

# Chemical Science

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## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 17(1) 1–674 (2026)



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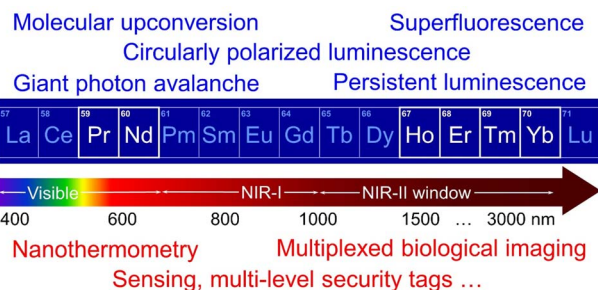
**Inside cover**  
See Kirill Nikitin, Declan G. Gilheany *et al.*, pp. 164–175. Image reproduced by permission of Anna Vetter and Kirill Nikitin from *Chem. Sci.*, 2026, 17, 164. Image generated in part using Adobe Firefly's generative AI platform, Adobe Inc.

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Alon Grinberg Dana\*



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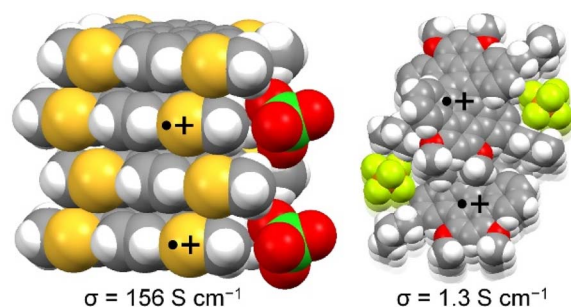
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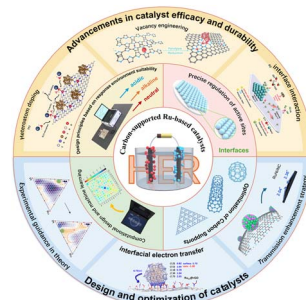
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**Multidimensional design of carbon-supported Ru-based catalysts: a journey to hydrogen evolution reaction performance breakthroughs**

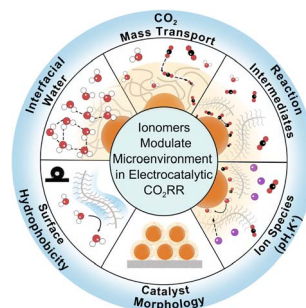
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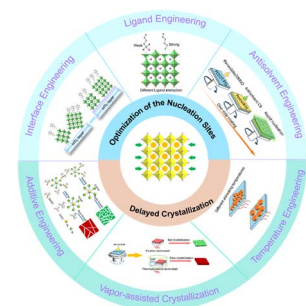
Sunhong Ruan,\* Gangjun Tang, Zhiming Zhang, Qinghong Zhang,\* Ye Wang\* and Shunji Xie\*

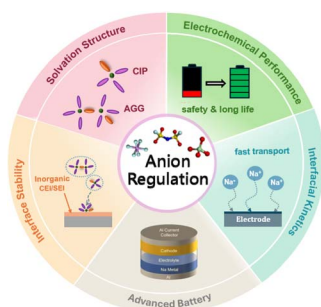


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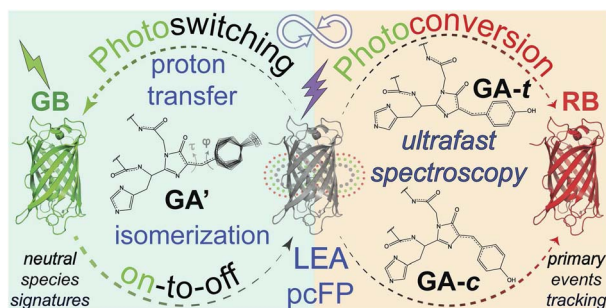
Long-Xue Cao, Yu-Hang Zhang, Yang Shen,\* Yan-Qing Li\* and Jian-Xin Tang\*





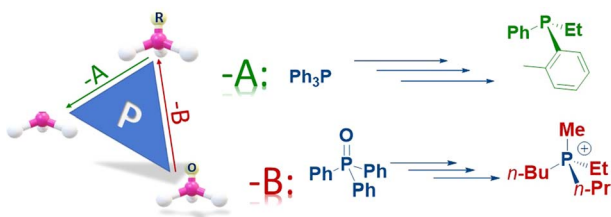
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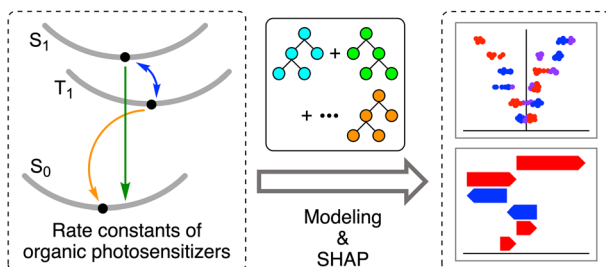
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### The organophosphorus synthesis triangle: introducing methods for the missing quaternization and de-quaternization routes

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### Data-driven approach to elucidate the correlation between photocatalytic activity and rate constants from excited states

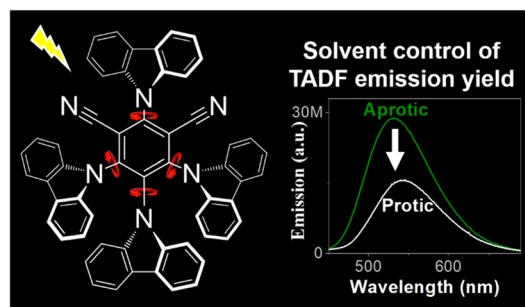
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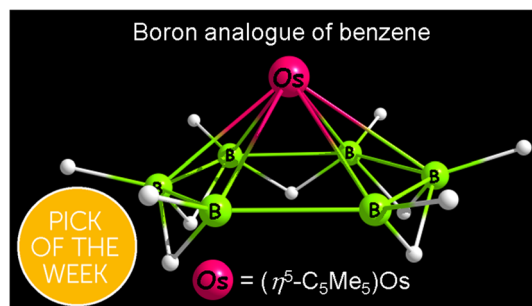
Sushree Suhani Puan, Laxmipriya Dash and Palas Roy\*



