

## IN THIS ISSUE

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### Cover

See Olexandr Isayev *et al.*, pp. 10228–10244. Image reproduced by permission of Olexandr Isayev and Tetiana Zubatyuk from *Chem. Sci.*, 2025, 16, 10228.



### Inside cover

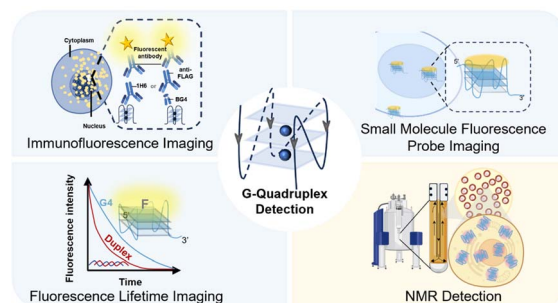
See Shi-Hua Chen, Meng Yang, Zong-Yin Song, Pei-Hua Li, Xing-Jiu Huang *et al.*, pp. 10245–10254. Image reproduced by permission of Rui-Ze Xia from *Chem. Sci.*, 2025, 16, 10245.

## PERSPECTIVES

10083

### Precise detection of G-quadruplex in living systems: principles, applications, and perspectives

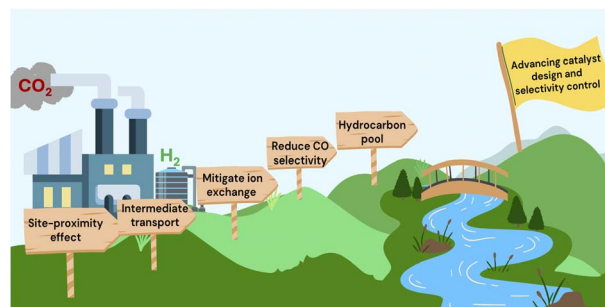
Huanhuan Li, Zelong Jin, Shuxin Gao, Shi Kuang,\*  
Chunyang Lei and Zhou Nie\*



10106

### Interrogating the missing links in tandem CO<sub>2</sub> hydrogenation: role of intermediate transport, active site proximity, and ion exchange in zeolites

Fatima Mahnaz, Andrew Iovine and Manish Shetty\*



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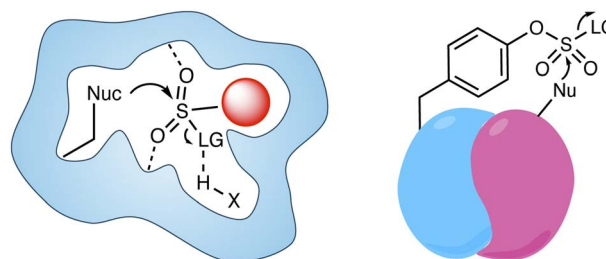
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## PERSPECTIVES

10119

**Advances in sulfonyl exchange chemical biology: expanding druggable target space**

Lyn H. Jones\*

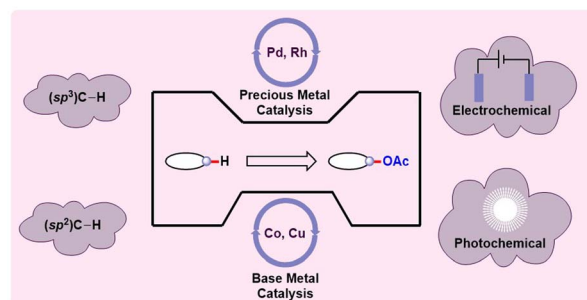


## REVIEWS

10141

**Harnessing C–H acetoxylation: a gateway to oxygen-enriched organic frameworks**

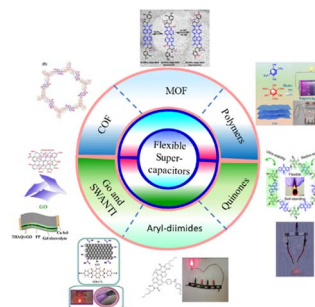
Jagrit Grover, Bishal Dutta, Devika Ghosh, Prakash K. Shee, Siddhartha Maiti, Daniel B. Werz\* and Debabrata Maiti\*



