

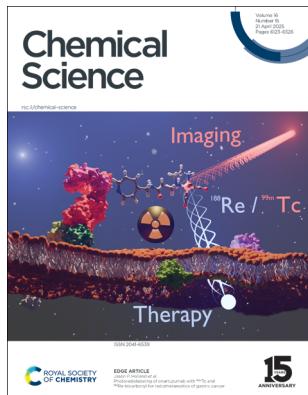
# Chemical Science

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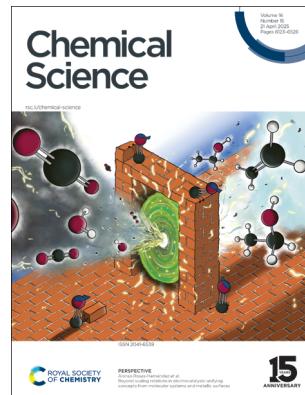
## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 16(15) 6123–6526 (2025)



### Cover

See Jason P. Holland *et al.*, pp. 6219–6230. Image reproduced by permission of Jason P. Holland and Cesare Berton from *Chem. Sci.*, 2025, 16, 6219.



### Inside cover

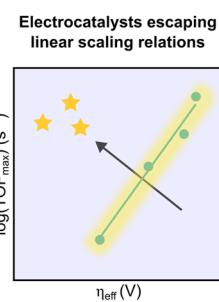
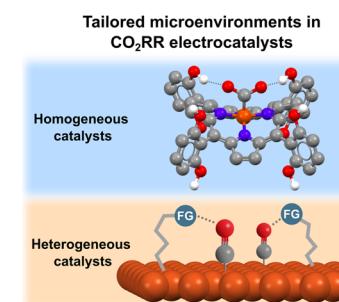
See Alonso Rosas-Hernández *et al.*, pp. 6136–6159. Image reproduced by permission of Kirstine N. Kolding, Kristian Torbensen and Alonso Rosas-Hernández from *Chem. Sci.*, 2025, 16, 6136.

## PERSPECTIVE

6136

### Beyond scaling relations in electrocatalysis: unifying concepts from molecular systems and metallic surfaces

Kirstine Nygaard Kolding, Kristian Torbensen and Alonso Rosas-Hernández\*

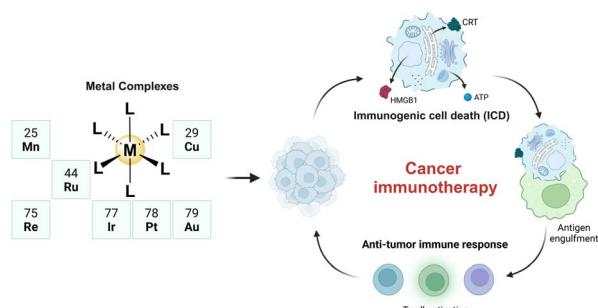


## REVIEWS

6160

### Metal-based immunogenic cell death inducers for cancer immunotherapy

Jiao Xia Zou, Meng Rui Chang, Nikita A. Kuznetsov, Jia Xuan Kee, Maria V. Babak\* and Wee Han Ang\*



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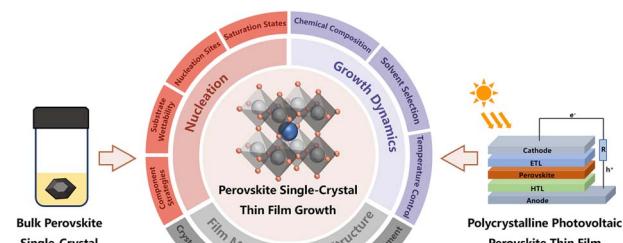


