

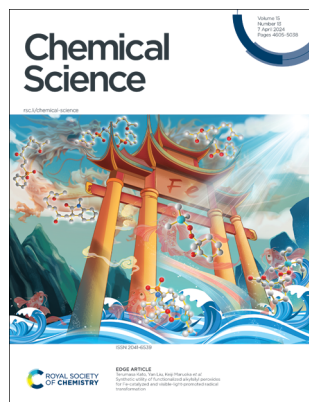
# Chemical Science

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## IN THIS ISSUE

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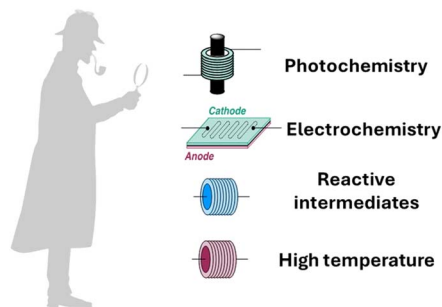
**Inside cover**  
See Monika Raj *et al.*, pp. 4763–4769. Image reproduced by permission of Monika Raj from *Chem. Sci.*, 2024, **15**, 4763.

## PERSPECTIVE

4618

### Continuous flow synthesis enabling reaction discovery

Antonella Ilenia Alfano, Jorge García-Lacuna, Oliver M. Griffiths, Steven V. Ley\* and Marcus Baumann\*

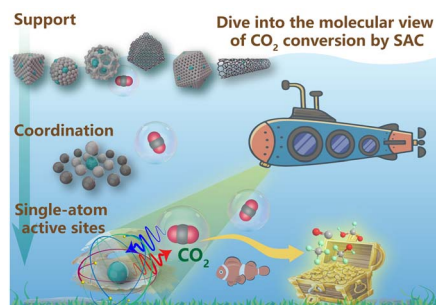


## REVIEWS

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### A molecular view of single-atom catalysis toward carbon dioxide conversion

Xin Shang, Xiaofeng Yang, Guodong Liu, Tianyu Zhang\* and Xiong Su\*



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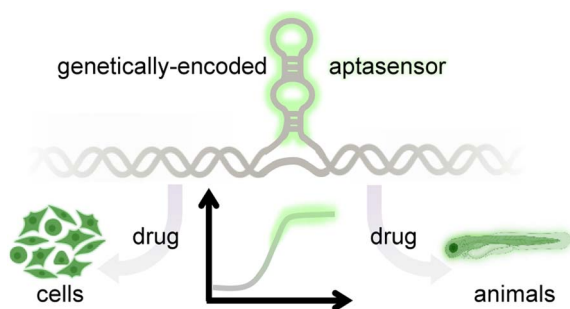
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Fundamental questions  
Elemental answers





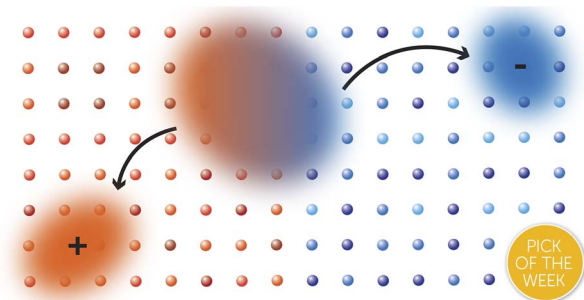
4770



### Non-invasive single cell aptasensing in live cells and animals

Eiman A. Osman, Thomas P. Rynes, Y. Lucia Wang, Karen Mruk and Maureen McKeague\*