10159

**Advancements in supercapacitors: breaking barriers and enabling amazing applications**

Sidhanath V. Bhosale\* and Sheshanath V. Bhosale\*

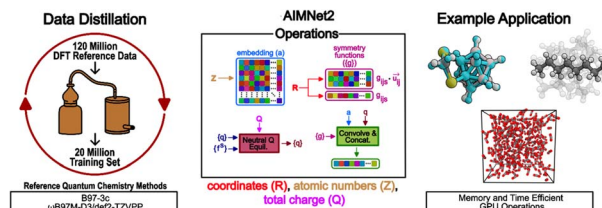


## EDGE ARTICLES

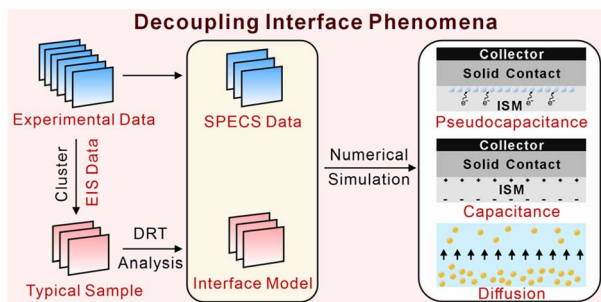
10228

**AIMNet2: a neural network potential to meet your neutral, charged, organic, and elemental-organic needs**

Dylan M. Anstine, Roman Zubatyuk and Olexandr Isayev\*



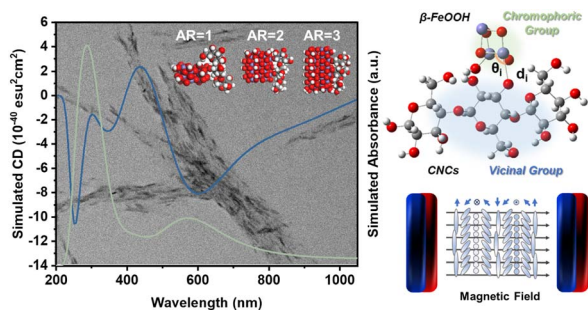
10245



### Inhibitions imposed by kinetic constraints of membranes in all-solid-state ion-selective electrodes: characteristics of interfacial capacitance in solid contacts

Rui-Ze Xia, Xin Cai, Jing-Yi Lin, Yong-Huan Zhao, Zi-Hao Liu, Chen-Lu Wang, Shi-Hua Chen,\* Meng Yang,\* Zong-Yin Song,\* Pei-Hua Li\* and Xing-Jiu Huang\*

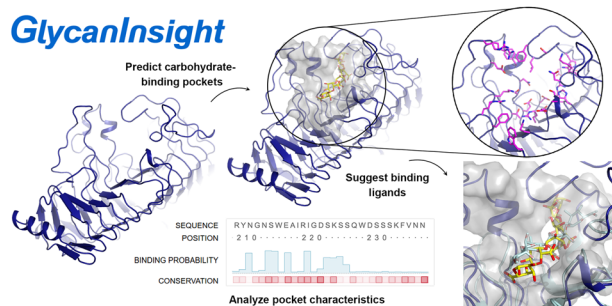
10255



### Anisotropy-dependent chirality transfer from cellulose nanocrystals to $\beta$ -FeOOH nanowhiskers

Jinyu Tang, Shouhua Feng and Ming Yang\*

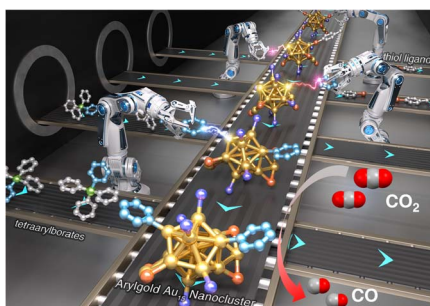
10264



### GlycanInsight: an open platform for carbohydrate-binding pocket prediction and characterization

Qinyu Chu, Xinheng He, Xinyi Tan, Zhiyong Gu, Yin Luo, Zifu Huang, Mingyue Zheng\* and Xi Cheng\*

10273



### Arylation of gold nanoclusters and insights into structure-related CO<sub>2</sub> reduction reaction performances

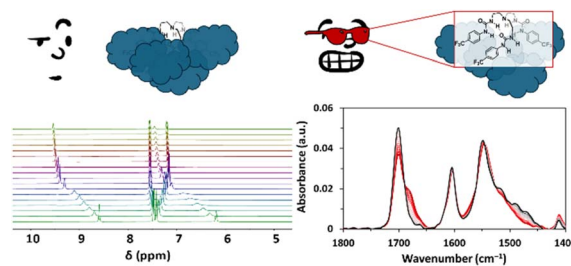
Chen Zhu, Bo Li, Chen Li, Luyao Lu, Hao Li, Xinhua Yuan, Xi Kang,\* De-en Jiang\* and Manzhou Zhu\*



