

## IN THIS ISSUE

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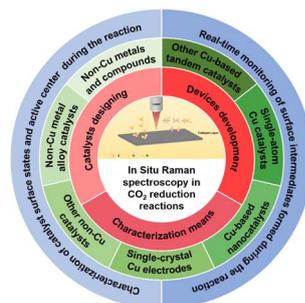
**Inside cover**  
See Hiromitsu Maeda *et al.*, pp. 4998–5006. Image reproduced by permission of Hiromitsu Maeda from *Chem. Sci.*, 2025, 16, 4998.

## REVIEWS

4916

### ***In situ* Raman spectroscopic studies of CO<sub>2</sub> reduction reactions: from catalyst surface structures to reaction mechanisms**

Dongao Zhang, Xuan Liu, Yu Zhao, Hua Zhang,\*  
Alexander V. Rudnev and Jian-Feng Li\*



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### **Biomass-derived carbon dots: synthesis, modification and application in batteries**

Dongyang Cai, Xue Zhong, Laiqiang Xu,\* Yu Xiong,\*  
Wentao Deng, Guoqiang Zou, Hongshuai Hou\*  
and Xiaobo Ji



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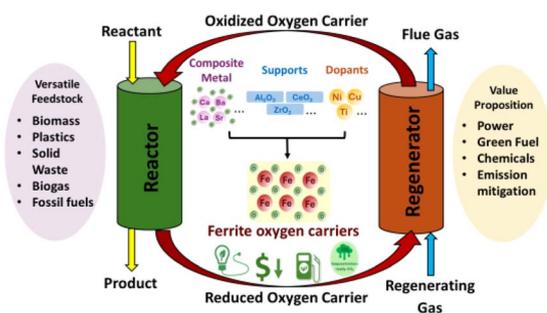
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## REVIEWS

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### Metal ferrite derivative chemical looping systems: a review towards a multiscale approach for technology readiness enabling clean energy conversion and carbon neutrality

Tanay A. Jawdekar, Ishani Karki Kudva, Sudeshna Gun, Shekhar G. Shinde, Ashin A. Sunny, Zhuo Cheng and Liang-Shih Fan\*

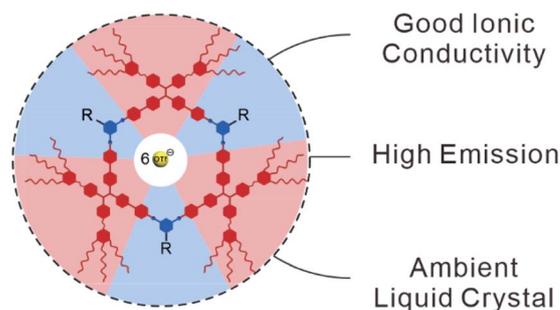


## EDGE ARTICLES

4992

### Metallacycle-cored luminescent ionic liquid crystals with trigonal symmetry

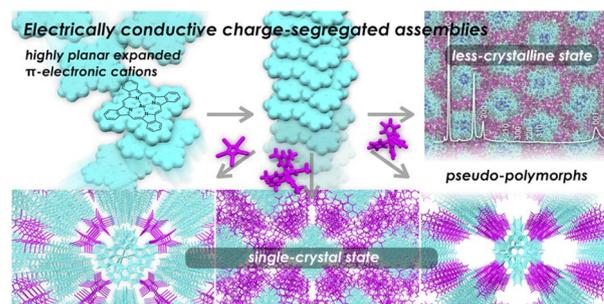
Long Chen, Yu Cao,\* Haohui Huo, Shuai Lu, Yali Hou, Tianyi Tan, Xiaopeng Li, Feng Liu and Mingming Zhang\*



4998

### Electrically conductive charge-segregated pseudo-polymorphs comprising highly planar expanded $\pi$ -electronic cations

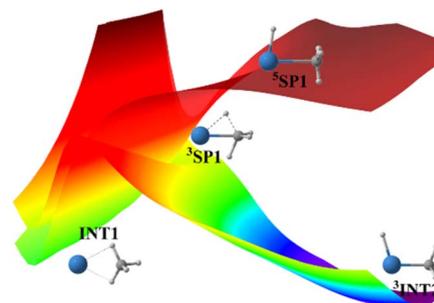
Yohei Haketa, Ryoya Nakajima, Yuto Maruyama, Hiroki Tanaka, Wookjin Choi, Shu Seki, Shunsuke Sato, Hitomi Baba, Yoshiki Ishii, Go Watanabe, Kirill Bulgarevich, Kazuo Takimiya, Kenzo Deguchi, Shinobu Ohki, Kenjiro Hashi, Takashi Nakanishi, Yukihide Ishibashi, Tsuyoshi Asahi, Kazuchika Ohta and Hiromitsu Maeda\*