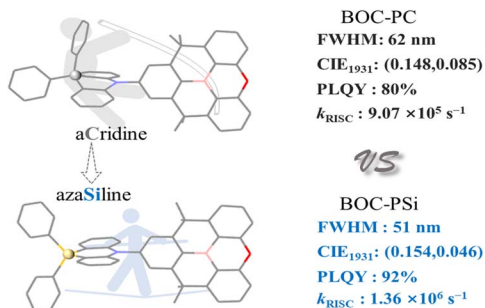
4779



### Delocalisation enables efficient charge generation in organic photovoltaics, even with little to no energetic offset

Daniel Balzer and Ivan Kassar\*

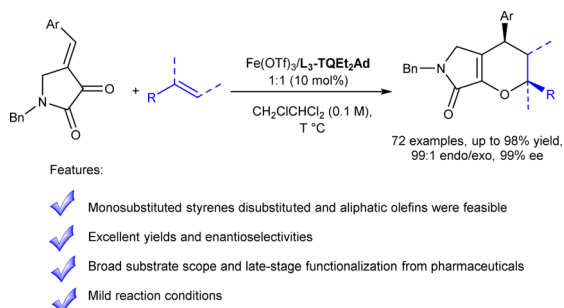
4790



### Realizing highly efficient deep-blue organic light-emitting diodes towards Rec.2020 chromaticity by restricting the vibration of the molecular framework

Chuan Li, Kai Zhang, Yanju Luo, Yang Yang, Yong Huang, Mengjiao Jia, Yuling He, Yue Lei, Jian-Xin Tang,\* Yan Huang and Zhiyun Lu\*

4797



### Iron<sup>III</sup>-catalyzed asymmetric inverse-electron-demand hetero-Diels-Alder reaction of dioxypyrrolidines with simple olefins

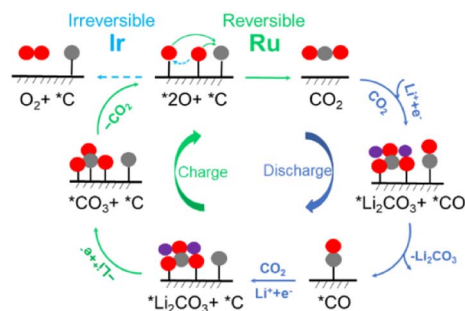
Tangyu Zhan, Liang Zhou, Yuqiao Zhou, Bingqian Yang, Xiaoming Feng\* and Xiaohua Liu\*



4804

## Reversible and irreversible reaction mechanisms of Li-CO<sub>2</sub> batteries

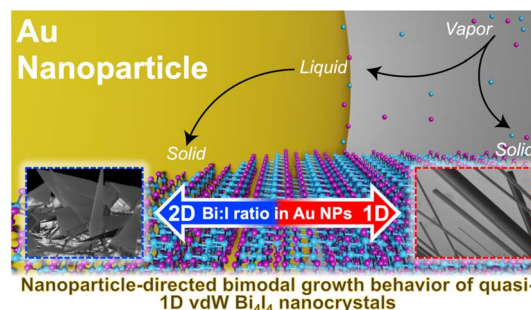
Xinxin Zhang, Yu Wang\* and Yafei Li\*



4811

## Nanoparticle-directed bimodal crystallization of the quasi-1D van der Waals phase, Bi<sub>4</sub>I<sub>4</sub>

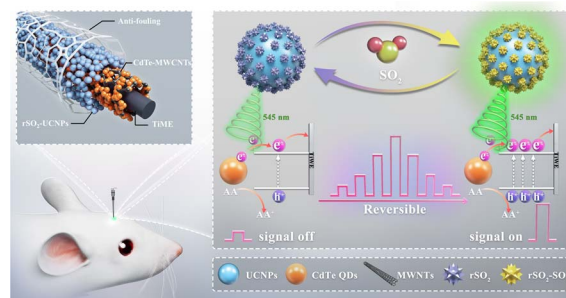
Steven Jay Allison, Dmitri Leo Mesoza Cordova, Maham Hasib, Toshihiro Aoki and Maxx Q. Arguilla\*



4824

## A reversible photoelectrochemical microsensor for dynamically monitoring sulfur dioxide in the epileptic brain

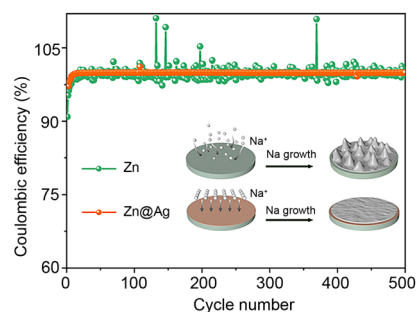
Danying Lin, Tao Lu, Xiao Wang, Xiaoxue Ye\* and Zhihong Liu\*