10282

### Expanding the toolbox for supramolecular chemistry: probing host–guest interactions and binding with *in situ* FTIR spectroscopy

Shiva Moaven, Douglas A. Vander Griend, Darren W. Johnson\* and Michael D. Pluth\*

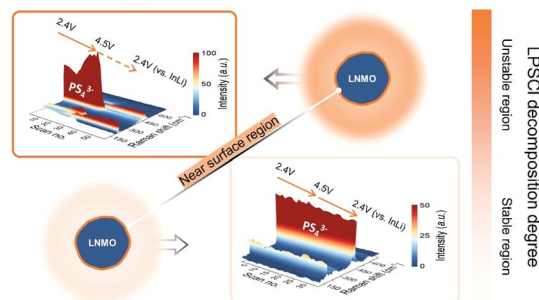


*in-situ* FTIR spectroscopy is a powerful technique to investigate host-guest interactions

10289

### Combined effect of high voltage and large Li-ion flux on decomposition of $\text{Li}_6\text{PS}_5\text{Cl}$

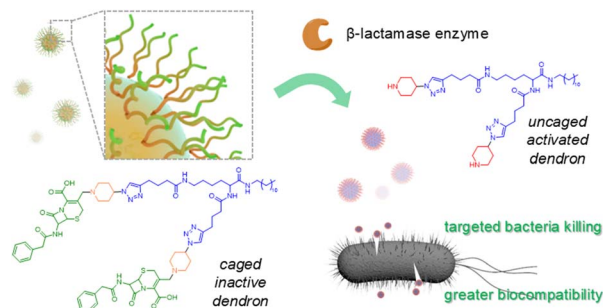
Deye Sun, Wenru Li, Yantao Wang, Jiangwei Ju, Pengxian Han, Shanmu Dong,\* Jun Ma\* and Guanglei Cui\*



10296

### $\beta$ -Lactamase-activated antimicrobial dendron via the amine uncaging strategy

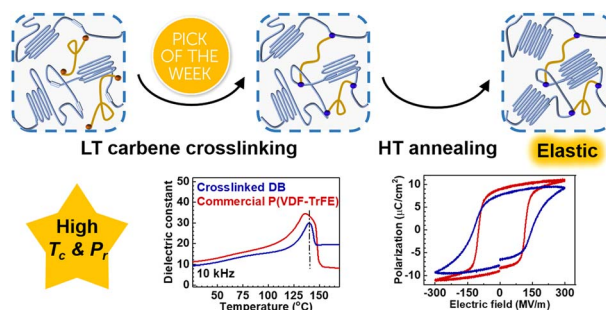
Hao Luo, Zeyu Shao, Karen Hakobyan, Jiangtao Xu, Rhiannon P. Kuchel, Shyam Kumar Mishra, Mark Willcox and Edgar H. H. Wong\*



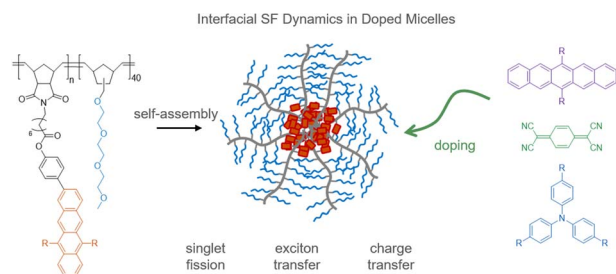
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### High-performance elastic ferroelectrics via low-temperature carbene crosslinking and high-temperature annealing

Liping Wang, Liang Gao, Xiaocui Rao, Fangzhou Li, Da Zu, Yunya Liu and Ben-Lin Hu\*



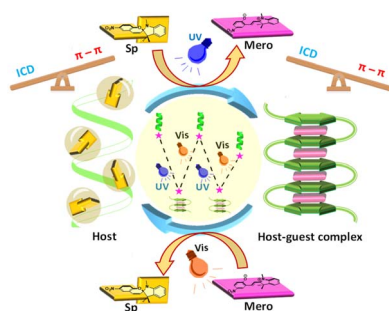
10315



### Exciton and charge transfer processes within singlet fission micelles

Daniel Malinowski, Guiying He, Bernardo Salcido-Santacruz, Kanad Majumder, Junho Kwon, Matthew Y. Sfeir\* and Luis M. Campos\*