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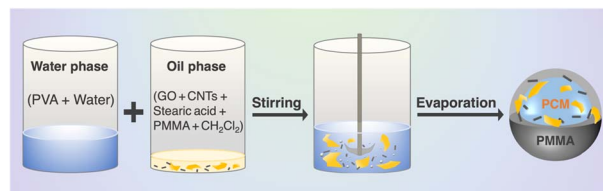
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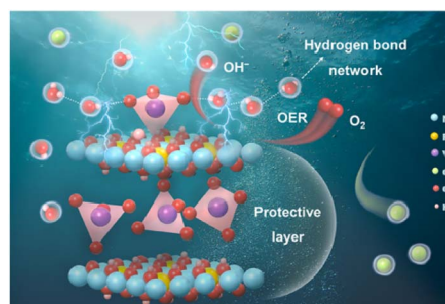
Bowei Du, Xinbing Jiang, Zhijie Zhang, Kai Xi, Borui Zhang, Qinghao Yang and Shujiang Ding\*



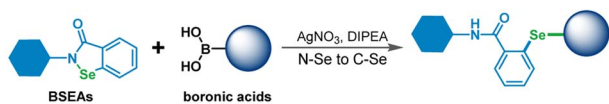
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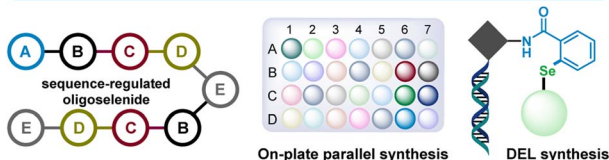
Shuxuan Yin, Zhixiang Zhai, Fangyuan Guan, Zihui Ning, Zelong Sun, Jia Wu, Wenjie Jiang, Lin Luo and Shibin Yin\*



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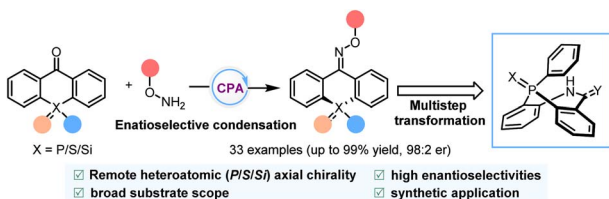
Highly selective and AI predictable SeNEx chemistry and its diversified performance



## Highly selective and AI-predictable Se–N exchange chemistry between benzoseleazolones and boronic acids for programmable, parallel, and DNA-encoded library synthesis

Wei Zhou, Yan Wang, Shuning Zhang, Chengwei Zhang, Jiacheng Pang, Shaoneng Hou, Jie Li, Ying Yao, An Su,\* Peixiang Ma,\* Hongtao Xu\* and Wei Hou\*

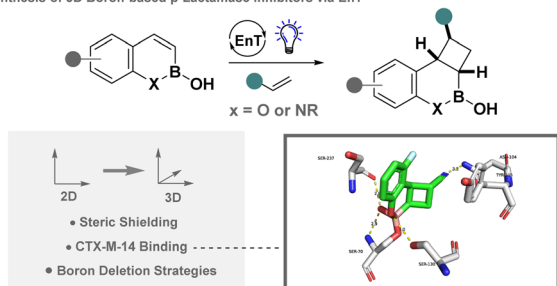
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## Catalytic asymmetric construction of remote P or other heteroatom (Si/S) stereogenic axially chiral scaffolds

Wenqi Liu, Zhijie Ling, Yang-Zi Liu\* and Wei-Ping Deng\*

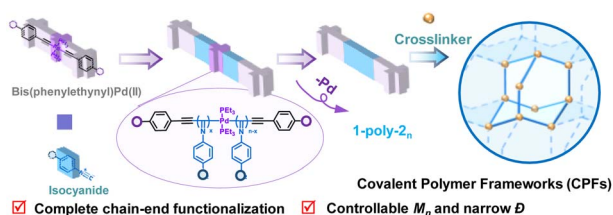
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Synthesis of 3D Boron-based  $\beta$ -Lactamase Inhibitors via EnT

## Fused 3D boron heterocycles via EnT catalysis: synthesis, modification and validation as beta-lactamase inhibitors

Hannah M. Kortman, Hao Fang, Kane A. C. Bastick, Charlotte Völkel, Dominik Oberthür, Peter H. Seeberger, Markus Perbandt\* and John J. Molloy\*

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## Precise synthesis of telechelic rodlike polyisocyanides: versatile building blocks for fabricating polymer frameworks with controllable pore-apertures

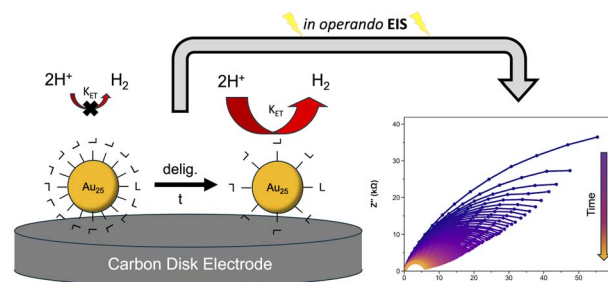
Yang Zong, Run-Tan Gao, Na Liu,\* Shixing Lei, Zhan-Ting Li and Zong-Quan Wu\*



