

Chemical Science

rsc.li/chemical-science

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 16(43) 20089–20616 (2025)



Cover
See Chi Zhang, Ke Hu *et al.*, pp. 20229–20238. Image reproduced by permission of Weijian Yang and Ke Hu from *Chem. Sci.*, 2025, 16, 20229. Cover design ideas by Weijian Yang and Ke Hu; image drawn by Zhiyuan Zheng from Changsha Keyanyihui Information Technology Co., Ltd.



Inside cover
See Anagha Sasikumar, Radek Marek *et al.*, pp. 20239–20244. Image reproduced by permission of Radek Marek from *Chem. Sci.*, 2025, 16, 20239.

EDITORIAL

20105

Sustainable chemical science and engineering: celebrating the 130th anniversary of Tianjin University

Jinlong Gong, Yingjin Yuan, Naiqin Zhao and Shi-Zhang Qiao

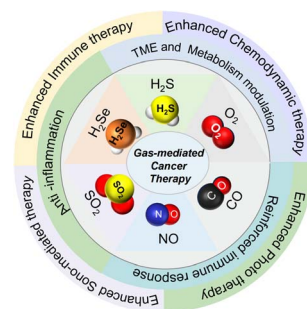


PERSPECTIVES

20108

Gas-mediated reinforcement of cancer therapies: emerging strategies and future perspectives

Fang Yuan, Lu Wang, Lulu Ning,* Jianjian Zhang* and Yuan Guo*



**GOLD
OPEN
ACCESS**

EES Batteries

**Exceptional research on
batteries and energy storage**

Part of the EES family

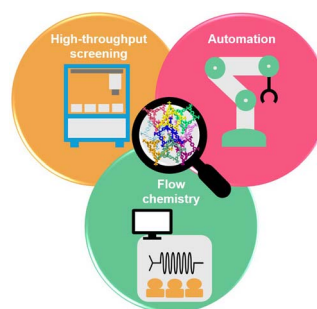
**Join
in** | Publish with us
rsc.li/EESBatteries

PERSPECTIVES

20124

Enabling technology for accelerated discovery of supramolecular materials

C. E. Shields, A. M. Scholes and A. G. Slater*

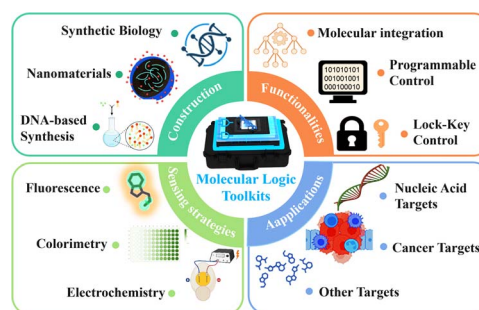


REVIEWS

20139

Intelligent molecular logic computing toolkits: nucleic acid-based construction, functionality, and enhanced biosensing applications

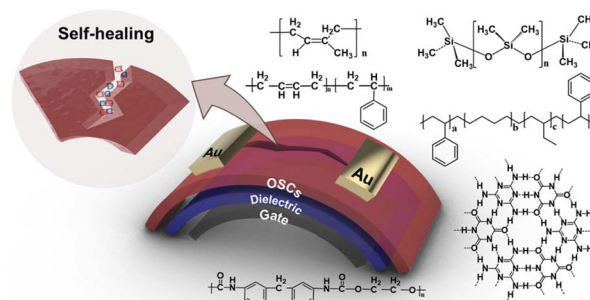
Yaxue Hu, Jinghui Zhang,* Ke Shen, Wei Shen, Hian Kee Lee* and Sheng Tang*



20181

The rise of rubber-like synthetic polymers in next-gen transistor technologies

Livy Laysandra, Dinda Bazliah, Daniel Muara Sentosa, Ayu Cahyarani Heksa, Hai-Khue Bui, Yu-Cheng Li and Yu-Cheng Chiu*