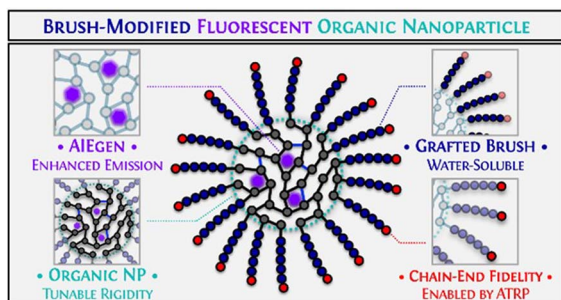
10325



### Light-induced twisting, untwisting, and retwisting of aromatic polyamides: an interplay between the induced chirality and the co-facial $\pi$ -stacking interactions

Subhendu Samanta and Raj Kumar Roy\*

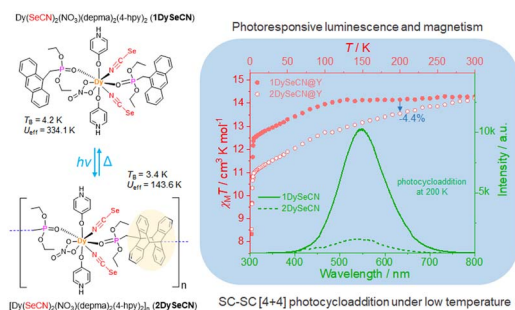
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### Brush-modified fluorescent organic nanoparticles by ATRP with rigidity-regulated emission

Rongguan Yin, Lianshun Luo, Xiaolei Hu, Hironobu Murata, Jaepil Jeong, Feng Gao, Zijie Qiu,\* Ben Zhong Tang, Michael R. Bockstaller\* and Krzysztof Matyjaszewski\*

10340



### A thermally and photoresponsive luminescent single-molecule magnet based on dysprosium-anthracene: effect of temperature on anthracene photocycloaddition

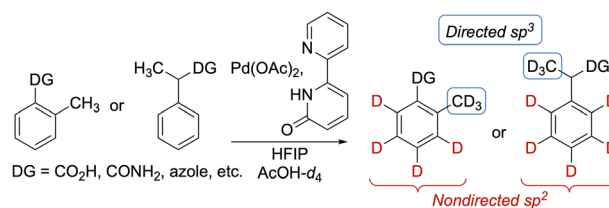
Xiu-Fang Ma, Xin-Lan Hou, Ye-Hui Qin, Qian Teng, Song-Song Bao, Yu-Xi Tian\* and Li-Min Zheng\*



10349

### Merging directed $sp^3$ and nondirected $sp^2$ C–H functionalization for Pd-catalyzed polydeuteration of (hetero)arenes

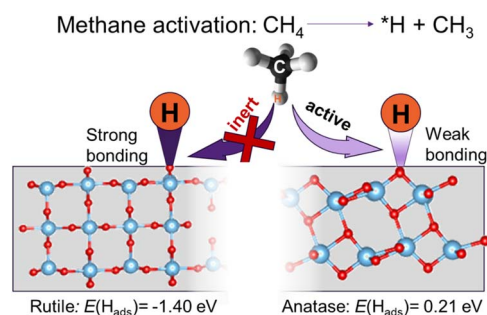
Soo Eun Park, Sungjun Choi, Chaewon Lim, Sang Hak Lee, Siyeon Jeong\* and Jung Min Joo\*



10357

### Phase effect of $TiO_2$ on surface hydrogen adsorption/desorption in controlling photocatalytic methane conversion

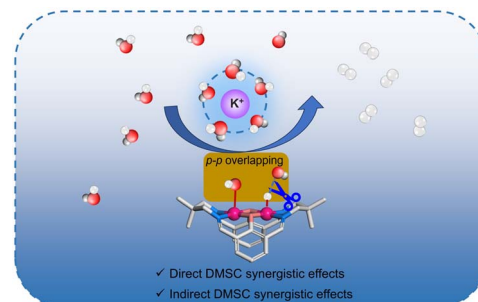
Jiakang You, Ardeshir Baktash, Dazhi Yao, Yanzhao Zhang, Shanshan Ding, Jingwei Hou, Guangyu Zhao, Yonggang Jin, Zhiliang Wang\* and Lianzhou Wang\*



10364

### A salen-based dinuclear cobalt(II) polymer with direct and indirect synergy for electrocatalytic hydrogen evolution

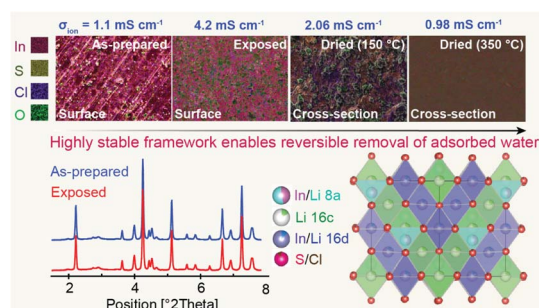
Xiao-Mei Hu, Wen-Jie Shi,\* Jian-Hua Mei, Yu-Chen Wang, Wei-Xue Tao, Di-Chang Zhong\* and Tong-Bu Lu\*