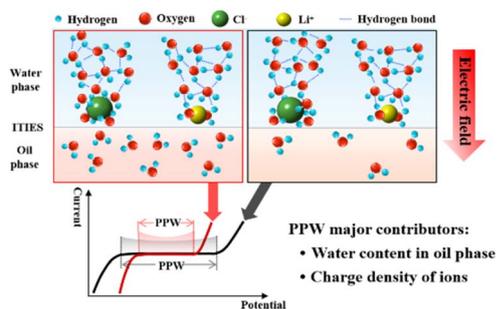
5007

### Insights into facile methane activation by a spin forbidden reaction with Ta<sup>+</sup> ions in the gas phase

Yang Liu, Milan Ončák,\* Tucker W. R. Lewis, Marcel Meta, Shaun G. Ard, Nicholas S. Shuman,\* Jennifer Meyer, Albert A. Viggiano and Hua Guo\*



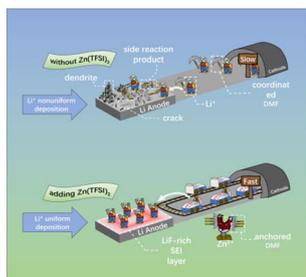
5017



### Polarizable potential window at soft molecular interfaces as a quantitative descriptor for the water content in organic solvents

Siqi Jin, Lifang Yang, Sijia He, Taoxiang Fang, Xiaohang Sun,<sup>\*</sup> Dandan Cai, Qiong Hu, Xinjian Huang and Haiqiang Deng<sup>\*</sup>

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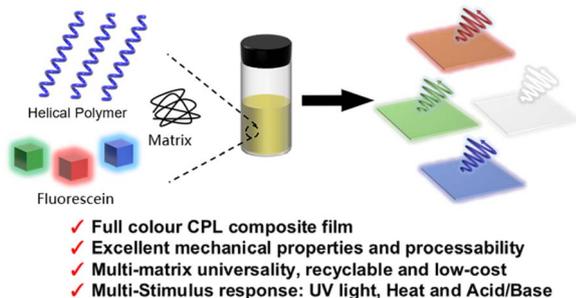


Schematic illustration for the action mechanism of Zn(TFS)<sub>2</sub> in PVDF-based electrolyte. The binding energy of Li-DMF, Na-DMF, K-DMF, Mg<sup>2+</sup>-DMF and Zn<sup>2+</sup>-DMF

### Regulating cation-solvent interactions in PVDF-based solid-state electrolytes for advanced Li metal batteries

Zhian Zhang, Meng Ye, Jianhua Chen, Xiaopeng Fu, Xunzhu Zhou, Limin Zheng, Liqing He, Zhenguo Wu, Amit Kumar, Lin Li,<sup>\*</sup> Fang Wan<sup>\*</sup> and Xiaodong Guo

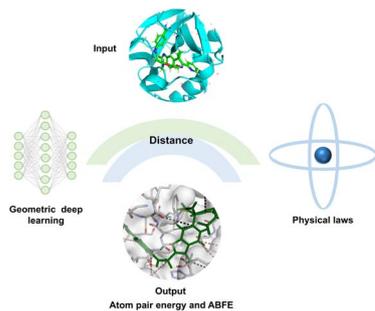
5036



### Helix-induced full-color circularly polarized luminescence films with multiple information encryption and multi-stimuli responsiveness

Shi-Yi Li, Yang Zong, Bing-Hao Liu, Na Liu and Zong-Quan Wu<sup>\*</sup>

5043



### Robust protein-ligand interaction modeling through integrating physical laws and geometric knowledge for absolute binding free energy calculation