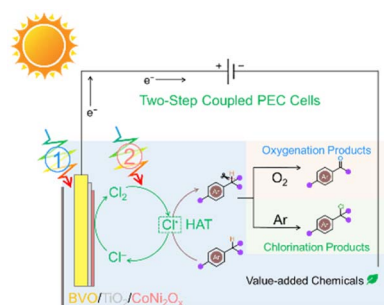


EDGE ARTICLES

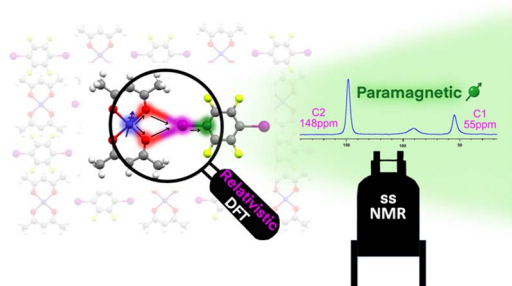
20229

Two-step coupled photoelectrochemical chlorination and oxygenation of C(sp³)-H bonds mediated by chlorine radicals over a modified BiVO₄ photoanode

Weijian Yang, Pengju Li, Yiming Han, Zijian Zhao, Limei Tian, Zhenghao Zhang, Mark G. Humphrey, Chi Zhang* and Ke Hu*



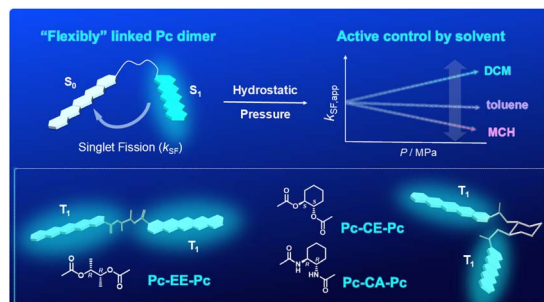
20239



Supramolecular covalency of halogen bonds revealed by NMR contact shifts in paramagnetic cocrystals

Anagha Sasikumar, Jan Novotný, Jan Chyba, Libor Kobera and Radek Marek*

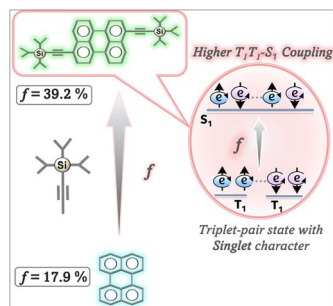
20245



Critical molecular design that can actively control intramolecular singlet fission by hydrostatic pressure

Rintaro Ogawa, Tomokazu Kinoshita, Tomoya Kuwabara, Hayato Sakai, Makoto Harada, Taku Hasobe* and Gaku Fukuhara*

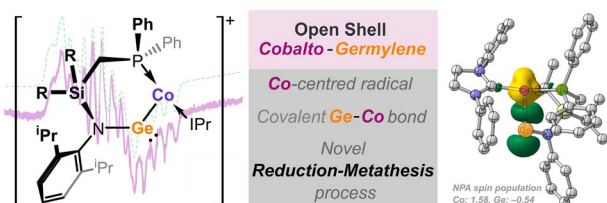
20255



Enhancing the statistical probability factor in triplet-triplet annihilation photon upconversion via TIPS functionalization

Lukas Naimovičius, Manvydas Dapkevičius, Edvinas Radiunas, Mila Miroshnichenko, Gediminas Kreiza, Carles Alcaide, Paulius Baronas, Yoichi Sasaki, Nobuhiro Yanai, Nobuo Kimizuka, Andrew B. Pun, Miquel Solà, Pankaj Bharmoria,* Karolis Kazlauskas and Kasper Moth-Poulsen*

20265



The path to an open-shell metallo-germylene: direct ligation, or reduction and metathesis?

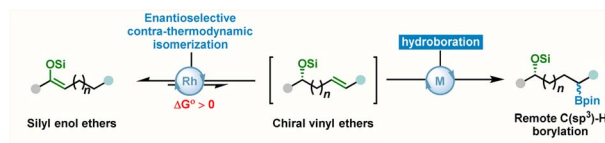
Annika Schulz, Myron Heinz, Max. C. Holthausen* and Terrance J. Hadlington*



20275

Catalytic asymmetric isomerization/hydroboration of silyl enol ethers

Yisen Yao, Jintao Sun, Jie Li and Wanxiang Zhao*



20286

eCarbonyls: an electrochemical thioether mediated oxidation of alcohols to aldehydes and ketones

Conall Molloy, Simon Kaltenberger, Lee Edwards, Katherine M. P. Wheelhouse and Kevin Lam*