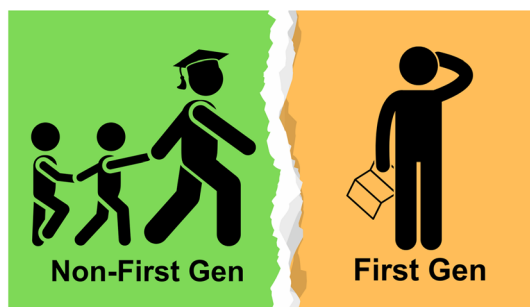
10372

### $Li_{3.6}In_7S_{11.8}Cl$ : an air- and moisture-stable superionic conductor

Ifeoluwa P. Oyekunle, Erica Truong, Tej P. Poudel, Yudan Chen, Yongkang Jin, Islamiyat A. Ojelade, Michael J. Deck, Bright Ogbolu, Md. Mahinur Islam, Pawan K. Ojha, J. S. Raaj Vellore Winfred, Dewen Hou, Hui Xiong, Chen Huang and Yan-Yan Hu\*



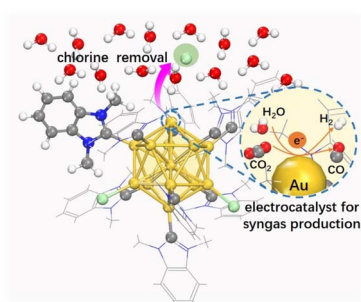
10386



### Being a first generation university graduate, the impact on a career in science

Mariam Yacoub, Sarah Koops, Panagiota Axelithioti, Claudia Caltagirone, Emily R. Draper, Cally J. E. Haynes, Charlotte K. Hind, Marion Kieffer, Larissa K. S. von Krbeke, Anna J. McConnell, Sarah J. Pike, Anna G. Slater, Jennifer R. Hiscock\* and Jennifer S. Leigh\*

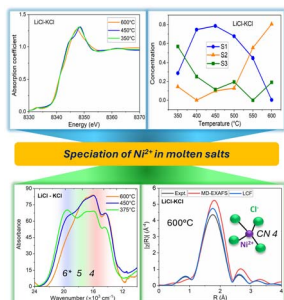
10397



### Electrochemical dechlorination promotes syngas production in N-heterocyclic carbene protected Au<sub>13</sub> nanoclusters

Zhimin Chen, Dongjie Zuo, Lancheng Zhao, Yuping Chen, Fang Sun, Likai Wang,\* Hui Shen\* and Qing Tang\*

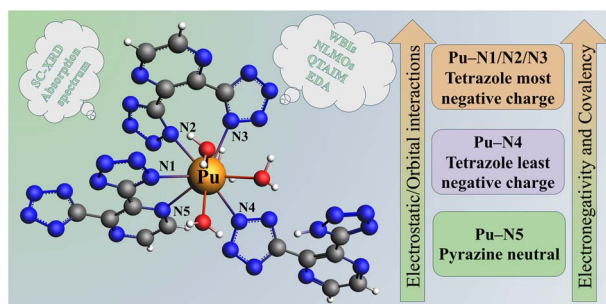
10414



### Correlative analysis of Ni(II) coordination states in molten salts using a combination of X-ray and optical spectroscopies and simulations

Yang Liu, Mehmet Topsakal, Kaifeng Zheng, Luis E. Betancourt, Michael Woods, Santanu Roy, Nirmalendu Patra, Denis Leshchev, Phillip Halstenberg, Dmitry S. Maltsev, Sheng Dai, Alexander S. Ivanov, Vyacheslav S. Bryantsev, James F. Wishart,\* Ruchi Gakhar,\* Anatoly I. Frenkel\* and Simerjeet K. Gill\*

10424



### Unveiling the covalency of versatile Pu(III)-N bonds in a unique plutonium(III) complex

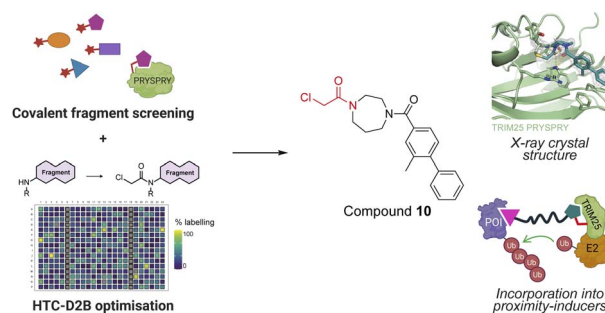
Zhuanling Bai, Madeline C. Martelles, Joseph M. Sperling\* and Thomas E. Albrecht\*