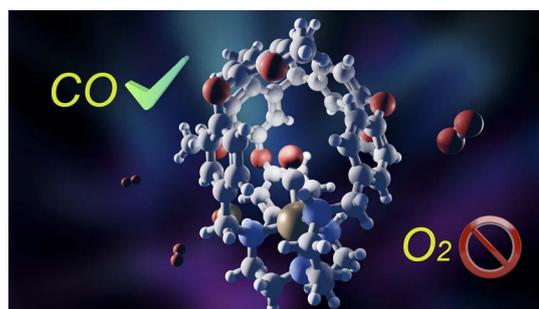
Qun Su, Jike Wang, Qiaolin Gou, Renling Hu, Linlong Jiang, Hui Zhang, Tianyue Wang, Yifei Liu, Chao Shen, Yu Kang, Chang-Yu Hsieh<sup>\*</sup> and Tingjun Hou<sup>\*</sup>



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### Unusually air-stable copper(I) complexes showing high selectivity for carbon monoxide

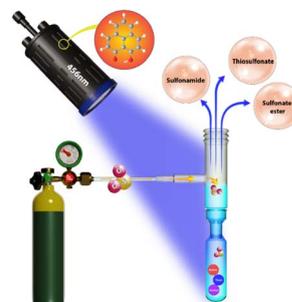
Borna Saeednia, Aria M. Sragow, Yannan Lin, Colton J. Sheehan, Amy S. Metlay, Michael R. Gau, Samantha A. Dye, Sarah P. O'Konski, Thomas E. Mallouk and Ivan J. Dmochowski\*



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### An organophotocatalytic redox-neutral strategy for late-stage drug functionalization with SO<sub>2</sub> gas

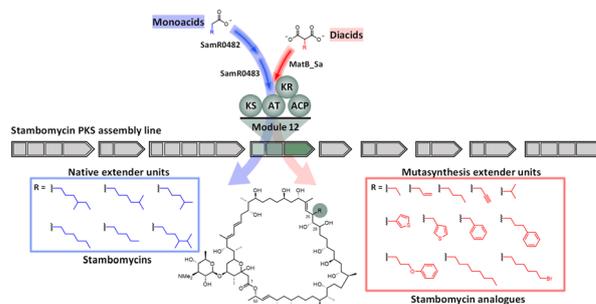
Paramita Datta, Subir Maji, Prativa Biswas, Divya Jain, Partha Protim Dey and Swadhin K. Mandal\*



5076

### Exploiting the inherent promiscuity of the acyl transferase of the stambomycin polyketide synthase for the mutasynthesis of analogues

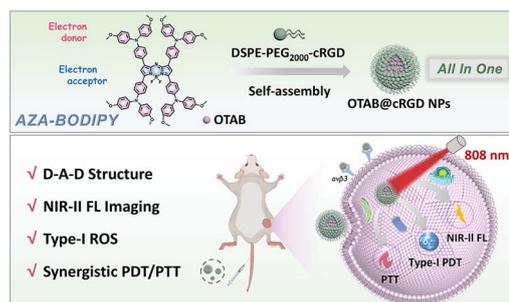
Li Su, Yaouba Souaibou, Laurence Hôtel, Christophe Jacob, Peter Grün, Yan-Ni Shi, Alicia Chateau, Sophie Pinel, Helge B. Bode, Bertrand Aigle\* and Kira J. Weissman\*



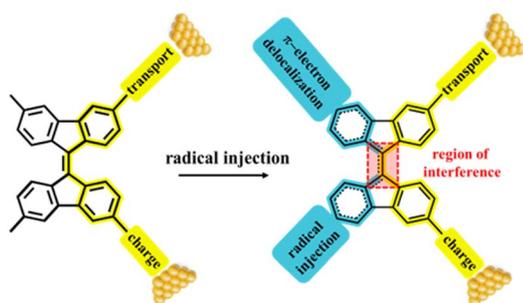
5089

### Donor modulation brings all-in-one phototheranostics for NIR-II imaging-guided type-I photodynamic/photothermal synergistic cancer therapy

Yuxin Ren, Xinyi Zhang, Ling Li, Qiong Yuan, Benkai Bao, Meiqi Li and Yanli Tang\*



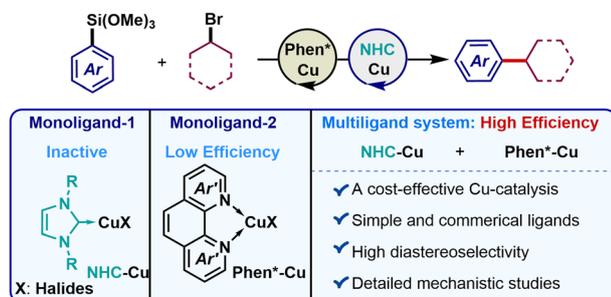
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### Radical-induced single-molecule conductance tuning in 9,9'-bifluorenylidene derivatives