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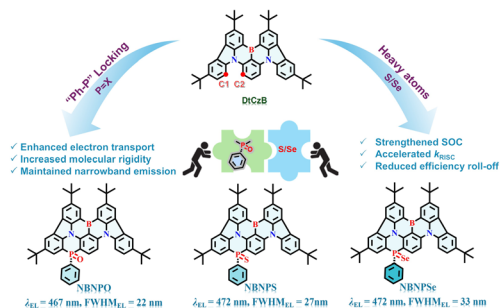
Eric Z. Liu, Samuel D. Parker, Dylan P. Tietje-Mckinney, Miguel Orozco, Trevor W. Hayton and Lior Sepunaru\*



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### Phenphosphine-X(O, S, Se) locking multi-resonance thermally activated delayed fluorescence materials

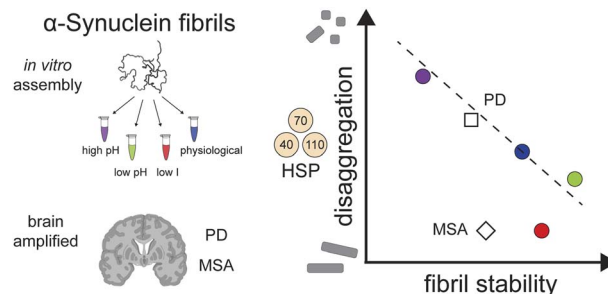
Xian-Fang Hong, Yi Wei, Hao-Ran Xing, Yu Wang, Jia-Qi Xi, Chen-Yang Wu, Li Yuan,\* Cheng-Hui Li and You-Xuan Zheng\*



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### Thermodynamic stability modulates chaperone-mediated disaggregation of $\alpha$ -synuclein fibrils

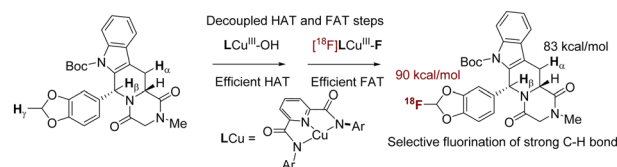
Celia Fricke, Antonin Kunka, Rasmus K. Norrild, Shuangyan Wang, Thi Lieu Dang, Jonas Folke, Mohammad Shahnawaz, Claudio Soto, Susana Aznar, Anne S. Wentink, Bernd Bukau and Alexander K. Buell\*



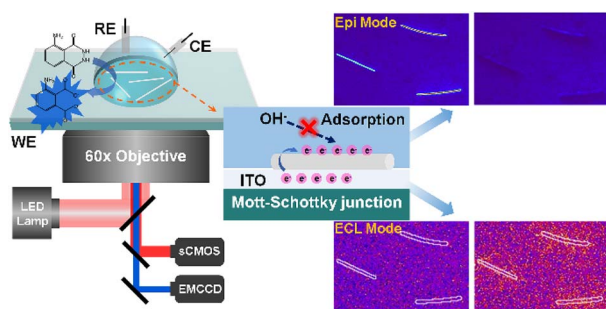
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### Distinct hydrogen atom transfer and radical capture reactivity of copper(III) OH/F complexes enables site-selective C(sp<sup>3</sup>)-H <sup>18</sup>F-fluorination

Joshua A. Queener, Angela Asor, Margaret A. P. Ball, Jinghua Tang, Jinda Fan\* and Shiyu Zhang\*



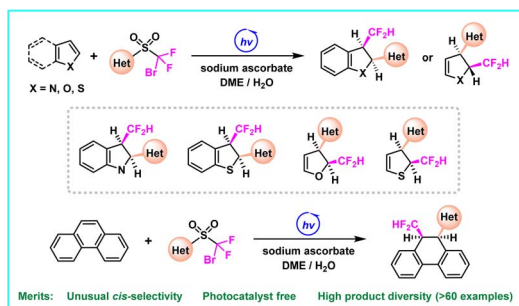
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### Reaction-pathway resolved multimode imaging of electrocatalytic oxygen evolution on single silver nanowires@ITO Mott–Schottky junctions

Yu Cui, Lisi Wen, Houkai Chen, Guopeng Li, Zhe Zhang and Rui Hao\*

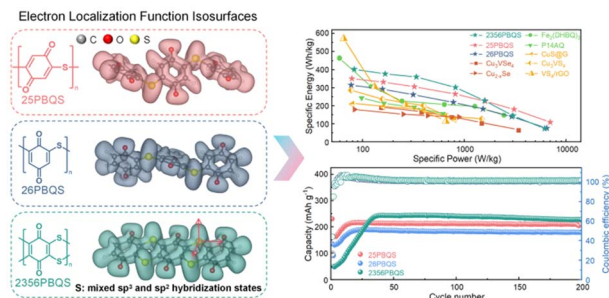
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### *Cis*-difluoromethyl hetarylation dearomatization by a radical docking-migration cascade

Jie Wang, Hao Kang, Shan Yang, Zhu Cao, Xiangyang Chen\* and Chen Zhu\*

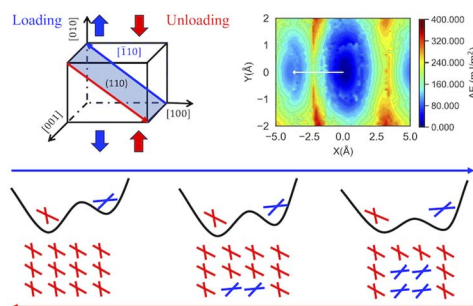
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### Hybridization-tuned dual-chain conjugated polythioether quinones for high-energy rechargeable magnesium batteries