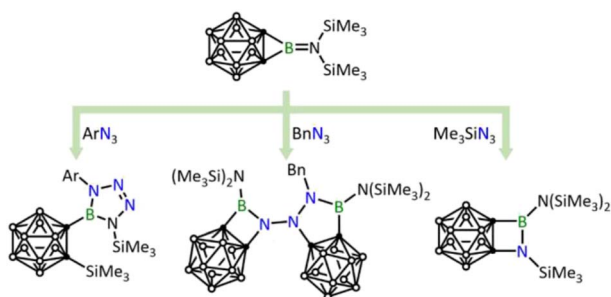
4833

## A conductive and sodiophilic Ag coating layer regulating Na deposition behaviors for highly reversible sodium metal batteries

Xiaomin Chen, Xunzhu Zhou, Zhuo Yang, Zhiqiang Hao, Jian Chen, Wenxi Kuang, Xiaoyan Shi, Xingqiao Wu, Lin Li\* and Shu-Lei Chou\*



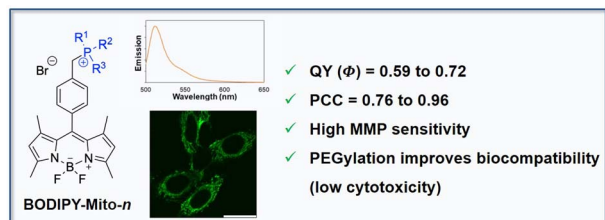
4839



### Avenue to novel *o*-carboranyl boron compounds – reactivity study of *o*-carborane-fused aminoborirane towards organic azides

Junyi Wang, Libo Xiang, Xiaocui Liu, Alexander Matler, Zhenyang Lin\* and Qing Ye\*

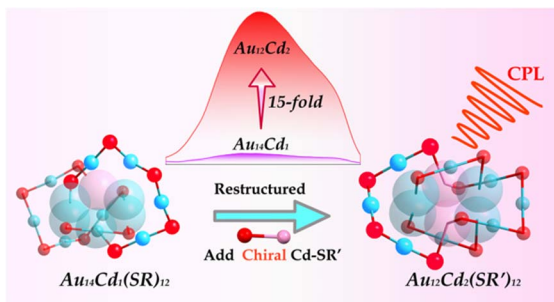
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### Mitochondria-targeting biocompatible fluorescent BODIPY probes

Edward R. H. Walter, Lawrence Cho-Cheung Lee, Peter Kam-Keung Leung, Kenneth Kam-Wing Lo\* and Nicholas J. Long\*

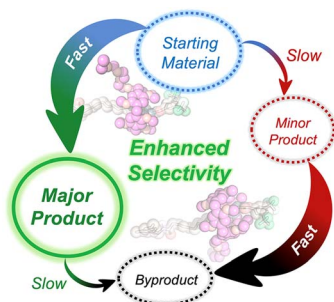
4853



### Construction of an Au<sub>12</sub>Cd<sub>2</sub> nanocluster with circularly polarized luminescence by a metal- and ligand-exchange strategy

Jun Zhou, Xiaofei Yang, Peisen Zheng, Qinzhen Li, Xiaowu Li, Jinsong Chai, Baoyu Huang,\* Sha Yang\* and Manzhou Zhu\*

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### Kinetically controlled synthesis of rotaxane geometric isomers

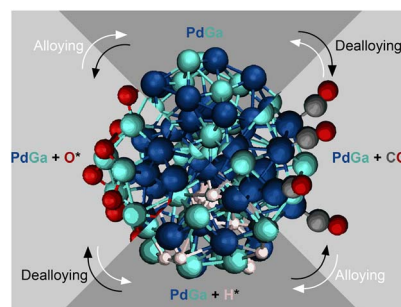
Dillon R. McCarthy, Ke Xu, Mica E. Schenkelberg, Nils A. N. Balemire, Huiming Liang, Shea A. Bellino, Jianing Li and Severin T. Schneebeli\*



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## Metadynamics simulations reveal alloying-dealloying processes for bimetallic PdGa nanoparticles under CO<sub>2</sub> hydrogenation