REVIEWS

6188

# Mechanistic insights and optimization strategies for perovskite single-crystal thin film growth

Jingyi Sun, Runda Li, Yang Gui, Xinyi Shao, Jingjing Xue\*  
and Rui Wang\*

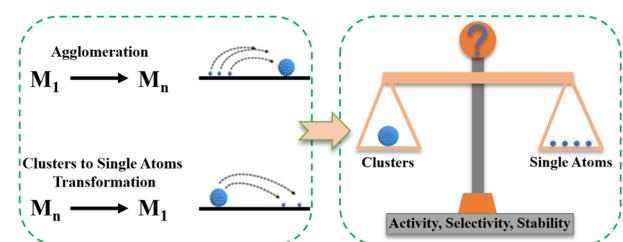


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6203

## Structural evolution of metal single-atoms and clusters in catalysis: Which are the active sites under operative conditions?

Shiyan Wang, Chaopeng Liu, Weiyao Hao, Yanling Zhuang,  
Jianmei Chen, Xianjun Zhu, Longlu Wang,\*  
Xianghong Niu, Jianjun Mao,\* Dongwei Ma\*  
and Qiang Zhao\*



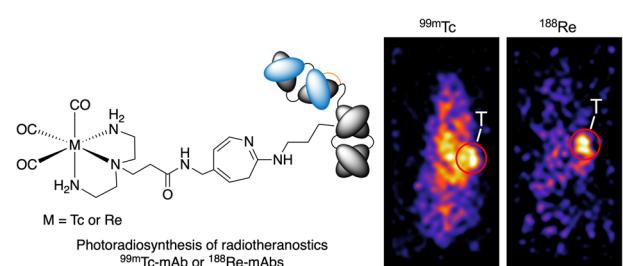
FDGE ARTICLES

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6219

# Photoradiolabeling of onartuzumab with $^{99m}\text{Tc}$ and $^{188}\text{Re}$ -tricarbonyl for radiotheranostics of gastric cancer

Jonas Genz, Cesare Berton, Samy Kichou, Simon Klingler,  
Miria C. Nolff, Henrik Braband and Jason P. Holland\*

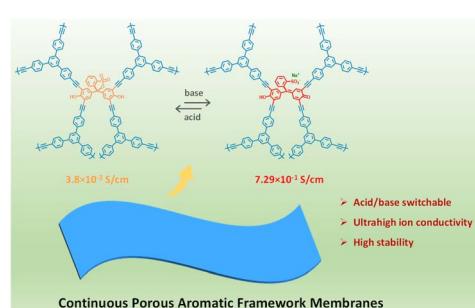


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6231

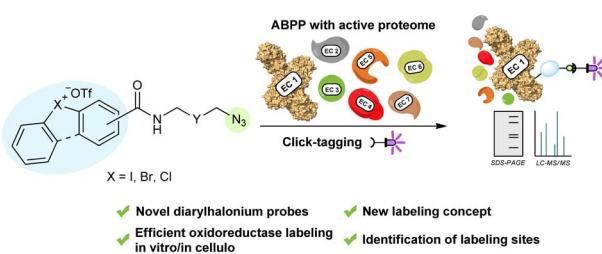
# Continuous porous aromatic framework membranes with acid-/base-induced reversible isomerization for switchable ion conductivity

Jian Song, Hengtao Lei, Lin Lin, Mengxiao Sun,  
Xueyan Han, Zilong Dou, Yuyang Tian\*  
and Guangshan Zhu\*



## EDGE ARTICLES

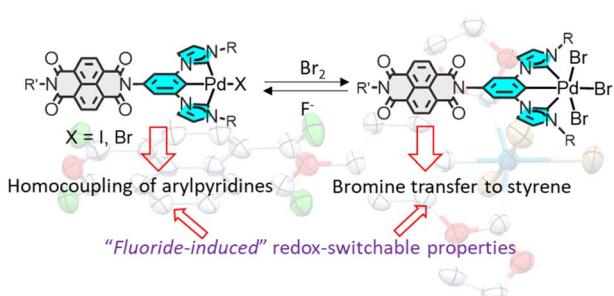
6240



### A general approach for activity-based protein profiling of oxidoreductases with redox-differentiated diarylhalonium warheads

