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# Chemical Science

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**Cover**
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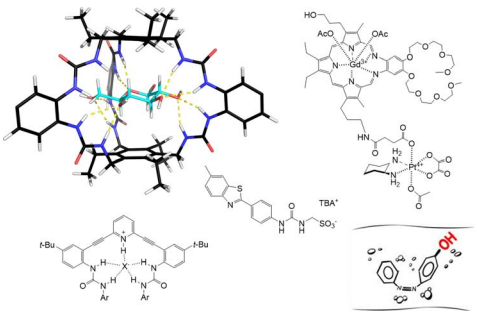
**Inside cover**
See Nikolay V. Tkachenko, K. Birgitta Whaley, Martin Head-Gordon *et al.*, pp. 22299–22313. Image reproduced by permission of Martin Head-Gordon from *Chem. Sci.*, 2025, **16**, 22299. Image concept created by Nikolay and Anastasiia Tkachenko.

## EDITORIAL

22195

**Making molecules work – stories of supramolecular translation**

Anthony P. Davis,* Arri Priimagi,* Matti Virkki, Jennifer R. Hiscock,* Calden N. Carroll,* Michael M. Haley,* Darren W. Johnson,* Jonathan F. Arambula,* Krystle Karoscik and Jonathan L. Sessler

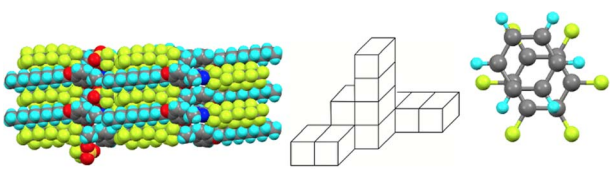


## PERSPECTIVE

22213

**Employing fluorine for supramolecular control in self-assembled and self-organised molecular systems**

Duncan W. Bruce



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## REVIEWS

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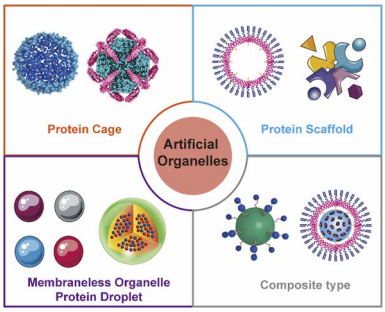
**Construction of artificial organelles *via* protein self-assembly and their applications**

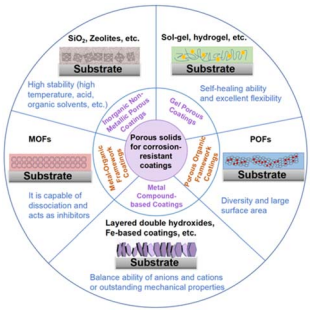
Jiachen Sun, Ruikui Gao, Zhongxuan Yang, Zefeng Deng, Lei Qin,* Haiyang Jia* and Chun Li*




22250

**Strategic microstructure manipulation of porous materials for advanced corrosion protection in metallic alloys**

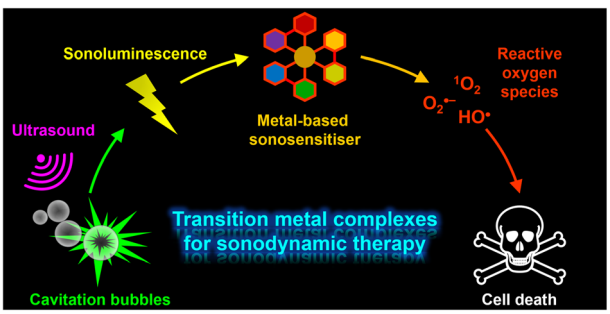
Yajie Yang, Yonghao Zhu, Zhuojun Yan,* Doudou Cao, Yingbo Song, Yue Zheng, Ya Wu, Jiakun Yue, Jiarui Cao, Sirui Li, Lu Luo and Ye Yuan*