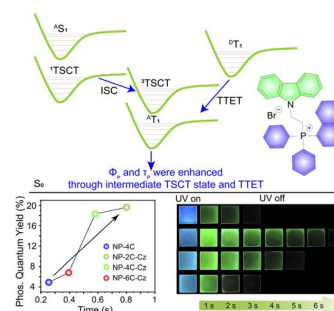
Julian F. Baumgärtner, Andreas Müller, Scott R. Docherty, Aleix Comas-Vives, Pierre-Adrien Payard\* and Christophe Copéret\*



4881

## Simultaneously enhancing organic phosphorescence quantum yields and lifetimes for triphenylphosphine salt doped polymer films

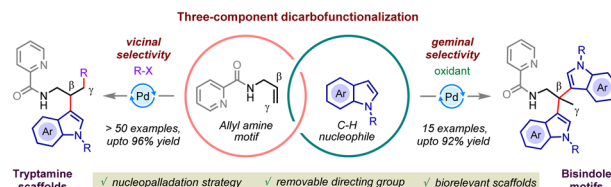
Jiangang Li, Kuanjian Wei, Jilong Wu, Yuchang Wang, Shujuan Liu, Yun Ma\* and Qiang Zhao\*



4890

## Three-component dicarbofunctionalization of allylamines via nucleopalladation pathway: unlocking vicinal and geminal selectivity

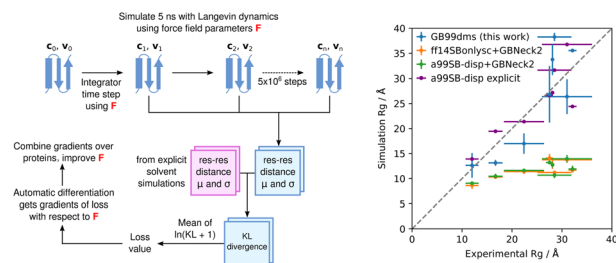
Nityananda Ballav, Shib Nath Saha, Shailesh Yadav and Mahiuddin Baidya\*



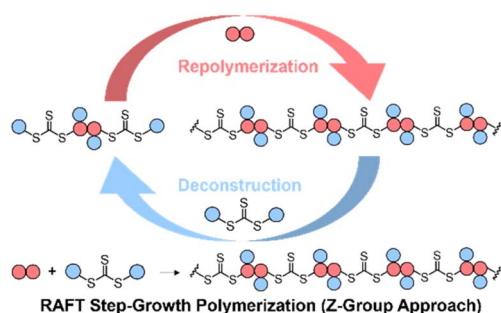
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## Differentiable simulation to develop molecular dynamics force fields for disordered proteins

Joe G. Greener



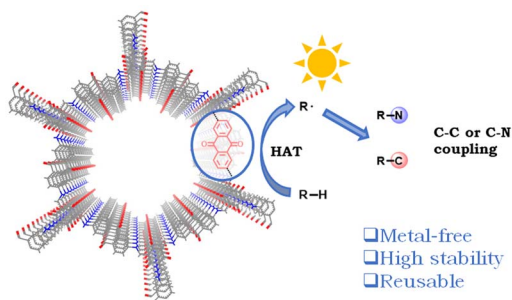
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### RAFT step-growth polymerization via the Z-group approach and deconstruction by RAFT interchange

Jiajia Li, Joji Tanaka,\* Qing Li, Claire Jing Jing Wang, Sergei Sheiko, Samantha Marie Clouthier, Jian Zhu and Wei You\*

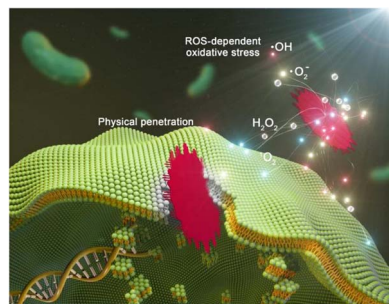
4920



### Anthraquinone-based covalent organic framework as a recyclable direct hydrogen atom transfer photocatalyst for C-H functionalization