Leo Krammer, Barbara Darnhofer, Marko Kljajic, Laura Liesinger, Matthias Schittmayer, Dmytro Neshchadin, Georg Gescheidt, Alexander Kollau, Bernd Mayer, Roland C. Fischer, Silvia Wallner, Peter Macheroux, Ruth Birner-Gruenberger\* and Rolf Breinbauer\*

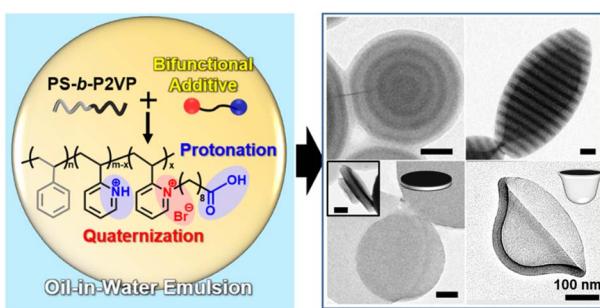
6257



### Fluoride-induced redox-switchable behaviour of a palladium(II)/(IV) couple

Sebastián Martínez-Vivas, Macarena Poyatos\* and Eduardo Peris\*

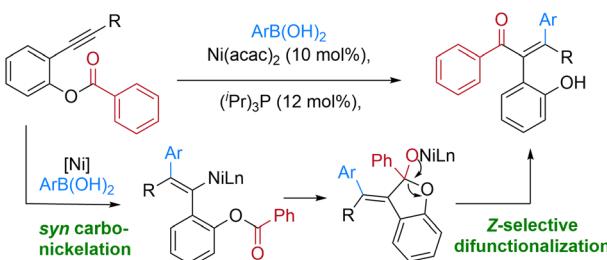
6265



### Bifunctional additive-driven shape transitions of block copolymer particles through synergistic quaternization and protonation

Zhengping Tan, Soohyun Ban, Younghyeon Ahn, Kang Hee Ku\* and Bumjoon J. Kim\*

6273



### Catalytic stereoselective synthesis of all-carbon tetra-substituted alkenes via Z-selective alkyne difunctionalization

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

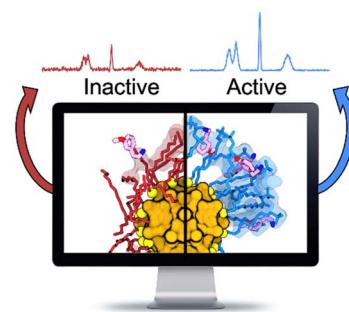


## EDGE ARTICLES

6282

**Rational design of gold nanoparticle-based chemosensors for detection of the tumor marker 3-methoxytyramine**

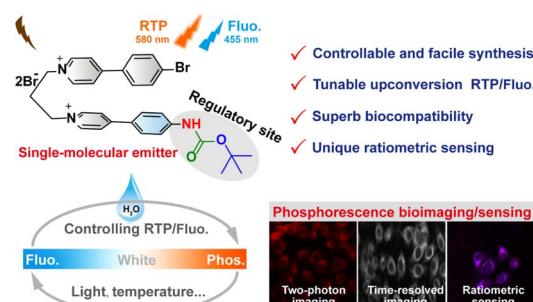
Sebastian Franco-Ulloa, Andrea Cesari, Giordano Zanoni, Laura Riccardi, Joseph Wallace, Beatrice Bernadette Mascitti, Federico Rastrelli, Fabrizio Mancin\* and Marco De Vivo\*



6290

**Aqueous up-conversion organic phosphorescence and tunable dual emission in a single-molecular emitter**

Yang Li, Zizhao Huang, Aixing Shao, Zhiqin Wu, Zhenyi He, He Tian and Xiang Ma\*



6298

**Catalytic insertion of nitrenes into B–H bonds**

Nikita M. Ankudinov,\* Nikita V. Alexeev, Evgeniya S. Podyacheva, Denis A. Chusov, Konstantin A. Lyssenko and Dmitry S. Perekalin\*