22266

**Ultrasound-activatable transition metal complexes to potentiate sonodynamic therapy**

Lawrence Cho-Cheung Lee and Kenneth Kam-Wing Lo*

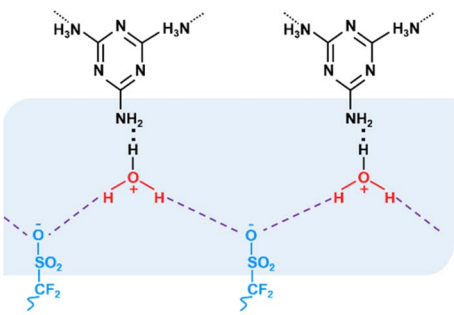



## EDGE ARTICLES

22291

**Triazine-ring protonation enables synergistic enhancement of proton conduction and membrane stability**

Yunfa Dong, Haodong Xie, Yupei Han, Quan Li, Jiecai Han and Weidong He*



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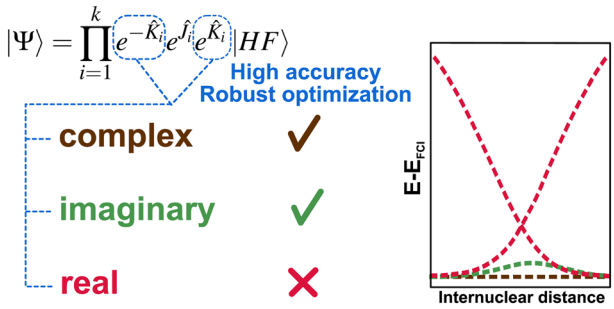
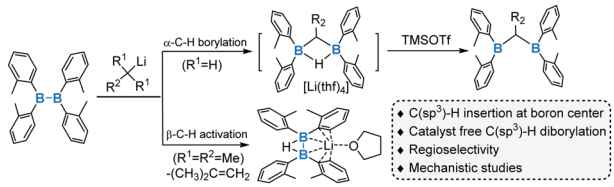



## Beyond real: alternative unitary cluster Jastrow models for molecular electronic structure calculations on near-term quantum computers

Nikolay V. Tkachenko,* Hang Ren, Wendy M. Billings, Rebecca Tomann, K. Birgitta Whaley* and Martin Head-Gordon*

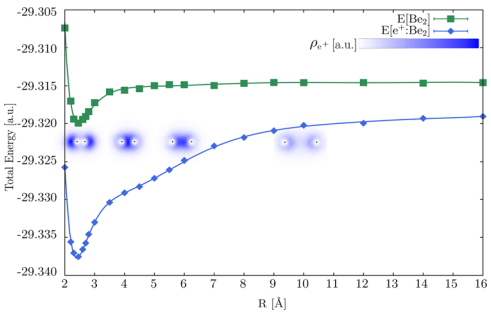
22314




## Regioselective C(sp$^3$)–H borylation *via* a diarylboryl anion surrogate in sp$^2$–sp$^3$ diboranes(5)

Xiaofeng Mao, Jie Zhang* and Zuowei Xie*

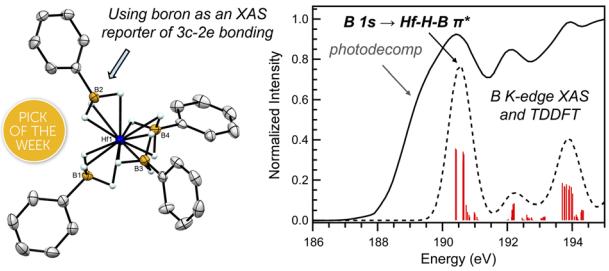
22322




## Watch out electrons!: positron binding redefines chemical bonding in $Be_2$

Rafael Porras-Roldan, Jorge Charry, Felix Moncada, Roberto Flores-Moreno, Márcio T. do N. Varella and Andrés Reyes*

22333




## Direct measurement of covalent three-center, two-electron M–H–B bonding in Zr and Hf borohydrides using B K-edge XAS

Hannah M. Hansen, Joshua C. Zgrabik, Peter A. Zacher, III, Jacob J. Schuely, Emily M. Amano, Mai Yer Yang, Daniel K. Unruh, Lucia Zuin, Jason M. Keith* and Scott R. Daly*

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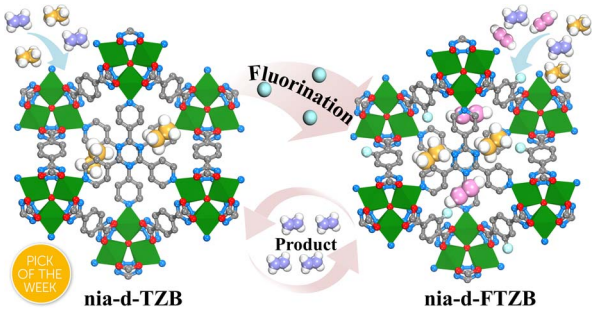
## EDGE ARTICLES

22348

**Fluorine-mediated single-step ethylene purification in face-transitive metal–organic frameworks from binary to ternary gas mixtures**