Hongda Gui, Ze Wang, Yuliang Cao and Fei Xu\*

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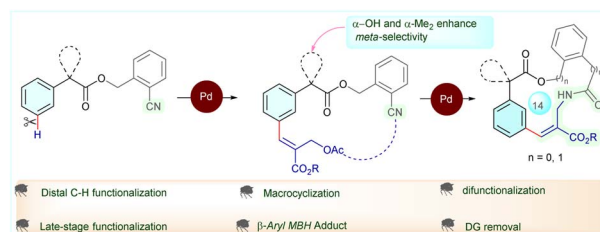
Zarif Fahim, Patrick Commins, Liang Li, Panče Naumov\* and Qiang Zhu\*



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### Pd-catalyzed sequential distal C–H alkenylation and $\pi$ -allylic amination of arylacetic acids using MBH acetates: access to macrocyclic lactams

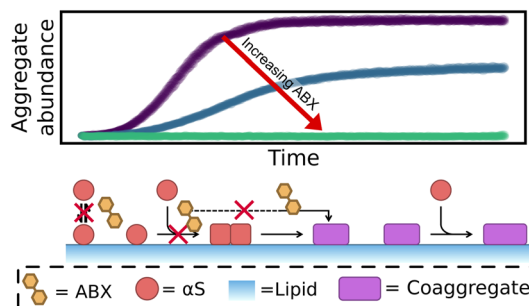
Perumal Muthuraja, Prabhat Kumar Maharana, Tamilthendral Veerappan, Subhadeep Kar and Tharmalingam Punniyamurthy\*



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### Ambroxol displaces $\alpha$ -synuclein from the membrane and inhibits the formation of early protein–lipid coaggregates

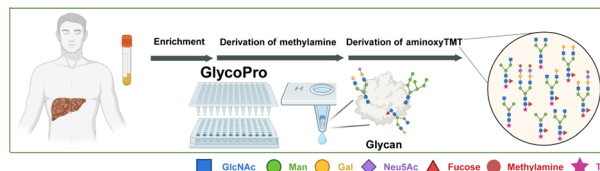
Jesper E. Dreier, Alisdair Stevenson, Elliot Carles, Katharina Schott, Thomas C. T. Michaels\* and Céline Galvagnion\*



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### A high-throughput N-glycan analysis strategy with targeted mass spectrometry (HTnGQs-target) for liver disease diagnosis

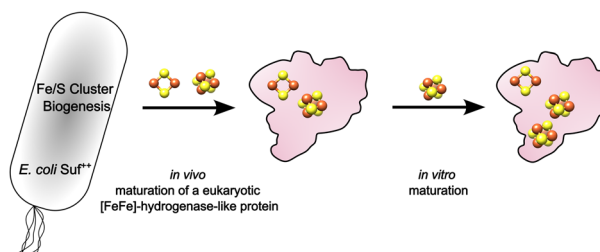
Xuejiao Liu, Jierong Chen, Bin Fu, Sanfeng Han, Dongdong Zheng, Ying Zhang\* and Haojie Lu\*



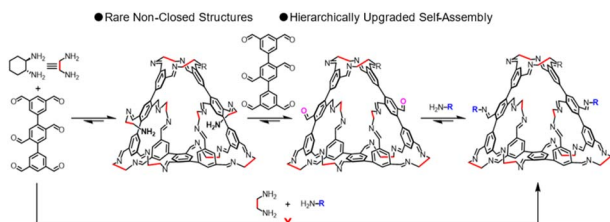
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### Yeast [FeFe]-hydrogenase-like protein Nar1 binds a [2Fe–2S] cluster

Joseph J. Braymer,\* Lukas Knauer, Jason C. Crack, Jonathan Oltmanns, Melanie Heghmanns, Jéssica C. Soares, Nick E. Le Brun, Volker Schünemann and Müge Kasanmascheff



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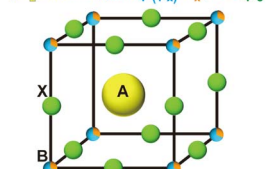


### A self-assembled macrocycle with a non-closed structure for hierarchically upgraded self-assembly

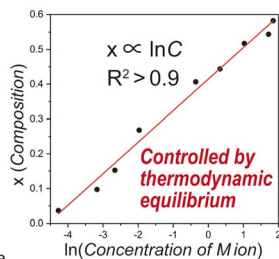
Ze Cao, Chenqi Ge, Guangcheng Wu,\* Hua Tang, Yating Wu, Yueyan Kuang, Yuyang Lu, Jiyong Liu and Hao Li\*

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### Energetic Perovskite Solid Solutions



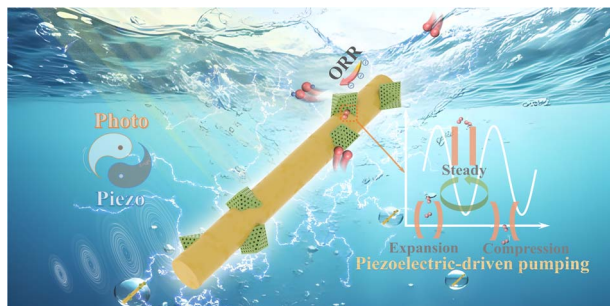
- ✓ Exceptional thermal stability
- ✓ Energy-safety optimization
- ✓ Enhanced detonation performance



### Controllable synthesis of perovskite solid solutions as novel energetic materials via thermodynamic equilibrium

Min Li, Dandan Han,\* Zheng Lin, Xiujuan Qi, Honglei Xia,\* Zhao Wang, Qinghua Zhang\* and Junbo Gong