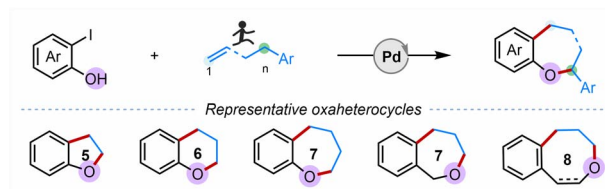
*Ceci n'est pas une Swern.*

- ✓ **Mild conditions:** operates at room temperature
- ✓ **Broad scope:** good functional group tolerance
- ✓ **Safe:** electrochemical approach avoids hazardous reagents
- ✓ **Scalable:** demonstrated in both batch and flow

20292

Modular and diverse synthesis of oxaheterocycles via Pd-catalyzed migratory 1,n-cycloannulation of alkenes

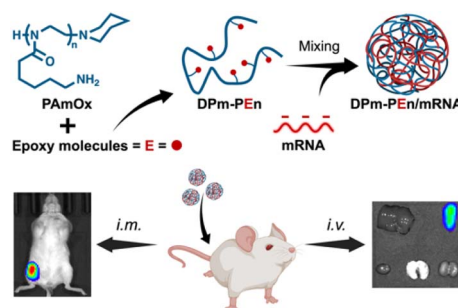
Jin-Ping Wang, Yichen Wu and Peng Wang*



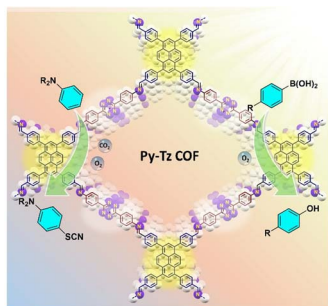
20300

A simple epoxide modification strategy to construct amino-functional poly(2-oxazoline) mRNA delivery vectors

Kuncheng Lv, Yibo Qi, Hanqin Zhao, Yuyan Zhang, Ziyue An, Sheng Ma and Wantong Song*



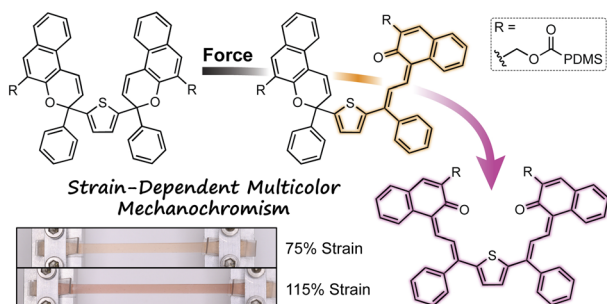
20314



Dual-functional photoredox catalytic thiocyanation and hydroxylation using a donor–acceptor COF

Tamagna Mandal, Anupam Dey, Dipayan Mandal and Tapas Kumar Maji*

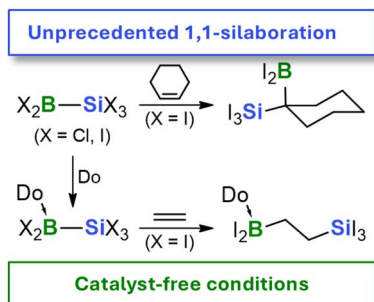
20323



Strain-dependent multicolor mechanochromism of 3H-bis-naphthopyran in solid polymeric materials

Skylar K. Osler, Audrey V. Conner, Molly E. McFadden and Maxwell J. Robb*

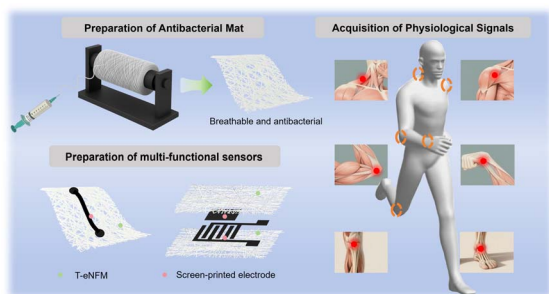
20329



Synthesis of perhalogenated silylboranes (X = Cl, I) and their application in regiodivergent alkene silaboration

Jan Heller, Christoph D. Buch, Alexander V. Virovets, Eugenia Peresykina, Hans-Wolfram Lerner, Felipe Fantuzzi and Matthias Wagner*

20344



Antimicrobial and breathable membranes with printed carbon nanotube-silver composite conductive layers for electronic sensing

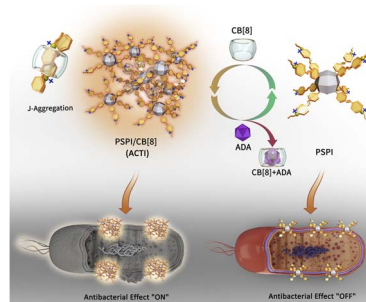
Huacui Xiang, Daniel Verrico, Taher Hafiz, Enjian He, Gary E. Wnek, Kun Hu, Guojun Liu,* Yen Wei* and Jiujiang Ji*