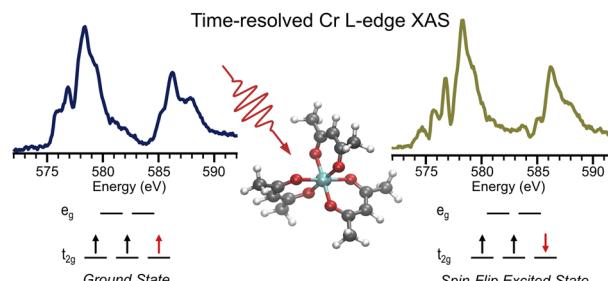


● new method for B–N bond formation      30+ examples  
● chiral-at-boron amidoboranes      up to 91:9 er

6307

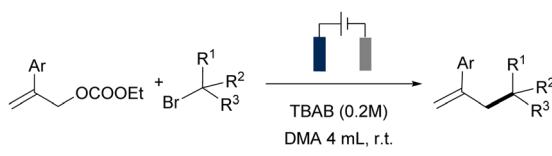
**Identification of metal-centered excited states in Cr(III) complexes with time-resolved L-edge X-ray spectroscopy**

Nahid Ghodrati, Sebastian Eckert, Mattis Fondell, Andreas Scherz, Alexander Föhlisch and Benjamin E. Van Kuiken\*



## EDGE ARTICLES

6317

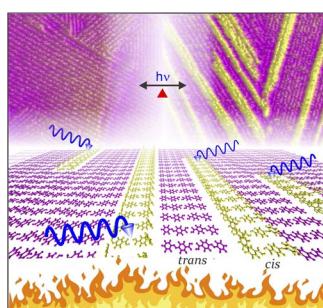
**Challenges: Potential-mismatched radical addition  
Competitive side reactions**

- Broad Scope ■ Mild conditions ■ Sterically hindered C(sp<sup>3</sup>)-C(sp<sup>3</sup>)
- Transition-metal-ligand free ■ Complex structure functionalization

**Facile, general allylation of unactivated alkyl halides via electrochemically enabled radical-polar crossover**

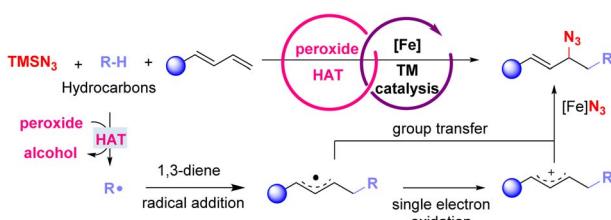
Haifeng Chen and Magnus Rueping\*

6325

**Unusual one dimensional cascade effect in the thermal and photo-induced switching of azobenzene derivatives on a graphite surface**

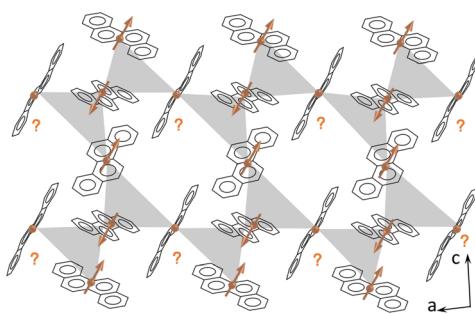
Hariom Birla, Showkat H. Mir, Khushboo Yadav, Thomas Halbritter, Alexander Heckel, Jayant K. Singh and Thiruvancheril G. Gopakumar\*