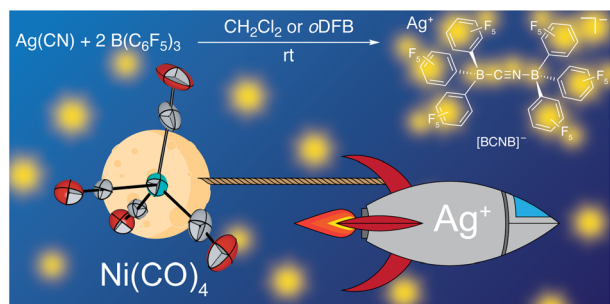
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### Accelerated confined mass transfer in piezoelectric semiconducting metal–organic frameworks for H<sub>2</sub>O<sub>2</sub> piezo-photosynthesis

Yuchen Lan, Ling Gao, Jin Qian, Jinzhou Liu, Bo Shen, Menghao Yang, Wenguang Tu, Jiwei Zhai\* and Guanyu Liu\*

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### A facile route to 'naked' Ag<sup>+</sup> ions enabling the coordination of the weak Lewis base Ni(CO)<sub>4</sub>

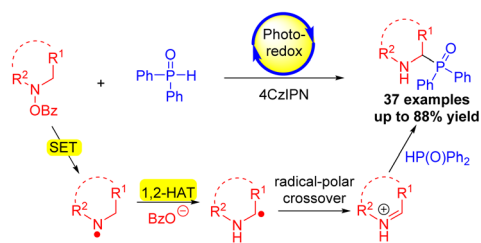
Willi R. Berg, Amina L. Moshtaha, Robin Sievers, Marc Reimann, Tim-Niclas Streit, Susanne M. Rupf, Martin Kaupp and Moritz Malischewski\*



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### 1,2-Hydrogen atom transfer of aminyl radicals under photoredox catalysis for the synthesis of $\alpha$ -amino phosphine oxides

Ailin Pan, Madeline E. Rotella, Yamiao Meng, Xun Tian, Shengzu Duan, Yonggang Jiang, Guogang Deng, Bart Limburg, Hongbin Zhang,\* Marisa C. Kozlowski,\* Patrick J. Walsh\* and Xiaodong Yang\*

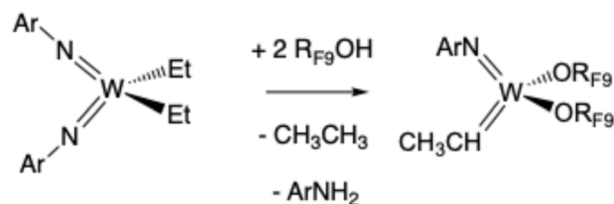


- Broad substrate scope and scalable
- Mild conditions (rt)
- Transition-metal free
- Weak base (leaving group)-promoted 1,2-HAT of N-centered radicals

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### Formation of tungsten ethylidene complexes from diethyl complexes through a proton-catalyzed rearrangement of ethylene

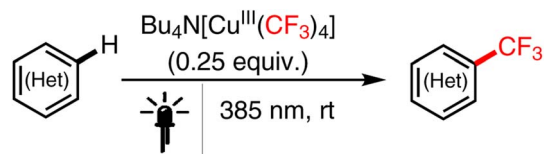
Milan Maji, Landley Zeng, Richard R. Schrock,\* Matthew P. Conley\* and Veronica Carta



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### Photochemical Cu(III)-mediated trifluoromethylation of (hetero)arenes and biomolecules

Petr Pospíšil, Vladimír Motornov,\* Ondřej Michal, Lucie Šálková, Soňa Boháčová, Tomáš Slanina, Ján Tarábek, Blanka Klepetářová and Petr Beier\*

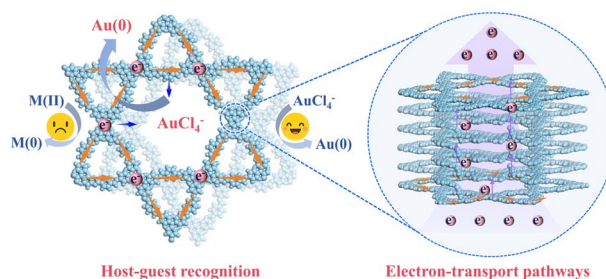


- Catalytic by copper
- Mild conditions
- Up to 98% yield (with respect to one CF<sub>3</sub> group)
- Late-stage functionalization of complex molecules

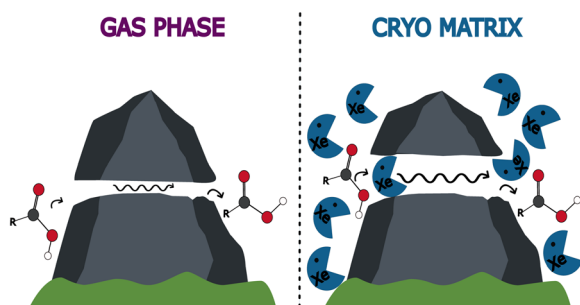
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### Topology engineering of COFs via localized 1D–2D unit interconnection to facilitate interfacial electron transfer for efficient gold recovery from e-waste leachates

Jiaying Xiong, Qi An, Hao Xiang, Yu Zhou, Yuan Zhang, WenJing Chen, Boxian Ren, Shixiong Wang, Huiping Bai,\* Hong Guo\* and Xiangjun Yang\*



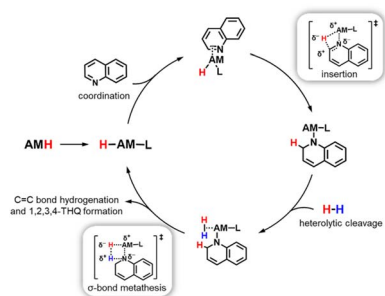
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### Solvation or not solvation: tunneling reactions of molecules embedded in cryogenic matrices