20355

Switchable supramolecular polycationic assemblies for tunable antibacterial strategies against antibiotic resistance

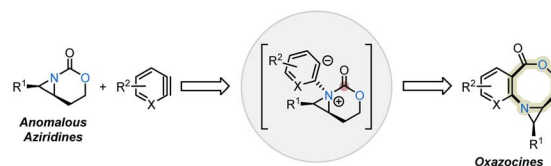
Jia Chen,* Xueqian Wang, Mengrui Zhang, Xue Wang, Ran Wang, Xinxing Lyu, Yunjian Xu, Xintian Shao,* Luling Wu* and Tony D. James



20368

Two-carbon ring expansion of bicyclic aziridines to oxazocines via aryne insertion into a σ C–N bond

Daniel S. Rampon, Tuan Anh Trinh, Yekun Pan, Sierra Thein, Jacob W. Kailing, Ilia A. Guzei, Israel Fernández* and Jennifer M. Schomaker*

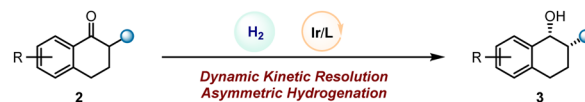


- Single step two-carbon ring expansion
- Retention of the stereochemical information
- DFT calculations
- Retention of aziridine handle
- Mild conditions

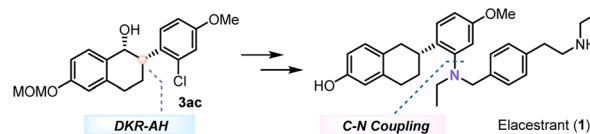
20376

Gram-scale synthesis of (+)-elacestrant streamlined by iridium-catalyzed dynamic kinetic asymmetric hydrogenation of α -substituted tetralones

Yan Zong,* Xiaomei Zou, Shaoke Zhang, Gen-Qiang Chen* and Xumu Zhang*



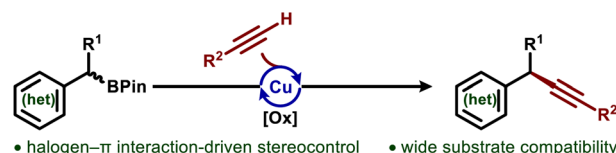
- Excellent yield and stereoselectivity
- Good functional group compatibility
- Up to 16,000 TON
- Gram scale synthesis



20382

Cu-catalyzed enantioconvergent deborylative alkylation

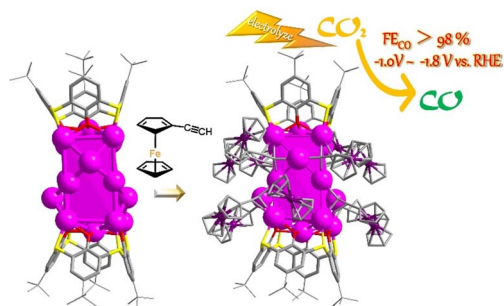
Joshua F. Head, Tanner J. Schubert, Biyu Zhao and Yuyang Dong*



- halogen- π interaction-driven stereocontrol
- wide substrate compatibility



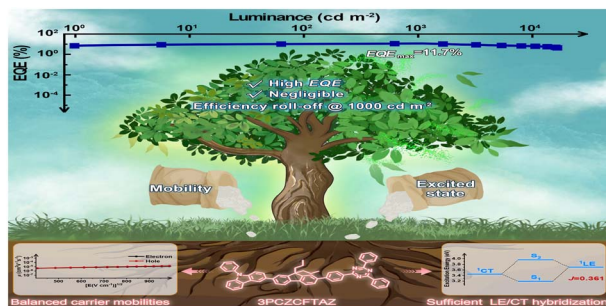
20389



Dynamic structural engineering of ferrocene-functionalized Ag₂₀ nanoclusters for enhanced CO₂ electroreduction performance

Hong-Yan Zhu, Xiao-Wei Wang, Xin-Yu Chen, Lan-Yan Li, Yi-Xin Li, Wei Dong Yu, Jun Yan and Chao Liu*