10432

### Discovery and optimisation of a covalent ligand for TRIM25 and its application to targeted protein ubiquitination

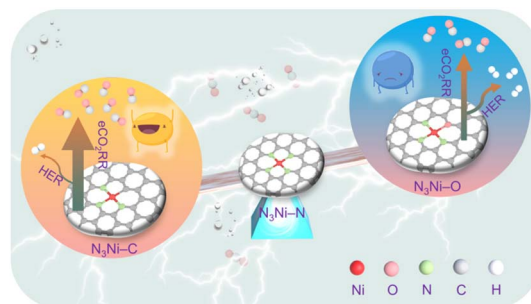
Katherine A. McPhee, Diego Esposito, Jonathan Pettinger, Daniel Norman, Thilo Werner, Toby Mathieson, Jacob T. Bush and Katrin Rittinger\*



10444

### Continuous coordination modulation with different heteroatoms unveils favorable single-atom Ni sites for near-unity CO selectivity in CO<sub>2</sub> electroreduction

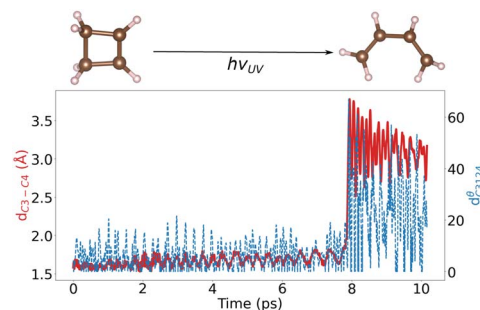
Shuangqun Chen, Tong Cao, Wen Yan, Ke Zhao, Yalin Guo,\* Tiantian Wu,\* Daliang Zhang, Ming Ma, Yu Han and Jianfeng Huang\*



10454

### The hole mass in Car–Parrinello molecular dynamics: insights into the dynamics of excitation

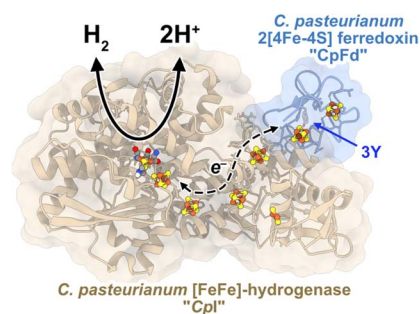
Sherif Abdulkader Tawfik\* and Tiffany R. Walsh



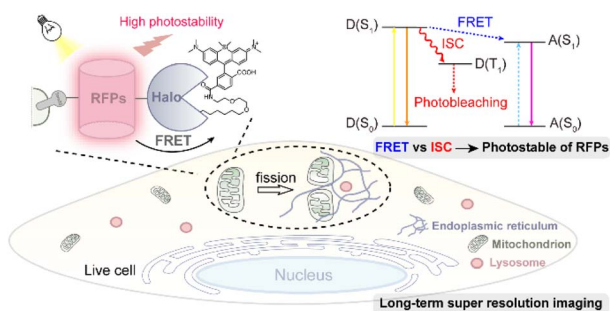
10465

### Probing the ferredoxin:hydrogenase electron transfer complex by infrared difference spectroscopy

Selmihan Sahin, Johanna Brazard, Kilian Zuchan, Takuji B. M. Adachi, Ulrich Mühlhoff, Ross D. Milton\* and Sven T. Stripp\*



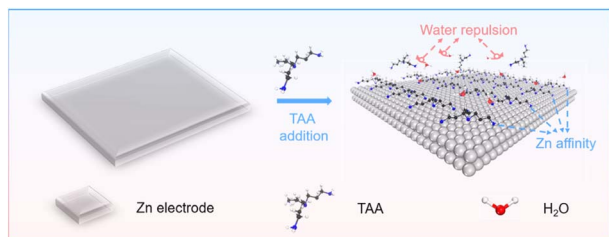
10476



## Enhancing the photostability of red fluorescent proteins through FRET with Si-rhodamine for dynamic super-resolution fluorescence imaging

Xuelian Zhou, Lu Miao,\* Wei Zhou, Yonghui Chen, Yiyang Ruan, Xiang Wang, Guangying Wang, Pengjun Bao, Qinglong Qiao\* and Zhaochao Xu\*