Zitong Wang, Pierce Yeary, Yingjie Fan and Wenbin Lin\*

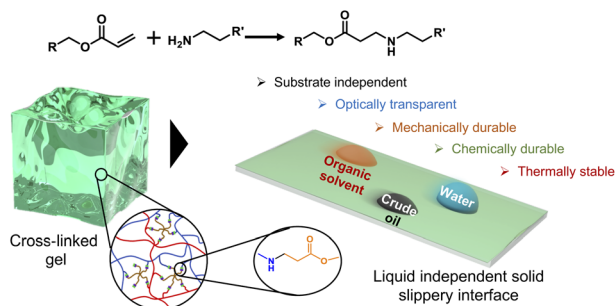
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### Bacterial elimination via cell membrane penetration by violet phosphorene peripheral sub-nanoneedles combined with oxidative stress

Qiudi Shen, Jing Kang,\* Xuwen Zhao, Wanqing Lou, Zhihao Li, Lihui Zhang, Bo Zhang, Jinying Zhang,\* Bailiang Wang\* and Alideertu Dong\*

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### Covalent crosslinking chemistry for controlled modulation of nanometric roughness and surface free energy

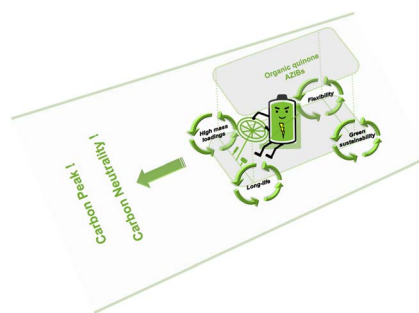
Debasmita Sarkar, Manideepa Dhar, Avijit Das, Sohini Mandal, Anirban Phukan and Uttam Manna\*



4952

### Constructing ultra-stable, high-energy, and flexible aqueous zinc-ion batteries using environment-friendly organic cathodes

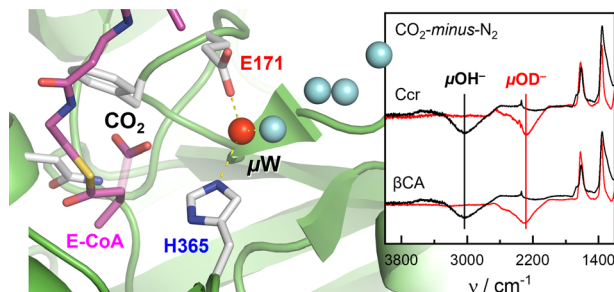
Chaojian Ding, Yonghui Wang, Chaobo Li, Jiawen Wang, Qichun Zhang\* and Weiwei Huang\*



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### Infrared spectroscopy reveals metal-independent carbonic anhydrase activity in crotonyl-CoA carboxylase/reductase

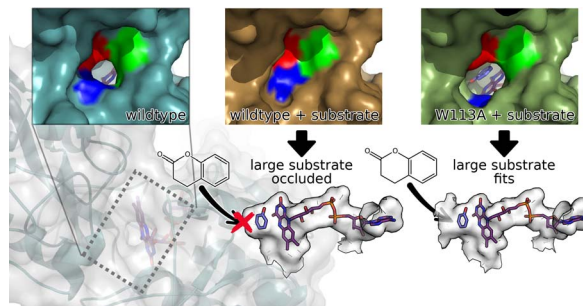
Aharon Gomez, Matthias Tinzl, Gabriele Stoffel, Hendrik Westedt, Helmut Grubmüller, Tobias J. Erb, Esteban Vöhlinger-Martinez\* and Sven T. Stripp\*



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### Rational design of a cyclohexanone dehydrogenase for enhanced $\alpha,\beta$ -desaturation and substrate specificity

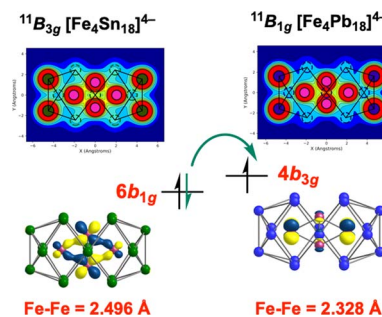
Warispreet Singh, Nicola L. Brown, Hannah V. McCue, Sophie R. Marriott, Richard C. Wilson, Justin Perry, Johan P. Turkenburg, Kshatresh D. Dubey, Stephen H. Prior, Andrew J. Carnell, Edward J. Taylor\* and Gary W. Black\*



