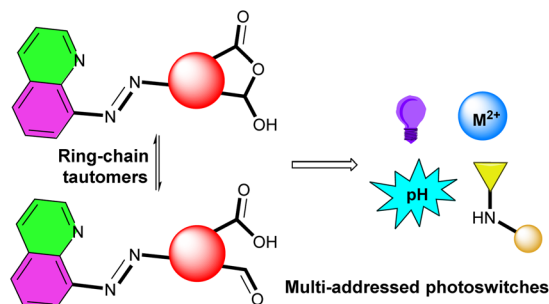


Construction of RBM-dUCC Ansatz utilizing Restricted Boltzmann Machine

### Machine learning assisted construction of a shallow depth dynamic ansatz for noisy quantum hardware

Sonaldeep Halder, Anish Dey, Chinmay Shrikhande and Rahul Maitra\*

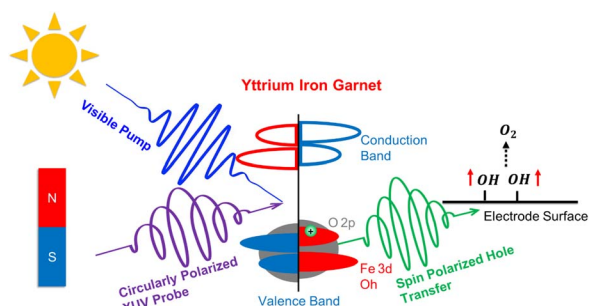
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### Multiple control of azoquinoline based molecular photoswitches

Younging Lv, Hebo Ye and Lei You\*

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### Spin polarized electron dynamics enhance water splitting efficiency by yttrium iron garnet photoanodes: a new platform for spin selective photocatalysis

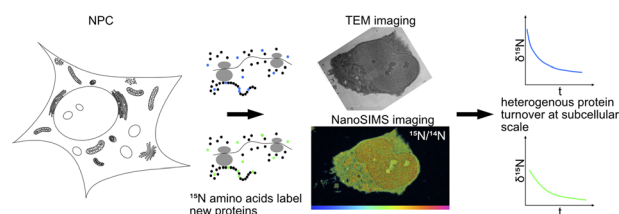
Harshad Gajapathy, Savini Bandaranayake, Emily Hruska, Aravind Vadakkayil, Brian P. Bloom, Stephen Londo, Jackson McClellan, Jason Guo, Daniel Russell, Frank M. F. de Groot, Fengyuan Yang, David H. Waldeck, Martin Schultze and L. Robert Baker\*



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### Subcellular protein turnover in human neural progenitor cells revealed by correlative electron microscopy and nanoscale secondary ion mass spectrometry imaging

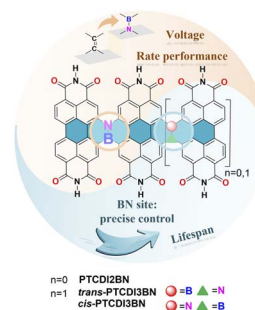
Alicia A. Lork, Stefania Rabasco, Carl Ernst, André du Toit, Silvio O. Rizzoli and Nhu T. N. Phan\*



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### Precise synthesis of BN embedded perylene diimide oligomers for fast-charging and long-life potassium–organic batteries

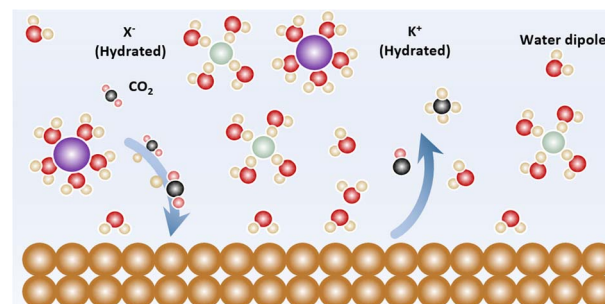
Guangwei Shao, Hang Liu, Li Chen, Mingliang Wu, Dongxue Wang,\* Di Wu\* and Jianlong Xia\*



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### Computational electrocatalysis beyond conventional hydrogen electrode model: CO<sub>2</sub> reduction to C<sub>2</sub> species on copper facilitated by dynamically formed solvent halide ions at the solid–liquid interface