6336

**Iron-catalyzed three-component 1,2-azidoalkylation of conjugated dienes via activation of aliphatic C–H bonds**

Zhen-Yao Dai, Chenxi Lin, Derek B. Hu and Jennifer M. Schomaker\*

6345

**Signatures of the quantum spin liquid state in triangular-based zig-zag polyaromatic hydrocarbon radicals**

Yongbing Shen,\* Mengxing Cui, Haitao Zhang, Hanjie Guo, Jumpei G. Nakamura, Jan Peter Embs, Jinkui Zhao, Masahiro Yamashita\* and Zhendong Fu\*

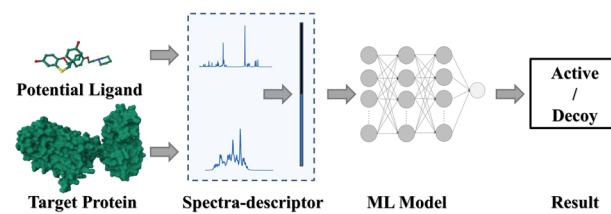


## EDGE ARTICLES

6355

**Spectra-descriptor-based machine learning for predicting protein–ligand interactions**

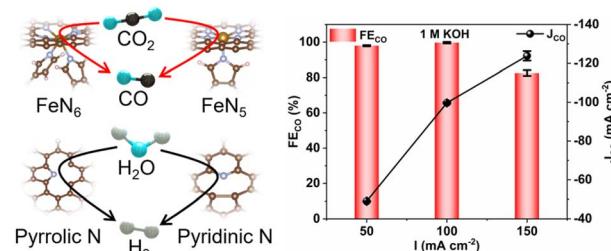
Cheng Chen, Ledu Wang, Yi Feng, Wencheng Yao, Jiahe Liu, Zifan Jiang, Luyuan Zhao, Letian Zhang, Jun Jiang and Shuo Feng\*  
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6366

**Unraveling the effect of alkali cations on Fe single atom catalysts with high coordination numbers**

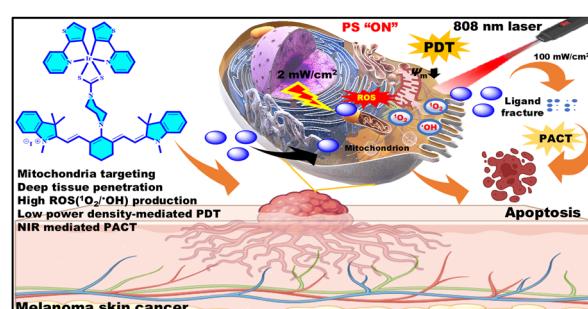
Yecheng Li, Songjie Meng, Zihong Wang, Hehe Zhang, Xin Zhao, Qingshun Nian, Digen Ruan, Lianfeng Zou,\* Zhansheng Lu\* and Xiaodi Ren\*



6376

**Near-infrared light-activatable iridium(III) complexes for synergistic photodynamic and photochemotherapy**

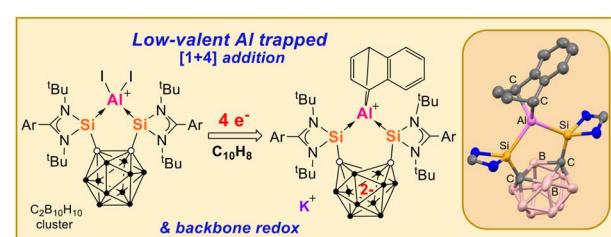
Monika Negi and V. Venkatesh\*



6383

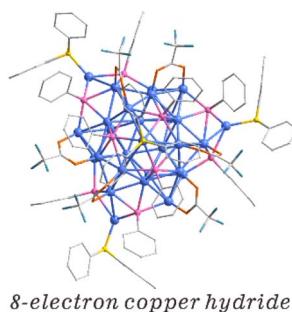
**Redox non-innocent bis-silylene aluminium complexes with a carborane backbone**