Hanjun Zhang, Lichuan Chen, Yunzhu Huang, Xiaodong Liu,<sup>\*</sup> Sergio Moles Quintero, Wenjing Hong, Dongsheng Wang,<sup>\*</sup> Juan Casado and Yonghao Zheng<sup>\*</sup>

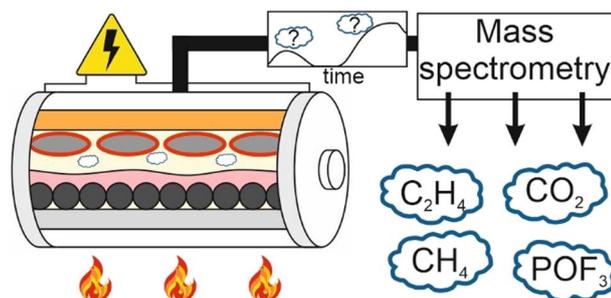
5109



### Multiligand-enabled, copper-catalyzed Hiyama coupling of arylsilanes with unactivated secondary alkyl halides: reaction development and mechanistic insights

Jiajing Zhou, Zhiqiang Zhang, Yan Cao and Weilong Xie<sup>\*</sup>

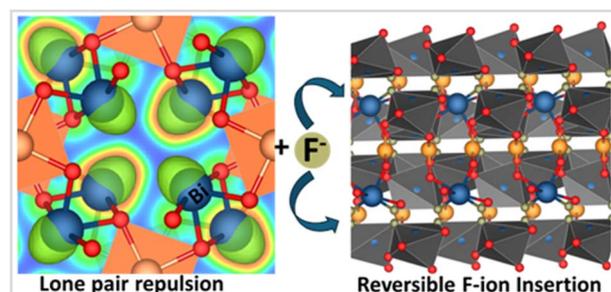
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### High temperature *in situ* gas analysis for identifying degradation mechanisms of lithium-ion batteries

Leon Schmidt, Kie Hankins, Lars Bläubaum, Michail Gerasimov and Ulrike Krewer<sup>\*</sup>

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### Stereochemical expression of Bi 6s<sup>2</sup> lone pairs mediates fluoride-ion (De)insertion in tunnel-structured Bi<sub>2</sub>PdO<sub>4</sub> and Bi<sub>1.6</sub>Pb<sub>0.4</sub>PtO<sub>4</sub>

George Agbeworvi, Anindya Pakhira, Shruti Hariyani, Wasif Zaheer, Alice Giem, Jaime R. Ayala, John D. Ponis, Saul Perez-Beltran, Chernó Jaye, Conan Weiland, Daniel A. Fischer, Hassan S. Bazzi, Mohammed Al-Hashimi and Sarbajit Banerjee<sup>\*</sup>

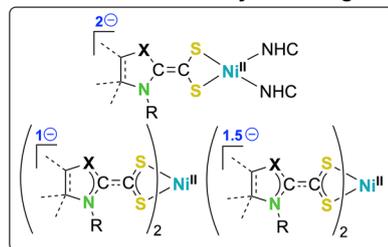


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### Azolium-2-dithiocarboxylates as redox active ligands in nickel chemistry

Martin S. Luff, Tin M. Filipovic, Celine S. Corsei, Kai Oppel, Ivo Krummenacher, Rüdiger Bertermann, Maik Finze, Holger Braunschweig and Udo Radius\*

#### Azolium-2-dithiocarboxylates as ligands

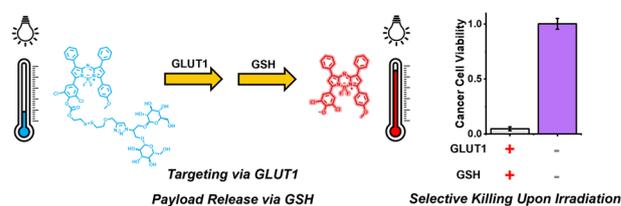


Redox-switches, NIR-Absorbers, Radicals

5155

### Logic-gated approach for targeted delivery and site-selective activation of photothermal agents in precision cancer treatment

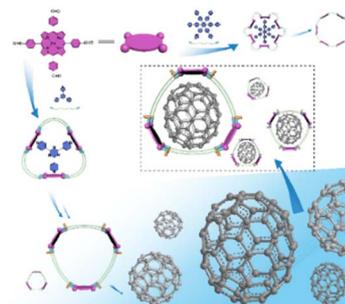
Chang Jiang, Zhengxiang Zhao, Amanda K. East, Suritra Bandyopadhyay, Ziyi Jiang and Jefferson Chan\*