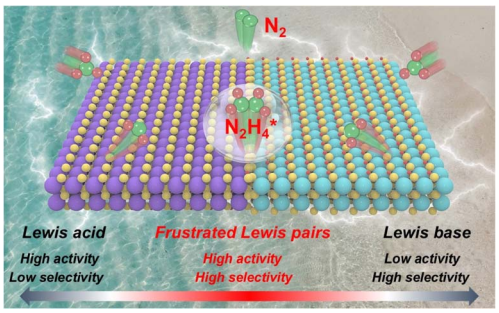
Wei-Hong Zhang, Ya-Nan Ma, Guo-Tong Du, Ping Wang and Dong-Xu Xue*




22357

**Accelerating $N_2H_{4(ads)}$ formation by frustrated Lewis pairs in an oxyhydroxide for electrocatalytic ammonia oxidation into $N_2$**

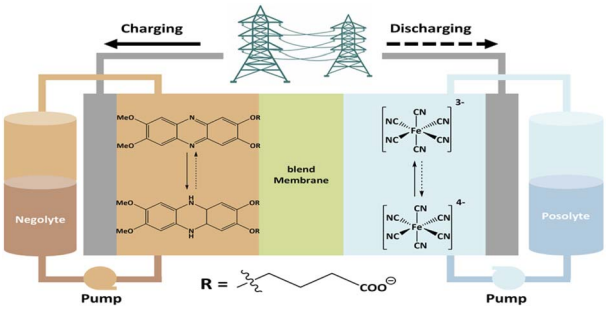
Meng-Ying Yin, Xing-Yuan Xia, Ting Dai, Xia Chen, Qiu-Ju Xing, Lei Tian* and Jian-Ping Zou*




22368

**A low-redox-potential phenazine-based negolyte with high stability for aqueous organic flow batteries**

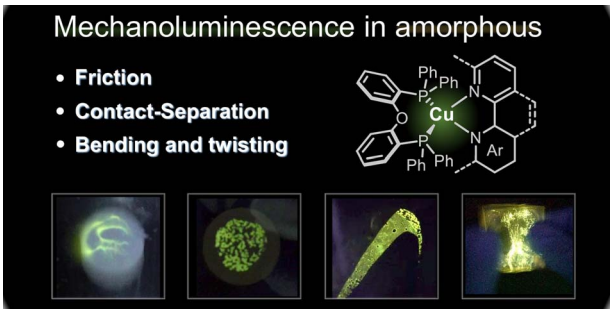
Xuanyu Xie, Taoyi Kong, Jiaming Gao, Ruiyang Li and Yonggang Wang*




22376

**Mechanoluminescence from amorphous solids of heteroleptic copper complexes and common luminophores induced by non-destructive mechanical stimuli and fabrication of flexible mechanoluminescent films**

Ayumu Karimata,* Daniil Ilatovskii, Robert R. Fayzullin, Shinya Komoto, Andrew Bruhacs, Eugene Khaskin and Julia R. Khusnutdinova*



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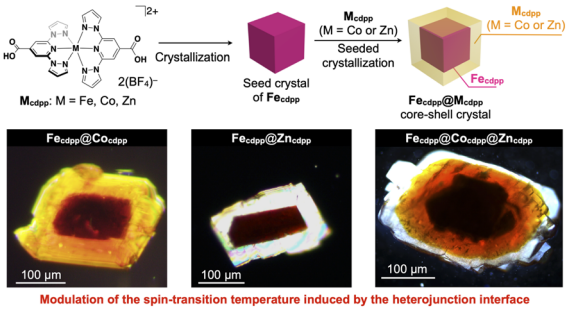


### Wrapping a single crystal spin-crossover complex with a single crystal non-spin-crossover complex to modulate the spin-transition temperature

Tomoya Fukui,* Masahiro Tsuchiya, Naoya Mita and Takanori Fukushima

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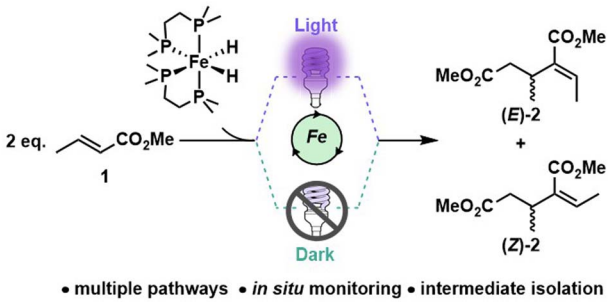
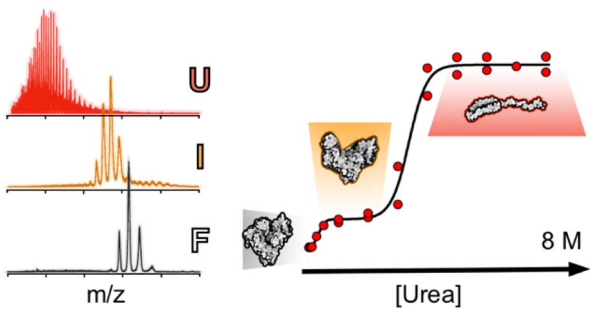