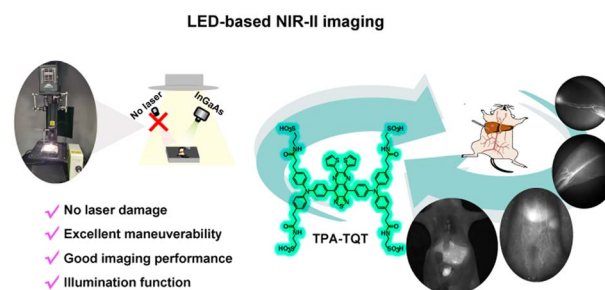
Xin Mao, Tianwei He, Gurpreet Kour, Hanqing Yin, Chongyi Ling,\* Guoping Gao,\* Yonggang Jin, Qingju Liu, Anthony P. O'Mullane and Aijun Du\*



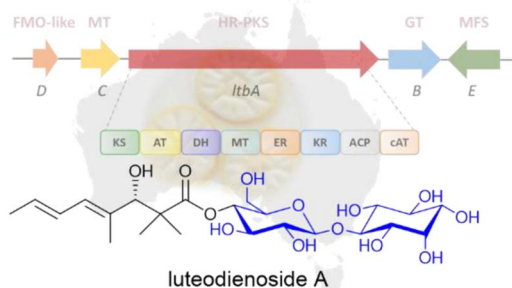
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### NIR-II fluorescence imaging without intended excitation light

Aiyan Ji, Hongyue Lou, Jiafeng Li, Yimeng Hao, Xiaonan Wei, Yibin Wu, Weili Zhao,\* Hao Chen\* and Zhen Cheng\*



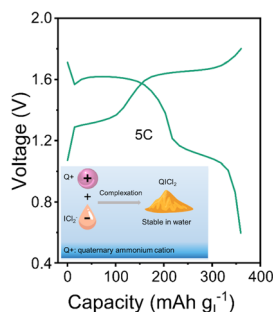
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### Discovery and heterologous biosynthesis of glycosylated polyketide luteodienoside A reveals unprecedented glucinol-mediated product offloading by a fungal carnitine O-acyltransferase domain

Amr A. Arishi, Zhuo Shang, Ernest Lacey, Andrew Crombie, Daniel Vuong, Hang Li, Joe Bracegirdle, Peter Turner, William Lewis, Gavin R. Flematti, Andrew M. Piggott\* and Yit-Heng Chooi\*

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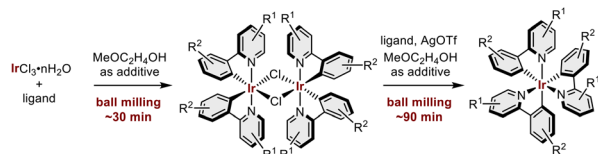


### Stabilized four-electron aqueous zinc–iodine batteries by quaternary ammonium complexation

Pengjie Jiang, Qijun Du, Chengjun Lei, Chen Xu, Tingting Liu, Xin He and Xiao Liang\*

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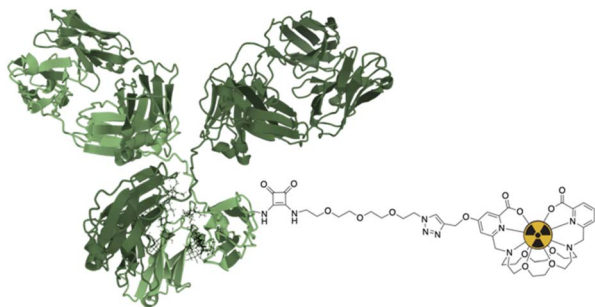
Mechanochemistry for the Rapid and Efficient Synthesis of Tris-Cyclometalated Iridium(III) Complexes



### Solid-state mechanochemistry for the rapid and efficient synthesis of tris-cyclometalated iridium(III) complexes

Koji Kubota,\* Tsubura Endo and Hajime Ito\*

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### Tumor targeted alpha particle therapy with an actinium-225 labelled antibody for carbonic anhydrase IX

Katherine A. Morgan, Christian W. Wichmann, Laura D. Osellame, Zhipeng Cao, Nancy Guo, Andrew M. Scott and Paul S. Donnelly\*



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## Structure and polymerization of liquid sulfur across the $\lambda$ -transition

Manyi Yang, Enrico Trizio and Michele Parrinello\*