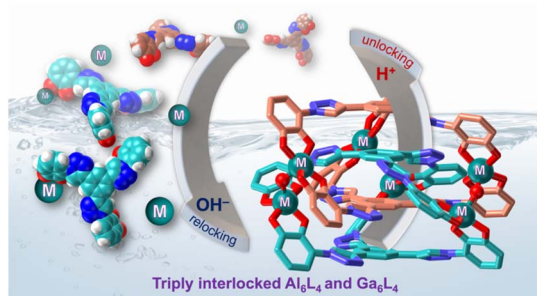
20397



Highly efficient and negligible efficiency roll-off non-doped blue electroluminescence with a synergistic effect of fast-balanced carrier transport and appropriate hybridized excited states

Huayi Zhou, Tengyue Li, Mizhen Sun, Yannan Zhou, Jingru Song, Jie Zhang, Qikun Sun, Shi-Tong Zhang, Xingrong Zhang* and Shanfeng Xue*

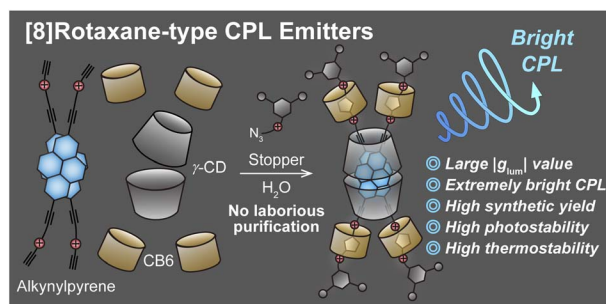
20406



Cooperative reversible assembly in triply interlocked Al₆L₄ and Ga₆L₄ cages

Ignacio Izquierdo, Laura Martínez-Castro, Gregori Ujaque and Antonio J. Martínez-Martínez*

20414



High-yield syntheses of doubly 2,7-dialkynylpyrene-threaded photostable [8]rotaxanes exhibiting extremely bright circularly polarized luminescence

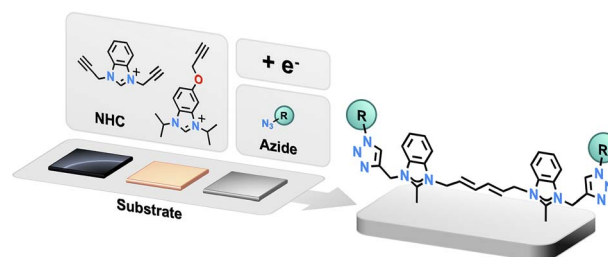
Kohei Nishioki, Asuka Kimura, Yuki Ohishi,*
Juri Yamashita, Masahiro Kitamoto, Munetaka Iwamura,
Koichi Nozaki, Junya Chiba and Masahiko Inouye



20422

N-heterocyclic carbenes as clickable molecular anchors for electrochemical surface functionalization of metals and glassy carbon

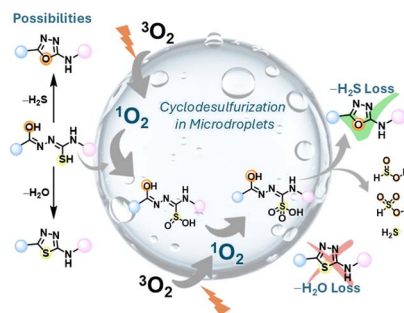
Antoine Juneau, Ahmadreza Nezamzadeh, Béatrice Laberge, Anastasia Messina, Justin Lomax, Thilini M. Suduwella, Jashanpreet Kaur, Vikram Singh, Mark D. Aloisio, Paul J. Ragogna,* Cathleen M. Crudden* and Janine Mauzeroll*



20438

Chemoselective cyclodesulfurization vs. dehydration enabled by aqueous microdroplet chemistry

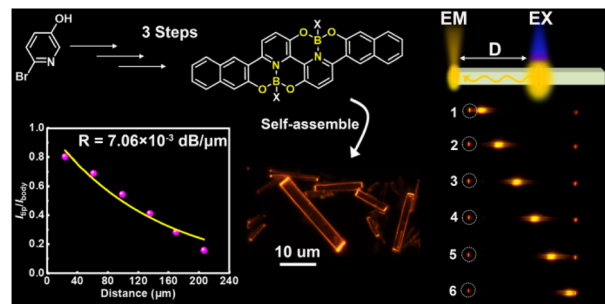
Manish Jana, Mousumi Saha and R. Graham Cooks*



20445

O–B ← N perturbed polycyclic aromatic hydrocarbons: a straightforward synthesis strategy, and their photophysical and optical waveguide properties