### Molecular-level insight into the multiple mechanistic pathways in iron-catalysed alkene dimerisation

Joseph H. P. Cockcroft, Annabel Flook, Patrick J. Boaler, Gary S. Nichol, Jarle Holt, Joost Smit, Jennifer A. Garden* and Stephen P. Thomas*

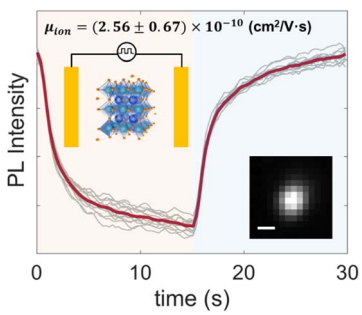
22407




### Mass spectrometry detects folding intermediates populated during urea-induced protein denaturation

Nicklas Österlund, Jacob S. Jordan, Eleonora Renzi, Gergo Peter Szekeres and Kevin Pagel*

22417




### Non-contact measurement of ion mobility in single halide perovskite particles

Yu-Ling Zou, Ke Li, Ben Niu, Bangyi Yue, Qiang Chen, Yuxi Tian* and Wei Wang*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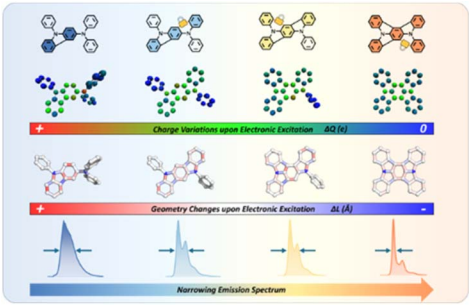
**Narrowing emission spectra based on indolocarbazole molecular model system: an experimental and theoretical study**

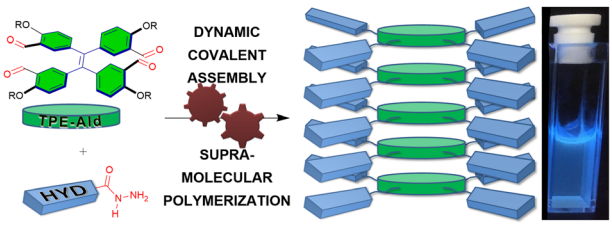
Yingbo Lv, Jingzhuo Bi, Runting Wang, Zhiqiang Yang, Xinqi Yang, Shuaiqiang Zhao, Shiyin Wang, Haichao Liu, Shi-Tong Zhang* and Bing Yang*




22438

**Emergence of fluorescent aggregates through hierarchical self-assembly**

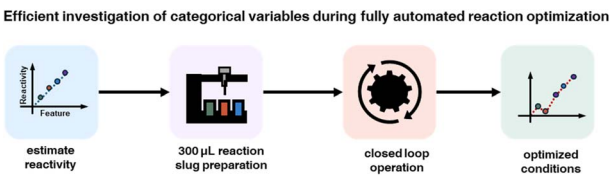
Maëva Coste and Sébastien Ulrich*




22447

**Leveraging an intelligent slug flow platform for self-optimization of reaction systems with categorical variables**

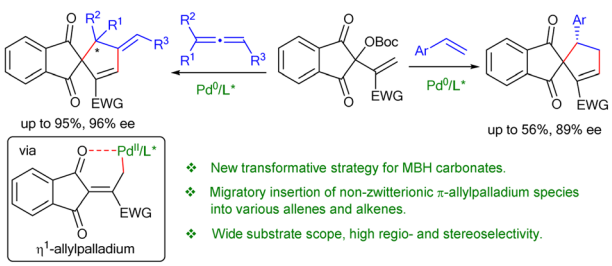
Florian L. Wagner, Gernot Neun, Thomas Tampone, Zhen Lei, Frederic G. Buono, Christopher A. Hone* and C. Oliver Kappe*




22456

**Palladium-catalysed asymmetric annulations of Morita–Baylis–Hillman carbonates with allenes or alkenes *via* migratory insertion**

Jin-Yu Huang, Xin-Ting Qin, Han-Wen Rao, Zhi-Chao Chen,* Lei Zhu, Qin Ouyang,* Wei Du and Ying-Chun Chen*