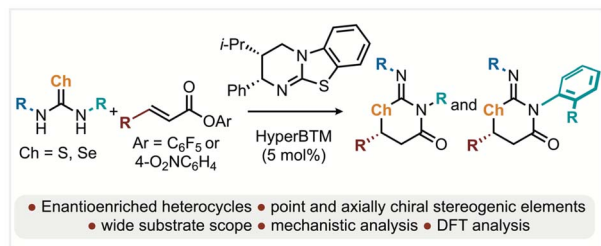
10487



## An amine electrolyte additive with claw structure promoting the stability of a Zn anode in aqueous batteries

Xiaoqi Sun,\* Hongtu Zhan, Qianrui Li and Kuo Wang\*

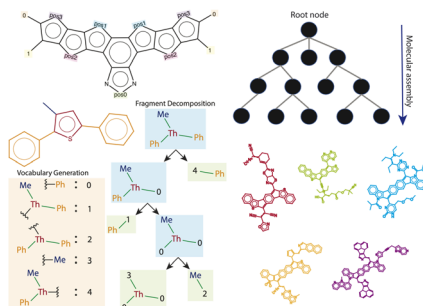
10494



## Isothiourea catalysed enantioselective generation of point and axially chiral iminothia- and iminoselenazinones

Alastair J. Nimmo, Alister S. Goodfellow, Jacob T. Guntley, Aidan P. McKay, David B. Cordes, Michael Bühl\* and Andrew D. Smith\*

10503



## Symmetry-constrained generation of diverse low-bandgap molecules with Monte Carlo tree search

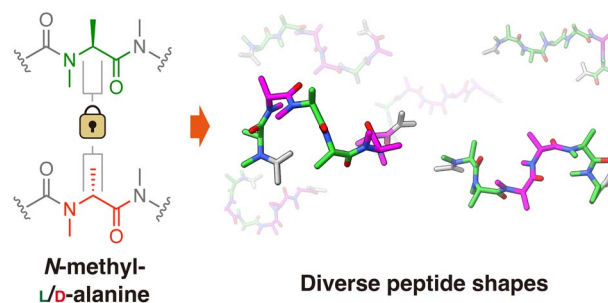
Akshay Subramanian, James Damewood, Juno Nam, Kevin P. Greenman, Avni P. Singhal and Rafael Gómez-Bombarelli\*



10512

### Bottom-up design of peptide shapes in water using oligomers of *N*-methyl-*L*/*D*-alanine

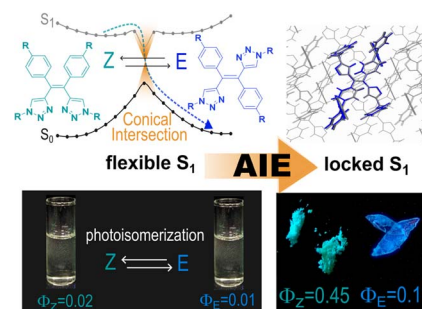
Jumpei Morimoto,\* Marin Yokomine, Yota Shiratori, Takumi Ueda, Takayuki Nakamuro, Kiyofumi Takaba, Saori Maki-Yonekura, Koji Umezawa, Koichiro Miyanishi, Yasuhiro Fukuda, Takumu Watanabe, Mayuko Suga, Ayumi Inayoshi, Takuya Yoshida, Wataru Mizukami, Koh Takeuchi, Koji Yonekura, Eiichi Nakamura and Shinsuke Sando\*



10523

### Stereoselective synthesis of heterocyclic tetraphenylethylene analogues with configuration-dependent solid-state luminescence

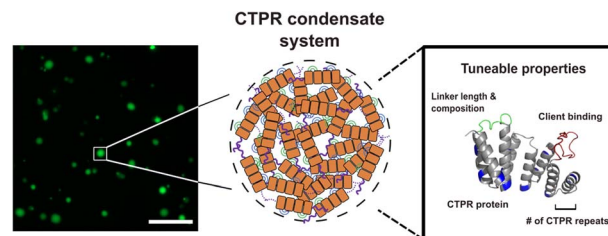
Mathilde Seinfeld,\* Jean Rouillon, Raphael Rullan, Erwann Jeanneau, Stephan N. Steinmann, Chantal Andraud, Tangui Le Bahers\* and Cyrille Monnereau