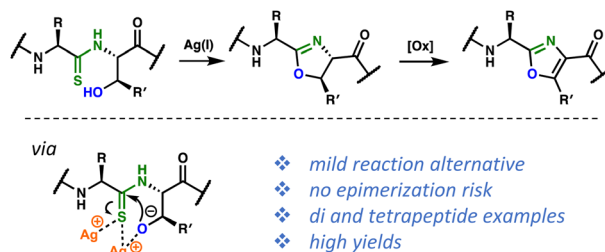
Jinying Zhao, Qihang Yang, Weibin Chen, Nuo Xu, Qing Zhang, Wenhao Zhao, Geng-Geng Luo, Qihong Cui* and Jianhua Huang*



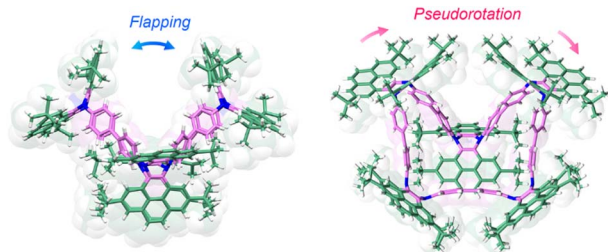
20457

Silver(I)-mediated oxazoline formation: a mild route to 2,4-oxazoles in peptides

Adam S. Pickett, Jacob W. Campbell, Katherine M. Cox, Zainab A. Bello, Erin R. Johnson and Carlie L. Charron*



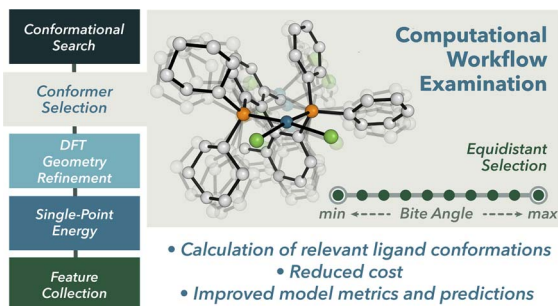
20464



Supercycloalkanes: dihydropyrazine-embedded macrocycles with flexible conformations resembling cycloalkanes

Shuhai Qiu, Li Zhang, Da-Hui Qu* and Zhaohui Wang*

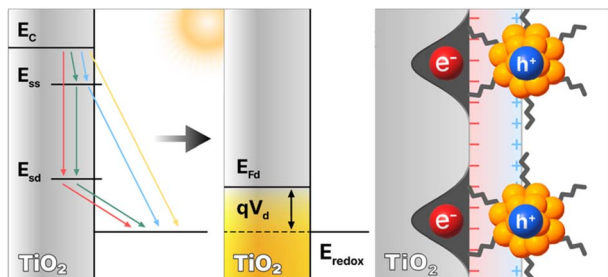
20473



Bisphosphine ligand conformer selection to enhance descriptor database representation: improving statistical modelling outcomes

Jamie A. Cadge, Sierra D. Hart, Richard C. Walroth, Kyle A. Mack and Matthew S. Sigman*

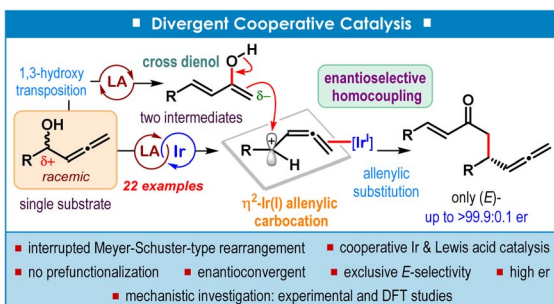
20486



Illumination-induced deep trap state activation at the nanocluster/TiO₂ interface: the origin of intrinsic photocapacitance in sensitized solar cells

Muhammad A. Abbas, Raju Thota, Minwook Jeon and Jin Ho Bang*

20495



Enantioselective homocoupling of allenyl alcohols through divergent cooperative catalysis

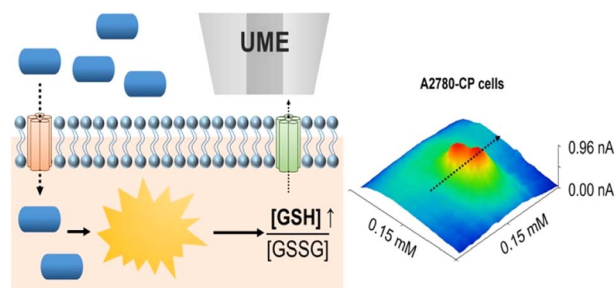
Aditya Chakrabarty, Ritwika Chatterjee and Santanu Mukherjee*