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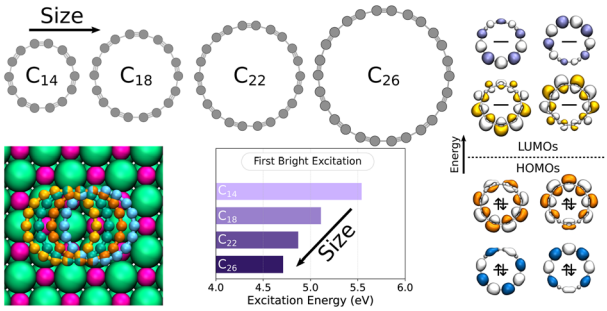


### The optical response of aromatic cyclocarbons

Simone Grillo,* Olivia Pulci and Tommaso Giovannini*

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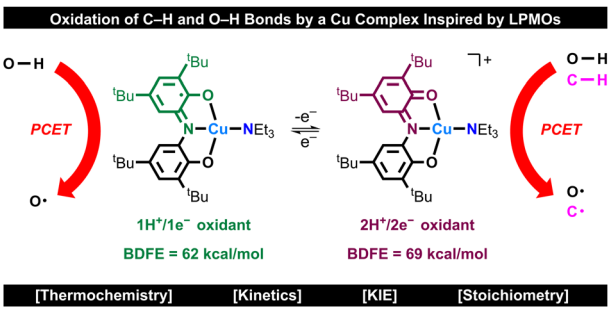
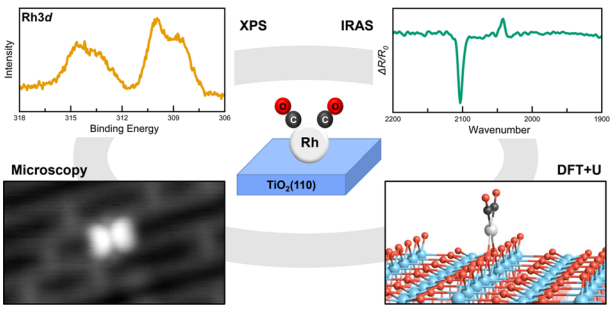



### Oxidation of C–H and O–H bonds by a copper complex inspired by the Cu(II)–tyrosyl species formed in LPMOs

David D. Hebert, Daniel Ye and Isaac Garcia-Bosch*

22481




### Multi-technique characterization of rhodium gem-dicarbonyls on $TiO_2$(110)

Moritz Eder,* Faith J. Lewis, Johanna I. Hütner, Panukorn Sombut, Maosheng Hao, David Rath, Paul Ryan, Jan Balajka, Margareta Wagner, Matthias Meier, Cesare Franchini, Gianfranco Pacchioni, Ulrike Diebold, Michael Schmid, Florian Libisch, Jiři Pavelec* and Gareth S. Parkinson

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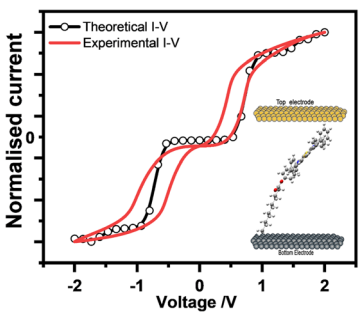


### High-performance room-temperature molecular switches enabled by resonant tunnelling in dithia-porphyrins

Kavita Garg,* Nikshay Bisht and Praveen C. Ramamurthy



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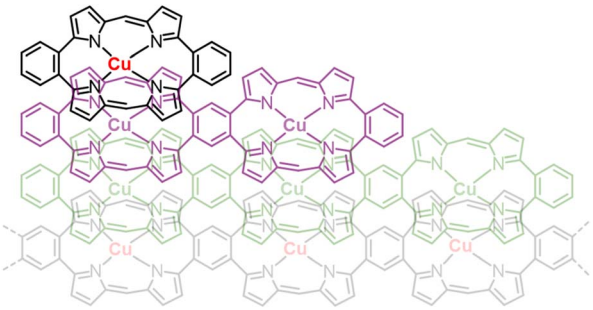
**Synthesis of wave-shaped Cu(II) porphyrin arrays and their electrocatalytic hydrogen evolution activity**