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### Template-directed self-assembly of porphyrin nanorings through an imine condensation reaction

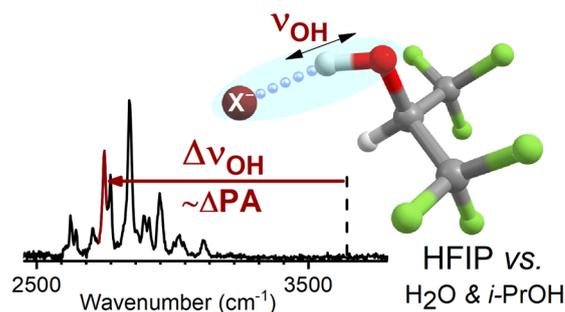
Ziwei Xu, Xinwen Ying, Yi Li, Xiaoyan Dong, Jiyong Liu, Shuping Wang, Marc A. Little, Dahao Zhang, Yongshu Xie, Zibin Zhang, Ling Yu, Feihe Huang and Shijun Li\*



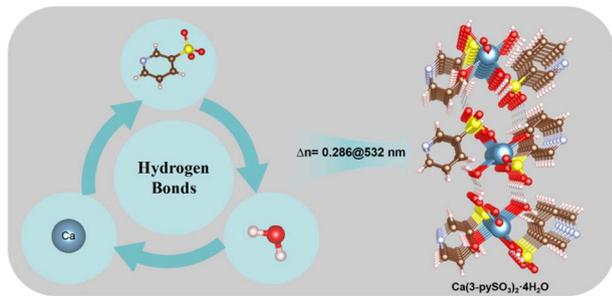
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### Quantifying hexafluoroisopropanol's hydrogen bond donor ability: infrared photodissociation spectroscopy of halide anion HFIP complexes

Milena Barp, Florian Kreuter, Qian-Rui Huang, Jiaye Jin, Franka E. Ninov, Jer-Lai Kuo,\* Ralf Tonner-Zech\* and Knut R. Asmis\*



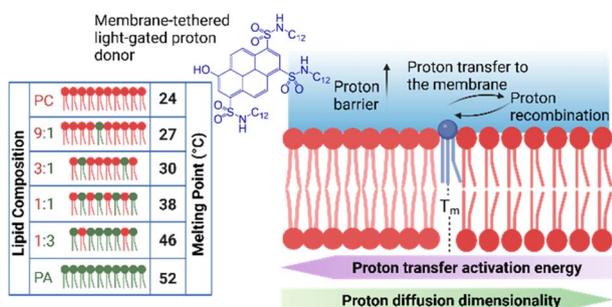
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### Hydrogen bonding regulation-oriented design of pyridine sulfonate as a promising UV birefringent crystal characterized by enhanced structural anisotropy

Longyun Xu, Conggang Li,\* Shuaifeng Li, Huijian Zhao, Xianghao Kong, Zaixin Qu, Wenjie Feng, Kaidong Xu, Ning Ye\* and Zhanggui Hu\*

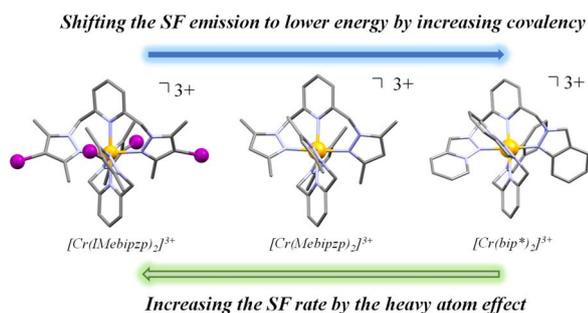
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### The role of lipid phase and temperature in proton barrier and proton migration on biological membranes

Ambili Ramanthrikkovil Variyam, Mateusz Rzycki, Ramesh Nandi, Alexei A. Stuchebrukhov, Dominik Drabik and Nadav Amdursky\*