Artemis Saddington, Shenglai Yao, Christian Lorent and Matthias Driess\*



## EDGE ARTICLES

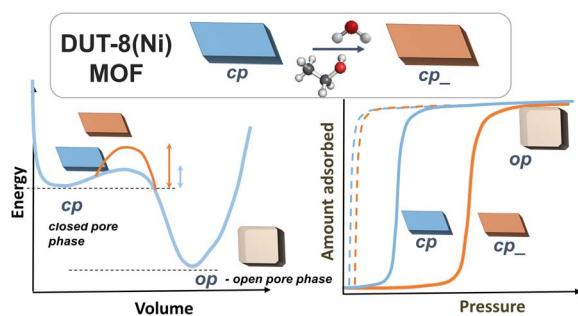
6392



### Eight-electron copper-hydride nanoclusters: synthesis, structure, alloying chemistry and photoluminescence

Jing Sun, Jiahe Liu, Hai-Feng Su, Simin Li, Xiongkai Tang, Zhenlang Xie, Zhen Xu, Wenya Jiang, Jianyu Wei, Xuekun Gong, Ayisha He, Song Wang,\* De-en Jiang, Nanfeng Zheng\* and Hui Shen\*

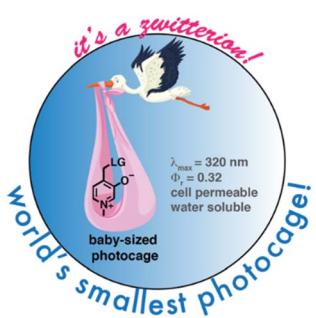
6402



### The role of surface deformation on responsivity of the pillared layer metal–organic framework DUT-8(Ni)

Leila Abylgazina, Irena Senkovska,\* Mariia Maliuta, Christopher Bachetzky, Marcus Rauche, Kathrin Pöschel, Johannes Schmidt, Mark Isaacs, David Morgan, Michal Otyepka, Eva Otyepkova, Matthias Mendt, Yogeshwar D. More, Robin Buschbeck, Andreas Schneemann, Alla Syntska, Andreas Pöpll, Lukas M. Eng, Jin-Chong Tan, Eike Brunner and Stefan Kaskel\*

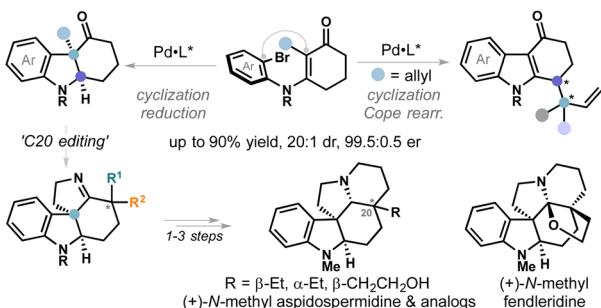
6418



### A structurally compact aqueous soluble oxypicolinium photocage with high photosensitivity

Komadbie C. Dissanayake, Mohammad K. I. Walid, Madelyn Austin, Emily A. Smith and Arthur H. Winter\*

6425



### Pd-catalyzed enantioselective access to hydrocarbazolones containing contiguous quaternary and tertiary stereocenters

Hao Sun, Cheng-Long Yu, Yu-Qing Zheng, Peng-Fei Shu, Zhan Dong, Yu-Chen Xia and Wen-Bo Liu\*

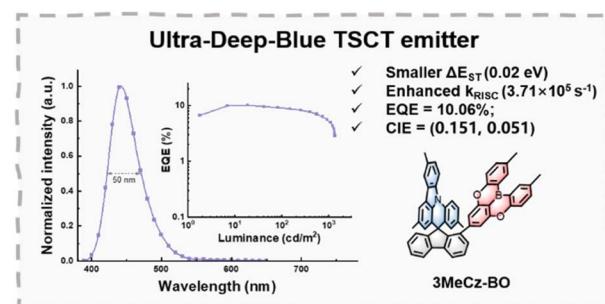


## EDGE ARTICLES

6434

**Enhancing electroluminescence performance of ultra-deep-blue through-space charge transfer emitters with  $\text{CIE}_y \approx 0.05$  via methyl-modification**