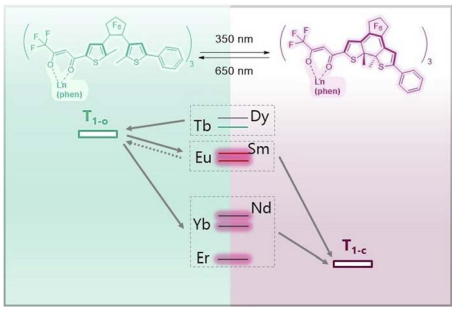
Tao Jiang, Yuanbo Zhou, Tao Ye, Shihao Liu, Ke Li, Xiaohui Zhao,* Zhongti Sun, Naoki Aratani, Hiroko Yamada, Fengxian Qiu,* Jianming Pan,* Toshiharu Teranishi and Songlin Xue*



22504

**From erbium(III) to samarium(III): generalized photomodulation of NIR to red lanthanide luminescence with a DTE ligand and its versatile role in the quenching processes**

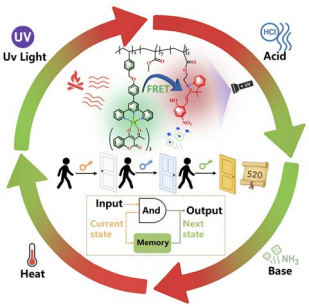
Tuan-Anh Phan, Frédéric Gendron, Salauat Kiraev, Olivier Galangau, Yoann Fréroux, Hassan Al Sabea, Cédric Mittelheisser, Marie Dallon, Aude Bouchet, François Riobé, Remi Métivier, Michel Sliwa, Boris Le Guennic, Olivier Maury,* Akos Banyasz, Bogdan Marekha, Lucie Norel* and Stéphane Rigaut*




22517

**Harnessing spiropyran isomerization in lanthanide metallopolymers for sequential logic encryption and anticounterfeiting**

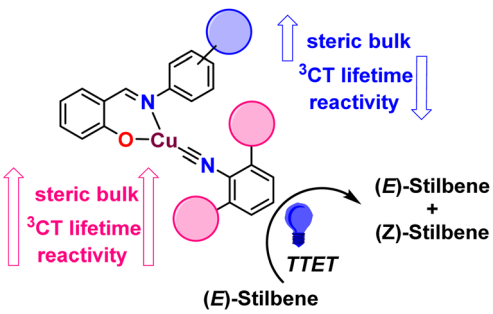
Weixu Feng, Xiaolin Liao, Sumin Lu, Dong Han, Qianrong Guo, Yan Zhao, Wei Tian and Hongxia Yan*




22527

**Ligand substituents modulate excited-state lifetime and energy-transfer reactivity in Cu(I) photosensitizers supported by salicylaldimine and isocyanide ligands**

Soumi Chakraborty, Kianna Agyekum, Dooyoung Kim and Thomas S. Teets*



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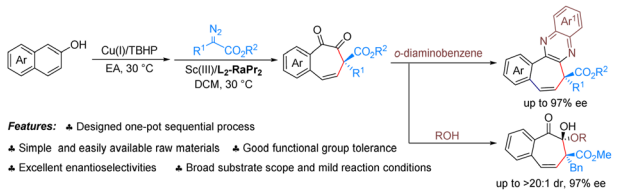


### Sequential oxidative dearomatization/asymmetric homologation: from simple naphthols to chiral benzocycloheptanes

Hongkun Zeng, Shiyang Li, Lichao Ning, Tao Huang, Xiaoming Feng* and Lili Lin*

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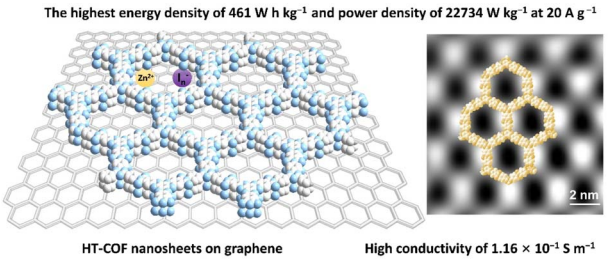
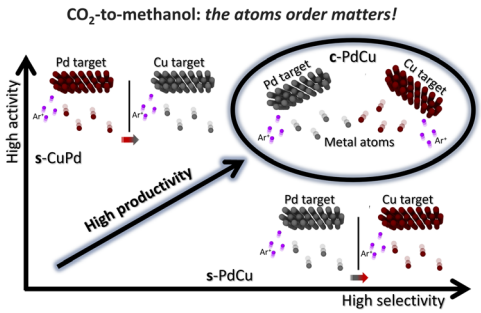



### Graphene-supported covalent organic framework nanosheets for high performance aqueous dual-ion batteries

Xiya Yang, Mengying Huang, Guang Lu, Rong Jiang, Xinxin Wang, Zhixin Liu, Lijuan Jiao, Erhong Hao, Dongdong Qi, Kang Wang,* Qian Chen* and Jianzhuang Jiang*