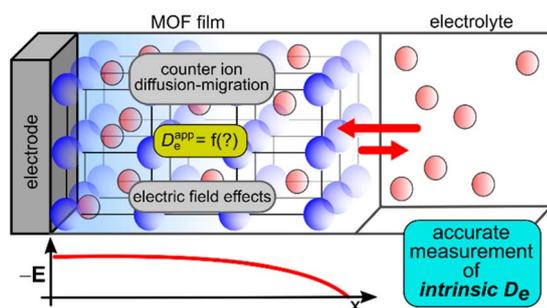
5205



### Modulating the spin-flip rates and emission energies through ligand design in chromium(III) molecular rubies

Yating Ye, Maxime Poncet, Polina Yaltseva, Pablo Salcedo-Abraira, Antonio Rodríguez-Diéguez, Javier Heredia Martín, Laura Cuevas-Contreras, Carlos M. Cruz, Benjamin Doistau, Claude Piguet, Oliver S. Wenger, Juan Manuel Herrera and Juan-Ramón Jiménez\*

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### Beyond diffusion: ion and electron migration contribute to charge transport in redox-conducting metal-organic frameworks

Ben A. Johnson,\* Ashleigh T. Castner, Hemlata Agarwala and Sascha Ott\*



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### 1,4-Dihydropyrrolo[3,2-*b*]pyrrole modified with dibenzoxazepine: a highly efficient core for charge-transfer-based OLED emitters

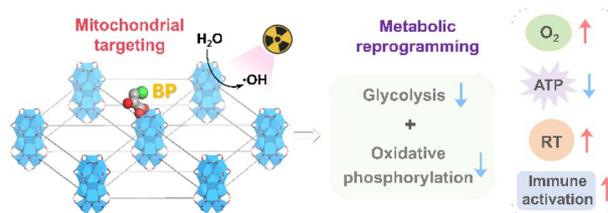
Krzysztof Górski, Steve Shelton, Jaijanarathanan Lingagouder, Przemyslaw Data,\* Denis Jacquemin\* and Daniel T. Gryko\*



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### Metal–organic layer delivers 3-bromopyruvate to mitochondria for metabolic regulation and cancer radio-immunotherapy

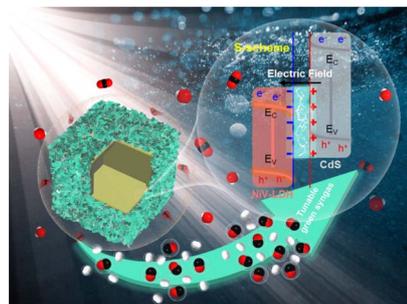
Wangqing Bian, Xiaomin Jiang, Jinhong Li, Langston Tillman, Chaoyu Wang, Wenyao Zhen, Ralph R. Weichselbaum, Tobias Fromme\* and Wenbin Lin\*



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### Modulating the PCET process *via* optimizing the local microenvironment of a CdS@NiV-LDH heterojunction for CO<sub>2</sub> reduction in tunable green syngas photosynthesis

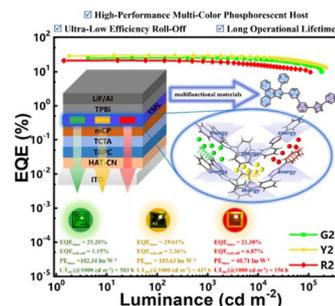
Senlin Zhang, Yuheng Ma, Changqiang Yu, Zhaohui Huang, Ruoning Zhan, Yingxinjie Wang, Xiuqiang Xie\* and Nan Zhang\*



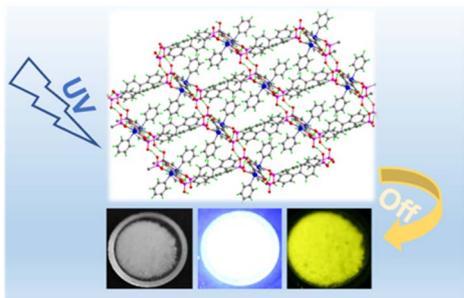
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### Multifunctional oxadiazole-based ultraviolet-emitting materials used as hosts for multicolor phosphorescence

Lizhi Chu, Chenglin Ma, Li Zhang, Yannan Zhou, Jingru Song, Qikun Sun, Shi-Tong Zhang,\* Wenjun Yang and Shanfeng Xue\*