Giacomo Mandelli, Chiara Aieta and Michele Ceotto\*

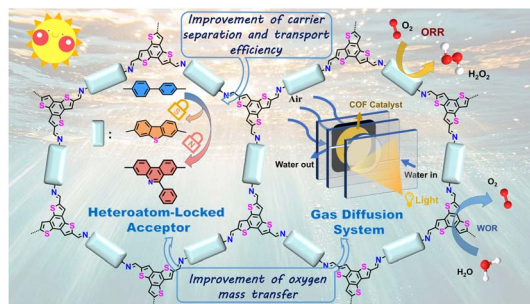
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### Simple s-block metal hydrides for selective hydrogenation of quinoline compounds

Shengyuan Zhang, Hong Wen, Qianru Wang,\* Yongli Cai, Zhao Li, Liang Liu, Xuanwei Chang, Jianping Guo and Ping Chen\*

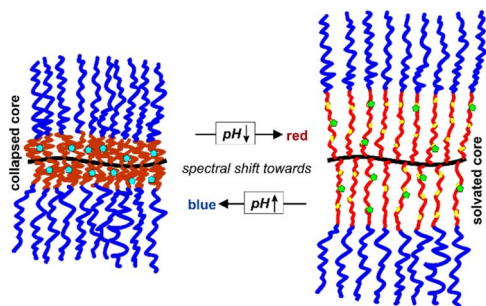
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### Boosting the photocatalytic H<sub>2</sub>O<sub>2</sub> production of covalent organic frameworks with a heteroatom-locked acceptor and gas diffusion system

Qianshuo Nan, Jing Ning, Bing Han, Hongtao Wei, Xuefeng Wang,\* Ying-Ying Gu,\* Shengxiang Zhou, Guangqiang Cao, Guangze Zhang, Xuehui Li, Yonggang Jia\* and Long Hao\*

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### A printable, unimolecular, core-shell polymer bottlebrush-based signal transducer using solvatochromatic reporting

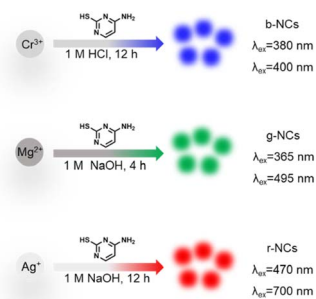
Chenyong Zhang, Samantha O. Catt, Tom Hawtrey, Ping Zeng, Haoxiang Zeng, Simran D. Kerai, Yen Theng Cheng, Moritz P. Hopp, Qingqin Yang, Elizabeth J. New, Eva Blasco\* and Markus Müllner\*



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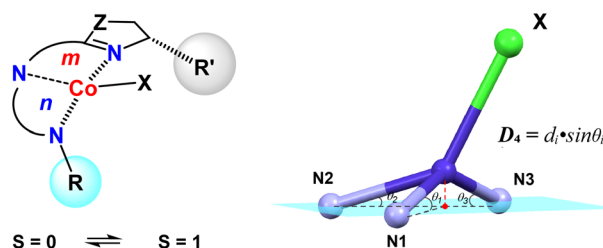
## Heterometallic ion-regulated full-color gold nanoclusters for multicolor bioimaging and circularly polarized luminescence

Yaguang Yin, Gan Zhao, Fanfan Yu and Honglin Liu\*



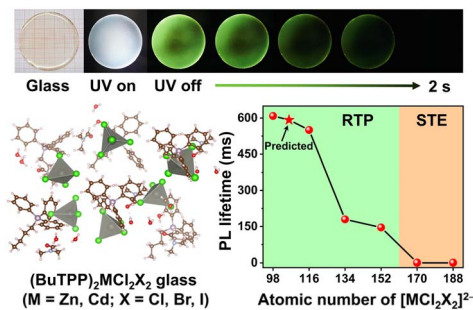
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## The structural parameter of spin states of $C_1$ -symmetric four-coordinate cobalt complexes: $D_4$

Chengcong Zheng, Jiyong Liu, Yongtao Wang,\*  
Haoran Li,\* Yuwen Wang\* and Zhan Lu\*

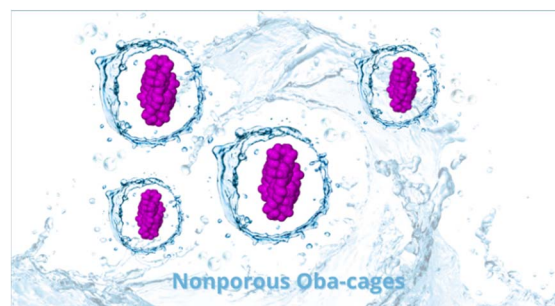
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## Heavy-atom effect regulating room temperature phosphorescence in hybrid metal halide glasses

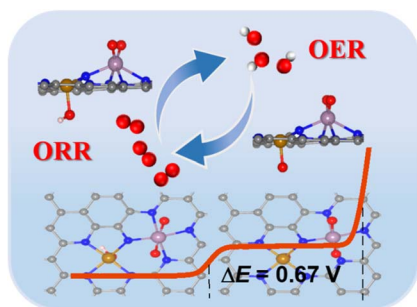
Linyuan Lian, Ming Ai, Daming Xiong, Tao Liang,  
Jibin Zhang, Mochen Jia, Ying Liu, Zhuangzhuang Ma,  
Xu Chen, Yanbing Han, Yongtao Tian, Xinjian Li  
and Zhifeng Shi\*

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## A nonporous crystalline organic cage for selective water uptake and storage

Lukman O. Alimi, Nida Khalfay, Soumaya Khelifi, Weibin Lin,  
Basem Moosa and Niveen M. Khashab\*