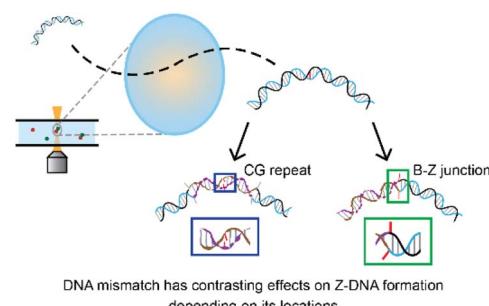
Quanwei Li, Haisong Zhao, Jinyang Zhao, Zhongxu Cao, Chao Yu, Shouke Yan\* and Zhongjie Ren\*



6443

**Contrasting effects of mismatch locations on Z-DNA formation under bending force**

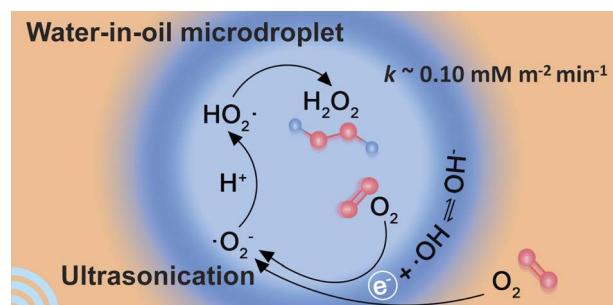
SoJung Park, Jaehun Yi and Nam Ki Lee\*



6450

**Deciphering the mechanism of hydrogen peroxide formation in ultrasound-mediated water-in-oil microdroplets**

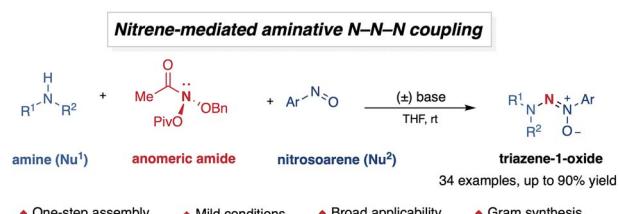
Xiaohu Zhou,\* Shutong Du, Wenjuan Zhang and Bo Zheng\*



6458

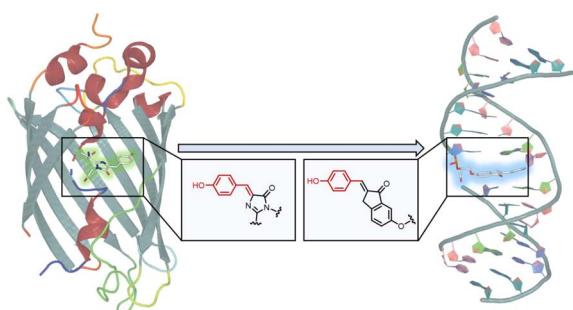
**Nitrene-mediated aminative N–N–N coupling: facile access to triazene 1-oxides**

Shiyang Zhu, Hairuo Zhang, Boyang Sun, Ziqian Bai, Gang He, Gong Chen and Hao Wang\*