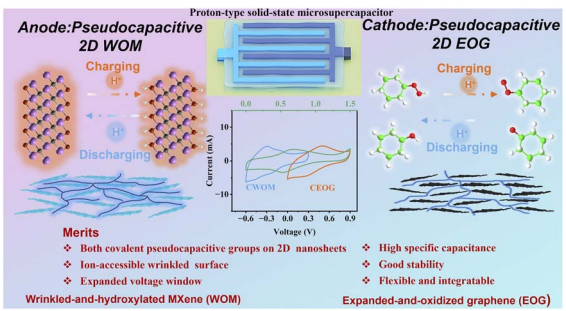
22554




### Atom-by-atom assembly reveals structure–performance control in PdCu catalysts for $CO_2$ hydrogenation to methanol

Louise R. Smith, Emerson C. Kohlrausch, Kieran J. Aggett, Mario Samperi, Sadegh Ghaderzadeh, Andreas Weilhard, Luke T. Norman, Isla E. Gow, Yifan Chen, Giuseppe Bonura, Catia Cannilla, Elena Besley, David J. Morgan, Thomas J. A. Slater, Andrei N. Khlobystov, Jesum Alves Fernandes* and Graham J. Hutchings*

22565




### Surface chemistry regulation of conductive two-dimensional nanosheets with highly pseudocapacitive covalent groups for a high-performance flexible asymmetric microsupercapacitor

Yuanming Wang,* Jinlong Wu, Jiayue Dong, Xiaoxu Xu, Huan Song, Libei Yuan, Xiaolong Li* and Zhaoqing Lu*

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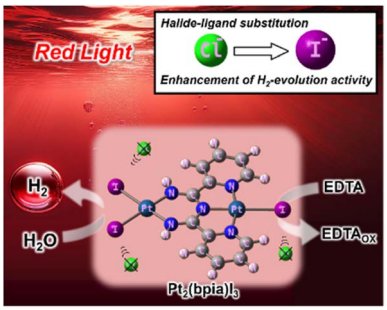
## EDGE ARTICLES

22580

**Enhanced red-light-driven hydrogen evolution by a diplatinum photocatalyst by the larger wavefunction leakage of iodide coordinated to the platinum center**

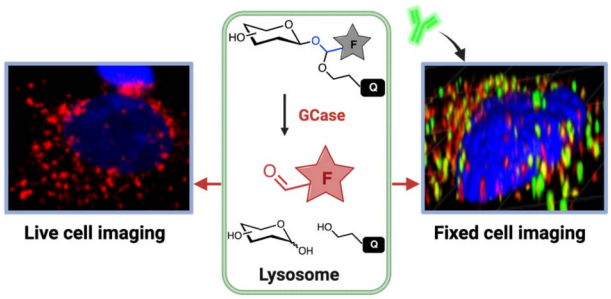
Toma Kunikubo, Raúl Castañeda, Muralee Murugesu, Jaclyn L. Brusso, Kosei Yamauchi, Hironobu Ozawa* and Ken Sakai*




22588

**A proto-aldehyde fluorescence quenched substrate for quantitative imaging of both protein and enzyme activity within cells**

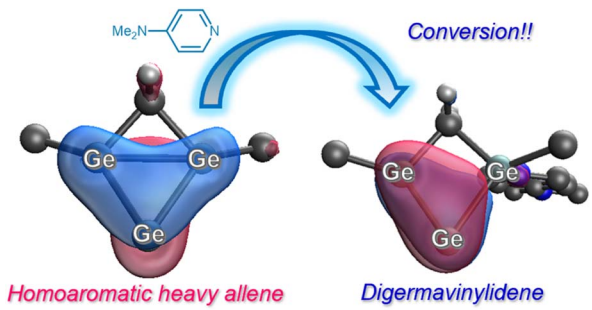
Sha Zhu, Matthew C. Deen, Samy Cecioni, Kim Lam Wong, Evan Perley-Roberston, Weifeng Benny Wu and David J. Vocadlo*




22597

**A neutral homoaromatic heavy allene as a platform for selective conversion to a germylene-coordinated digermavinylidene**

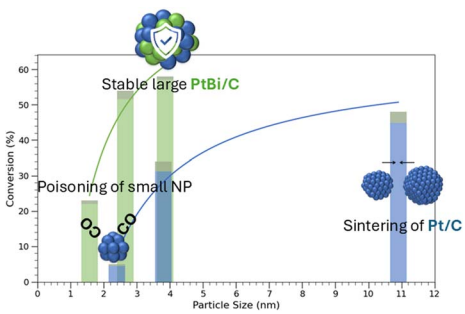
Daichi Uchida, Hiroko Yamada and Yoshiyuki Mizuhata*