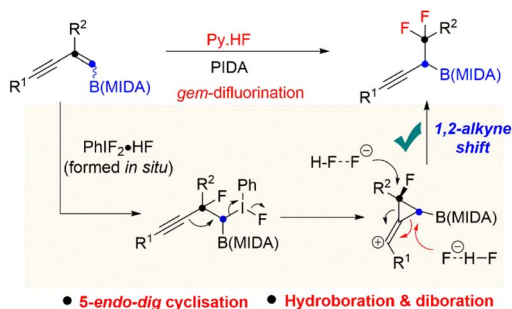
4981

### Fe-Fe bonding in the rhombic Fe<sub>4</sub> cores of the Zintl clusters [Fe<sub>4</sub>E<sub>18</sub>]<sup>4-</sup> (E = Sn and Pb)

Wei-Xing Chen, Zi-Sheng Li, Harry W. T. Morgan, Cong-Cong Shu, Zhong-Ming Sun\* and John E. McGrady\*



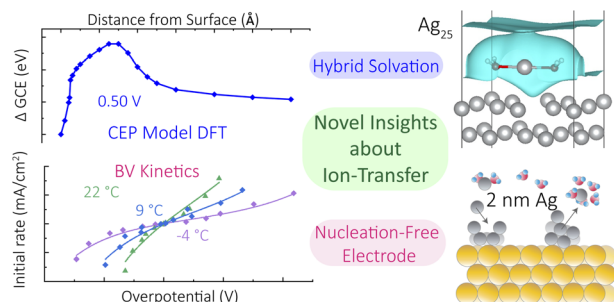
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### Reactivity of 1,3-enyne MIDA boronates: exploration of novel 1,2-alkyne shift via *gem*-difluorination

Samir Manna, Debasis Aich, Subrata Hazra, Shivam Khandelwal and Santanu Panda\*

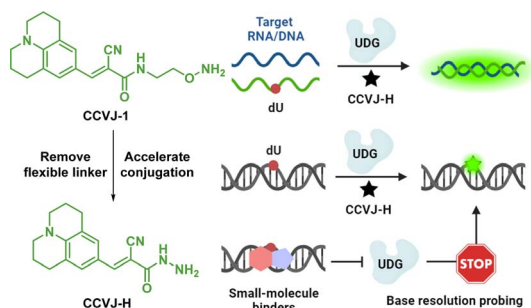
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### Understanding ion-transfer reactions in silver electrodisolution and electrodeposition from first-principles calculations and experiments

Richard Kang,\* Yang Zhao, Diptarka Hait, Joseph A. Gauthier, Paul A. Kempler, Kira A. Thurman, Shannon W. Boettcher\* and Martin Head-Gordon\*

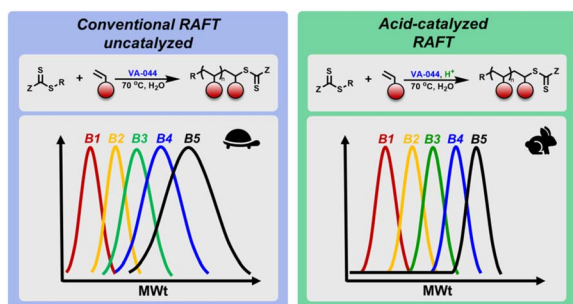
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### Multifaceted nucleic acid probing with a rationally upgraded molecular rotor

Tuan-Khoa Kha, Qi Shi, Nirali Pandya and Ru-Yi Zhu\*

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### Enhanced synthesis of multiblock copolymers via acid-triggered RAFT polymerization

Maria-Nefeli Antonopoulou, Nghia P. Truong and Athina Anastasaki\*



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## Discovery of potent PROTAC degraders of Pin1 for the treatment of acute myeloid leukemia

Yunkai Shi, Minmin Liu, Mengna Li, Yiwen Mao, Jingkun Ma, Ruikai Long, Miaomiao Xu, Yaxi Yang, Wenlong Wang,\* Yubo Zhou,\* Jia Li\* and Bing Zhou\*