20507

Tracking carboplatin chemoresistance in ovarian cancer by scanning electrochemical microscopy

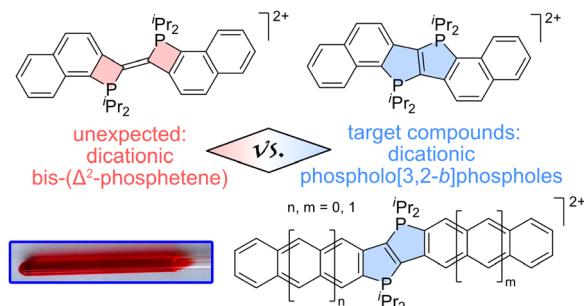
Roy Daou, Mengzhen Lyu, Katherine Bazin, Dao Trinh, Michael A. Saley, Dhésmon Lima, Mark W. Nachtigal and Sabine Kuss*



20517

π -Extended diphosphonium-bridged ladder stilbenes: water-soluble fluorophores with up to eight annulated rings

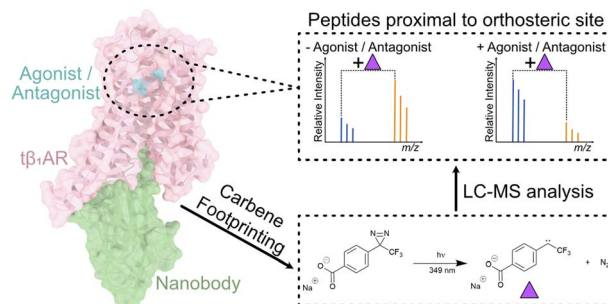
Sebastian Senn, Jean-Marc Mörsdorf,*
Maria-Sophie Bertrams, Christoph Kerzig*
and Joachim Ballmann



20527

Multi-region mapping of ligand binding and structural changes in the β -1 adrenergic receptor using carbene footprinting and mass spectrometry

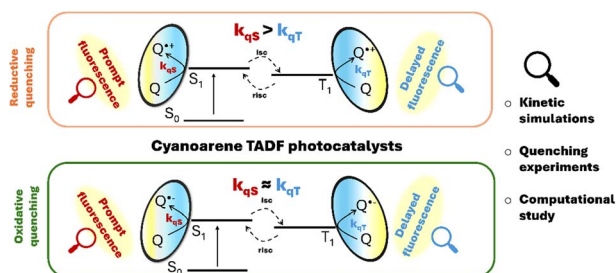
James R. Lloyd, Arpana S. Varughese, Parth Kapoor, Katharina L. Dürr, Hsin-Yung Yen, Ali Jazayeri, Jonathan T. S. Hopper* and Neil J. Oldham*



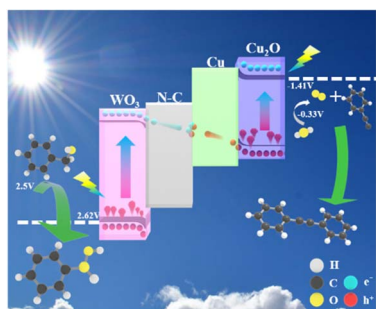
20536

Reactivity of organic photocatalysts displaying thermally activated delayed fluorescence (TADF): rationalizing unexpected differences between rates of quenching of the lowest singlet and triplet states

Federica Fina, Caterina Bellatreccia, Xia Wu, Pier Giorgio Cozzi, Alessandro Troisi, Sergei Vinogradov and Paola Ceroni*



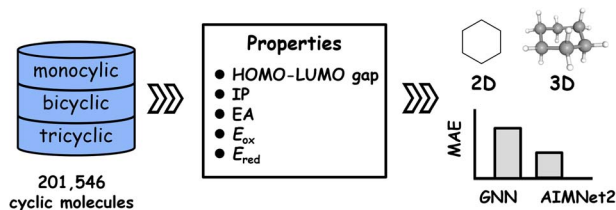
20544



Constructing a visible-light-excited Z-scheme heterojunction by engineering the directional N-C/Cu insertion layer: overcoming work function mismatches