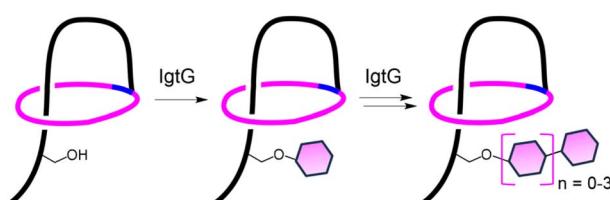
## EDGE ARTICLES

6468

**Modular access to nucleobase GFP-surrogates: pH-responsive smart probes for ratiometric nucleic acid diagnostics**

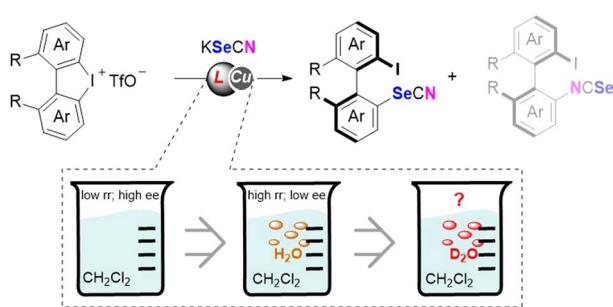
Keenan T. Regan, Austin Pounder, Ryan E. Johnson, Makay T. Murray, Hannah X. Glowacki, Stacey D. Wetmore\* and Richard A. Manderville\*

6480

**Iterative glycosylation on a single residue of a mature lasso peptide**

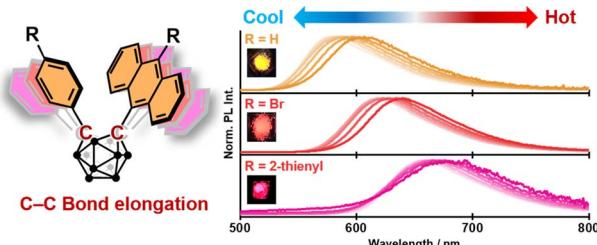
Ke Sun, Jiao-Jiao Cui, WeiKang Zhai, Xuan Su, Yi-Cheng Liu, Lu Ning, Jiang Xiong, Kun Gao, Shangwen Luo, Xinxiang Lei and Shi-Hui Dong\*

6488

**Observation of the solvent enantio-isotope effect in asymmetric ring-opening of cyclic diaryliodoniums with selenocyanate**

Yuanyuan Li, Chenyu Tao, Longhui Duan\* and Zhenhua Gu\*

6495

**Partial Restriction of Geometry Relaxation****Solid-state temperature-dependent luminescence of C,C'-diaryl-o-carboranes based on restriction of excited-state structural relaxation**

Kazuhiro Yuhara and Kazuo Tanaka\*

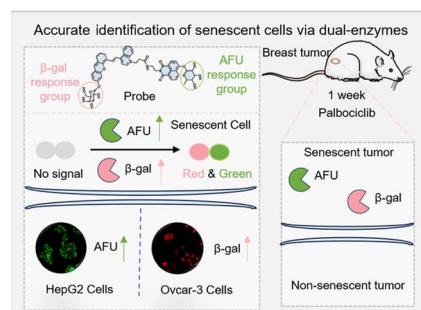


## EDGE ARTICLES

6507

**A dual-enzyme activated fluorescent probe for precise identification of tumor senescence**

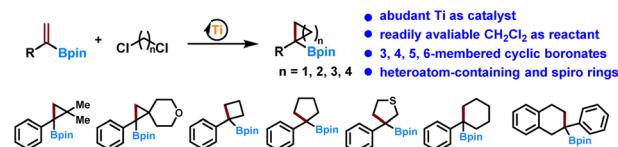
Xianzhu Luo, Erzhuo Hu, Fei Deng, Cuiling Zhang\* and Yuezhong Xian\*



6515

**Synthesis of  $\alpha$ -substituted cyclic boronates via titanium-catalyzed cyclization of vinyl boronates with dihaloalkanes**

Ximei Tian and Lipeng Wu\*



## CORRECTIONS

6522

**Correction: Low-energy electron distributions from the photoionization of liquid water: a sensitive test of electron mean free paths**

Titouan Gadeyne, Pengju Zhang,\* Axel Schild and Hans Jakob Wörner\*

6523

**Correction: DiffBP: generative diffusion of 3D molecules for target protein binding**

Haitao Lin, Yufei Huang, Odin Zhang, Siqi Ma, Meng Liu, Xuanjing Li, Lirong Wu, Shuiwang Ji, Tingjun Hou\* and Stan Z. Li\*