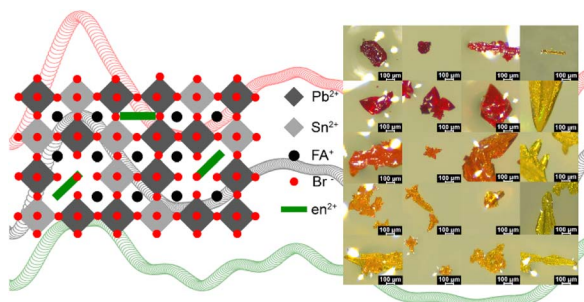
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### Engineering O–O formation on dual-atom Fe–Mo catalysts for oxygen electrocatalysis

Luoluo Qi, Yanan Tang,\* Tao Gan\* and Jingqi Guan\*

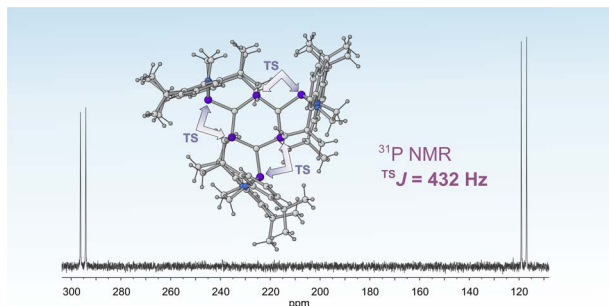
526



### Tuning optical properties and local lone-pair off-centering in “hollow” FA<sub>1-x</sub>(en)<sub>x</sub>Pb<sub>η-y</sub>Sn<sub>y</sub>Br<sub>3</sub> perovskites

Adam Balvanz, Anastasia Pournara, Robert P. Reynolds, Patricia E. Meza, Christos D. Malliakas, Jared D. Fletcher, Ram Seshadri, Vinayak P. Dravid and Mercouri G. Kanatzidis\*

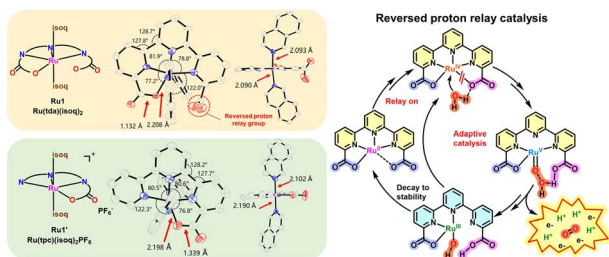
544



### Exceptionally large “through-space” nuclear spin coupling in a 2,4,6-tri(phosphanyl)-1,3,5-triphospha-benzene

David C. Meier, Álvaro García-Romero, Daniel González-Pinardo, Nicholas H. Rees, Alex Lovstedt, Israel Fernández\* and Jose M. Goicoechea\*

555



### Elucidating the reversed proton relay mechanism: dual regulatory role of pendant carboxylates relevant to water oxidation

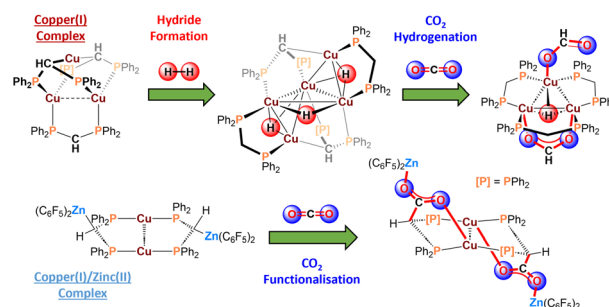
Taolue Liu, Yu Wei, Guojie Gao, Mingxia Guo, Jinxuan Liu, Xin Ding,\* Yingying Li\* and Yan Gao\*



564

## Structural and reactivity investigations using organo-copper(I) and zinc(II) complexes with hydrogen and carbon dioxide

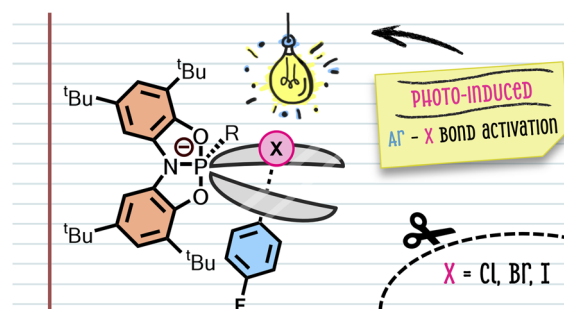
Bradley E. Cowie, Andreas Phanopoulos, Milo S. P. Shaffer\* and Charlotte K. Williams\*



579

## Photochemical activation of pincer-ligated phosphoranides: mechanistic insight for reduction of aryl halides

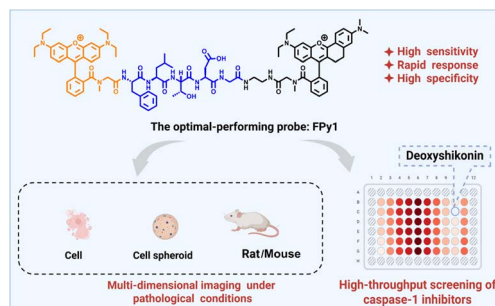
Emile Escoudé, Manuel Pedrón, Lilian Bourqui, Geoffrey Gontard, Maxime R. Vitale, Ilaria Ciofini,\* Sami Lakhdar\* and Laurence Grimaud\*



585

## Design and optimization of caspase-1-responsive fluorescent probes for pyroptosis imaging and anti-pyroptosis drug screening