10532

### Tandem-repeat proteins introduce tuneable properties to engineered biomolecular condensates

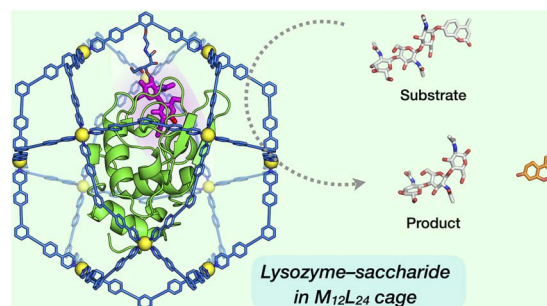
Tin Long Chris Ng, Mateo P. Hoare, M. Julia Maristany, Ellis J. Wilde, Tomas Sneideris, Jan Huertas, Belinda K. Agbetiamah, Mona Furukawa, Jerelle A. Joseph, Tuomas P. J. Knowles, Rosana Collepardo-Guevara, Laura S. Itzhaki\* and Janet R. Kumita\*



10549

### Proximity-induced saccharide binding to a protein's active site within a confined cavity of coordination cages

Takahiro Nakama,\* Miri Tadokoro, Risa Ebihara, Maho Yagi-Utsumi, Koichi Kato and Makoto Fujita\*

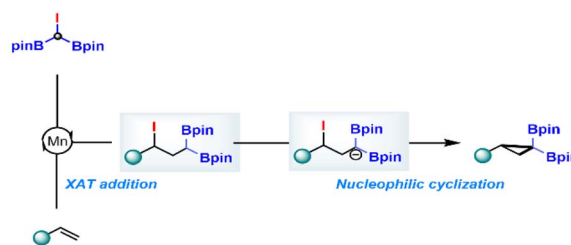




10595

### Synthesis of *gem*-di(boryl)cyclopropanes from non-activated olefins via Mn-photocatalyzed atom transfer radical addition

Jiefeng Hu,<sup>\*</sup> Kun Zhang, Jing Wang, Mingming Huang, Shuangru Chen, Zhuangzhi Shi and Todd B. Marder<sup>\*</sup>

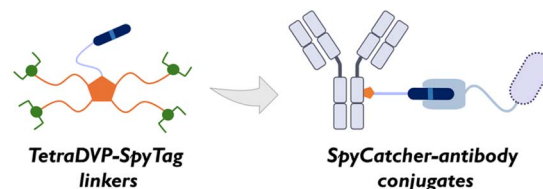


- ◆ practical, scalable
- ◆ high catalytic efficiency
- ◆ scalable and cheap precursors
- ◆ excellent selectivity
- ◆ broad substrate scope
- ◆ good functional group compatibility

10602

### A platform for SpyCatcher conjugation to native antibodies

Sona Krajcovicova, Thomas Wharton, Claudia L. Driscoll, Thomas A. King, Mark R. Howarth<sup>\*</sup> and David R. Spring<sup>\*</sup>

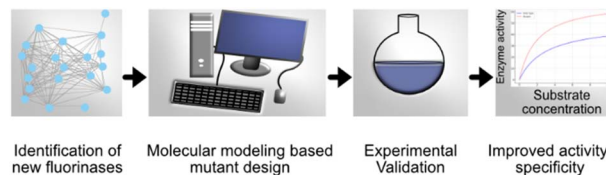


- ✓ Solid-phase linker synthesis
- ✓ SpyTag/SpyCatcher use with native antibodies
- ✓ Scalable to gram quantities
- ✓ Compatible with IgG1 and IgG4 antibodies
- ✓ Linkers used beyond ADCs
- ✓ SpyCatchers attached with great selectivity

10610

### Unveiling the molecular basis of selective fluorination of SAM-dependent fluorinases

Ravi Kumar Verma, Wan Lin Yeo, Elaine Tiong, Ee Lui Ang,<sup>\*</sup> Yee Hwee Lim,<sup>\*</sup> Fong Tian Wong<sup>\*</sup> and Hao Fan<sup>\*</sup>



- Identification of new fluorinases
- Molecular modeling based mutant design
- Experimental Validation
- Improved activity/specificity

10620

### Correction: Exciton and charge transfer processes within singlet fission micelles

Daniel Malinowski, Guiying He, Bernardo Salcido-Santacruz, Kanad Majumder, Junho Kwon, Matthew Y. Sfeir<sup>\*</sup> and Luis M. Campos<sup>\*</sup>



10621

**Correction: Site- and stereoselective silver-catalyzed intramolecular amination of electron-deficient heterobenzylic C–H bonds**

Tuan Anh Trinh, Stanislav Cherempei, Daniel S. Rampon and Jennifer M. Schomaker\*