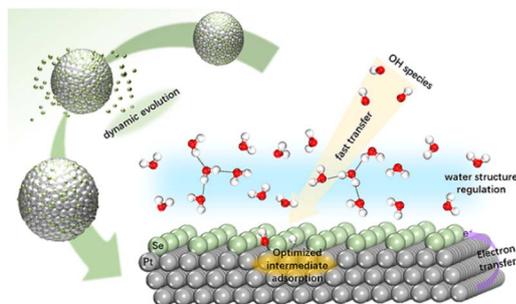
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### Preparation, single-crystal structure and room-temperature phosphorescence of a covalent organic polymer containing Te–O–P bonds

Miaomiao Xue, Guigui Ye, Lei Zhang, Qiang Dong, Chun-Sing Lee, Zhen Li\* and Qichun Zhang\*

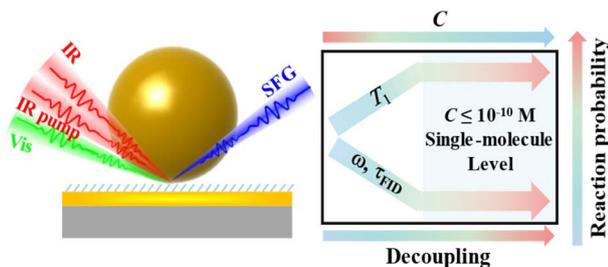
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### Dynamic surface reconstruction engineers interfacial water structure for efficient alkaline hydrogen oxidation

Chaoyi Yang, Zihao Dai, Jianchao Yue, Guangqin Wang and Wei Luo\*

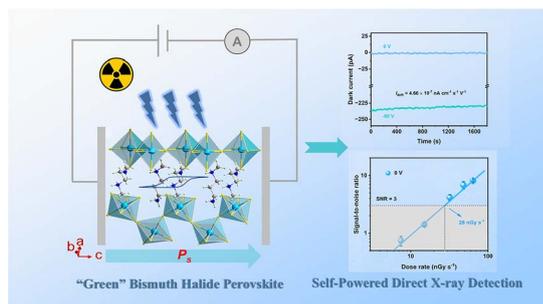
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### Single-molecule-level detection of interfacial molecular structures and ultrafast dynamics

Xiaoxuan Zheng, Junjun Tan,\* Quanbing Pei, Yi Luo\* and Shuji Ye\*

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### Stable self-powered X-ray detection with a low detection limit using a green halide hybrid perovskite ferroelectric crystal

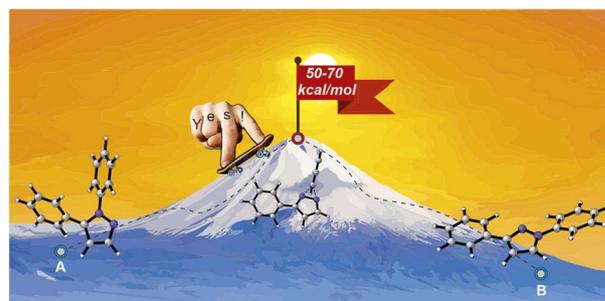
Yueying Wang, Qianwen Guan, Zeng-Kui Zhu,\* Huang Ye, Hang Li, Ying Zeng, Panpan Yu, Huawei Yang, Wenhui Wu and Junhua Luo\*



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## Are activation barriers of 50–70 kcal mol<sup>-1</sup> accessible for transformations in organic synthesis in solution?

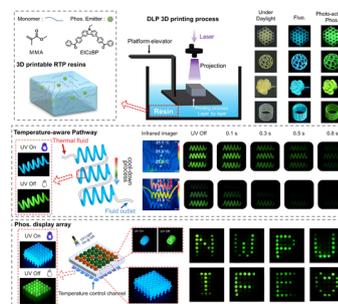
Ruslan R. Shaydullin, Alexey S. Galushko, Valentina V. Ilyushenkova, Yulia S. Vlasova and Valentine P. Ananikov\*



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## 3D printable organic room-temperature phosphorescent materials and printed real-time sensing and display devices

Haodong Sun, Yuxin Xiao, Yunfei He, Xiaoyu Wei, Jindou Zou, Yuanda Luo, Yazhang Wu, Jiaxin Zhao, Vonika Ka-Man Au and Tao Yu\*



5310

## Correction: Exploiting the inherent promiscuity of the acyl transferase of the stambomycin polyketide synthase for the mutasynthesis of analogues

Li Su, Yaouba Souaibou, Laurence Hôtel, Christophe Jacob, Peter Grün, Yan-Ni Shi, Alicia Chateau, Sophie Pinel, Helge B. Bode, Bertrand Aigle\* and Kira J. Weissman\*