Hao Gao, Xiaoxiao He, Jinbu Li, Qiang Zhu, Chengyu Qin, Liming Sun,* Shuting Zhi, Lei Yang, Wenwen Zhan,* Jianwei Zhao and Xiguang Han*

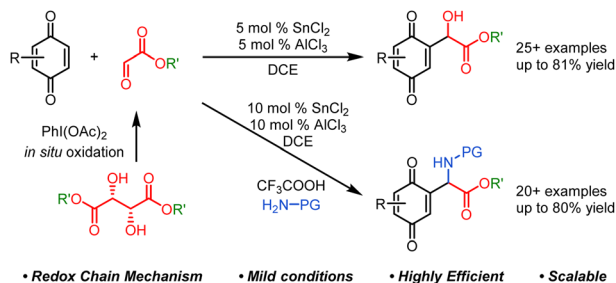
20553



High-throughput electronic property prediction of cyclic molecules with 3D-enhanced machine learning

Peikun Zheng and Olexandr Isayev*

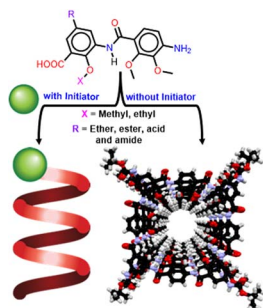
20564



Construction of α -quinonyl- α -hydroxy/amino acid esters through the redox chain reaction

Yu-Meng Ye and Zhi Li*

20570



Design and synthesis of macrocycles with tuneable diameters and helical foldamers with customizable peripheral side chains

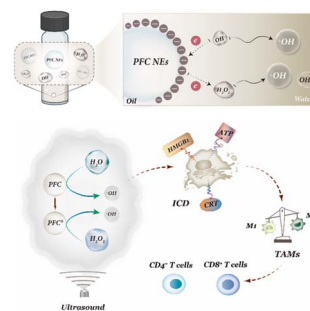
Saqib Farooq, Aurelien Crochet and Andreas F. M. Kilbinger*



20580

Hydroxyl radical generation from H_2O_2 via liquid–liquid contact-electro-catalysis

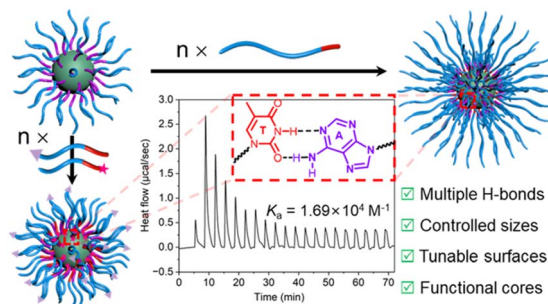
Haimei Li, Airong Xie, Chengzi Hong, Zichen Wang, Xu Chu, Zhong Lin Wang,* Yi Liu* and Peng Jiang*



20594

Quantitative and spatially defined functionalization of nanostructures by overcoming the strong steric hindrance through bioinspired nucleobase interactions

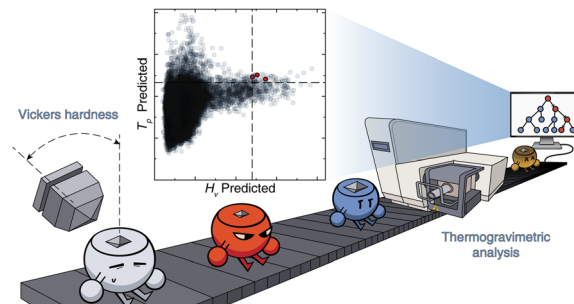
Huijuan Chen, Yuan Xue, Nan Yao, Rong Cheng, Jia Liu, Jiawen Bao and Zan Hua*



20601

Identifying inorganic solids for harsh environments via machine learning

Jacob C. Hickey, Arman M. Karimaghahi, Matt Flores, Sally Hoang, Roy Arrieta, Amit Kumar, Gonzalo Cuervo, Peter Zhu and Jakoah Brgoch*



20612

Correction: Construction of a homologous series of metal nanoclusters and implications for structure–activity correlations

Qinzheng Li, Tingting Jiang, Sha Yang, Jinsong Chai,* Haizhu Yu* and Manzhou Zhu*



20613

Correction: Two-carbon ring expansion of bicyclic aziridines to oxazocines via aryne insertion into a σ C–N bond

Daniel S. Rampon, Tuan Anh Trinh, Yekun Pan, Sierra Thein, Jacob W. Kailing, Ilia A. Guzei, Israel Fernández* and Jennifer M. Schomaker*