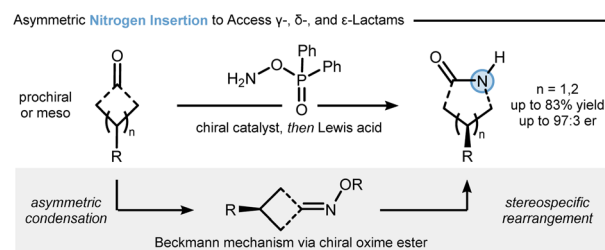
Wei Wang, Guanrui Huang, Yeting Zhou, Yue Wang, Luling Wu,\* Tony D. James, Weili Wang\* and Yi Wang\*



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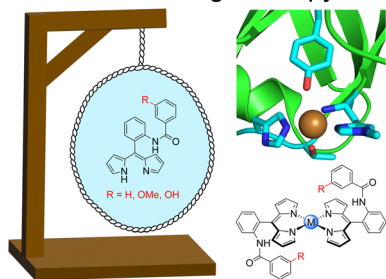
## Synthesis of chiral lactams by asymmetric nitrogen insertion

Jasmin Hammes, Clara Mañas, Abhilash Pedada, Marlene Arnold and Johannes M. Wacht\*



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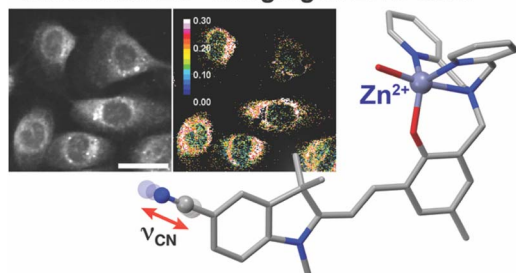
## Biomimetic Hangman Dipyrrins



## Hangman dipyrrin complexes

Isaac S. Schomberg-Sanchez, William C. Robinson, Makayla E. Sanderson, Martín A. Mosquera and Christopher M. Lemon\*

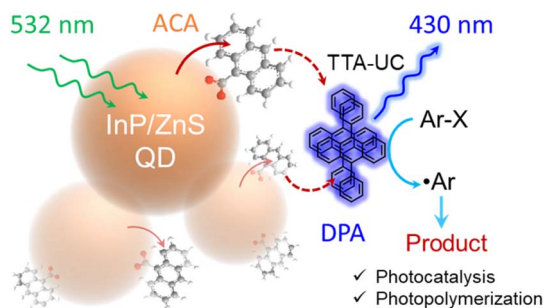
617

Vibrational  $Zn^{2+}$  Imaging in Live Cells

## Imaging intracellular zinc by stimulated Raman scattering microscopy with a small molecule vibrational probe

Elsy El Khoury, Symara de Melo Silva, Naixin Qian, Vinh Gia Vuong, Wei Min\* and Daniela Buccella\*

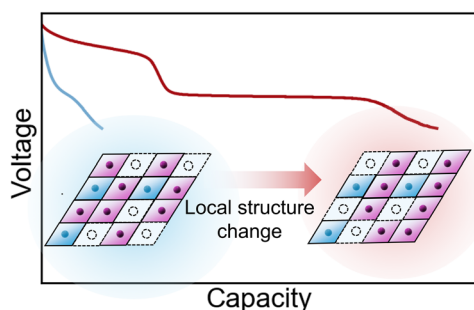
626



## Photon upconversion with indium phosphide quantum dots enables high-energy photoreactions using visible light

Indra Narayan Chakraborty, Adhra S. Sury, Aman Chaturvedi, Kaixing Wang, Ankit Dhankhar, Pankaj Mandal, Benjamin Dietzek-Ivanšić\* and Pramod P. Pillai\*

634

Impact of the  $d^0$  transition metal on local structural transformations in disordered rock salt cathodes

Tianyu Li, Otavio Marques, Tullio S. Geraci, Erick A. Lawrence, Arava Zohar, Jue Liu, Evans Avoka, Alexandra Navrotsky, Johanna Nelson Weker and Raphaële J. Clément\*

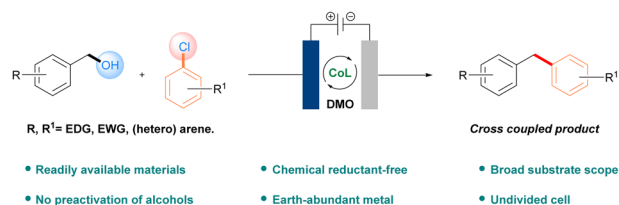


## EDGE ARTICLES

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### Low-valent cobalt catalyzed direct dehydroxylative cross-coupling of benzyl alcohols with aryl-chlorides

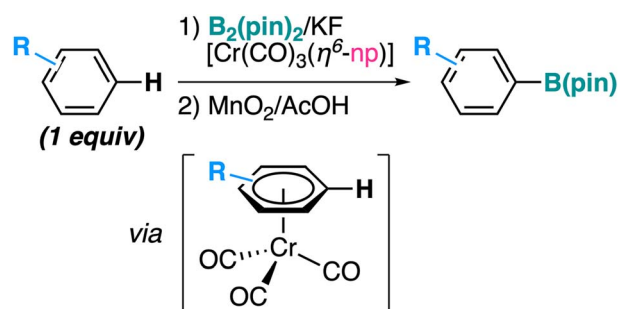
Prashant S. Shinde, Valmik S. Shinde\* and Magnus Rueping\*



664

### Transient $\pi$ -coordination enables nucleophilic borylation of simple arenes

Yuichiro Mutoh,\* Relam Khalaf, Sobi Asako and Laurean Ilies\*



## CORRECTION

671

### Correction: Photocatalytic [3 + 2]-annulation *via* sodium tetraarylborate: a fundamental approach for synthesizing 1,4,2-diazaborole analogs

Hao-Ni Qin, Hao-Wen Jiang, Yi Zhao, Saira Qurban, Ke-Chun Wang and Peng-Fei Xu\*