22603

**Selective aerobic oxidation of alcohols with supported Pt nanoparticles: effect of particle size and bismuth promotion**

Anna Giorgia Nobile, Enzo Brack, Milivoj Plodinec and Christophe Copéret*



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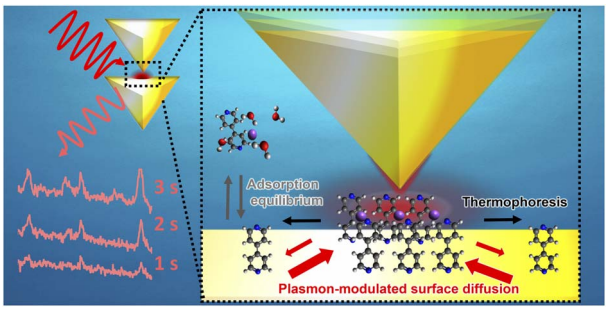
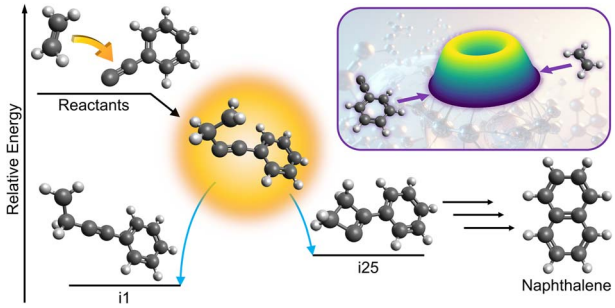
22611




**Formation of distinct condensed molecular phases at solid–liquid interfaces by plasmon-driven molecular trapping under ambient conditions**

Nobuaki Oyamada, Hiro Minamimoto and Kei Murakoshi*

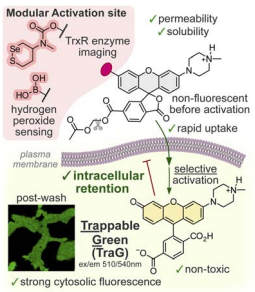
22621




**Gas-phase synthesis of naphthalene through an unconventional thermal alkyne–alkene [2 + 2] cycloaddition mechanism**

Shane J. Goettl, Iakov A. Medvedkov, Anatoliy A. Nikolayev, Chao He, Zhenghai Yang, Alexander M. Mebel,* Ankit Somani, Adrian Portela-Gonzalez, Wolfram Sander* and Ralf I. Kaiser*

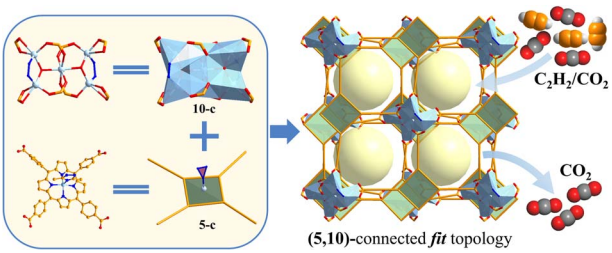
22630




**A modular scaffold for cellularly-retained fluorogenic probes for sensitive cell-resolved bioactivity imaging**

Philipp Mauker, Lucas Dessen-Weissenhorn, Carmen Zecha, Nynke A. Vepřek, Julia I. Brandmeier, Daniela Beckmann, Annabel Kitowski, Tobias Kernmayr, Julia Thorn-Seshold, Martin Kerschensteiner and Oliver Thorn-Seshold*

22638




**Precision pore engineering *via* fit-topology assembly in a Zn-porphyrin MOF for selective $C_2H_2$ capture**

Zhenliang Zhu, Jianfei Xiao, Min Zhang, Yaoqi Huang* and Shaojun Yuan*



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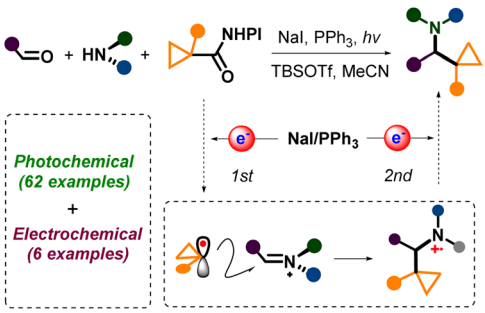
## EDGE ARTICLES

22647

**Photogenerated-radical cyclopropylation of *in situ* generated iminiums mediated by NaI/PPh$_3$: direct access to α-cyclopropyl tertiary alkylamines**

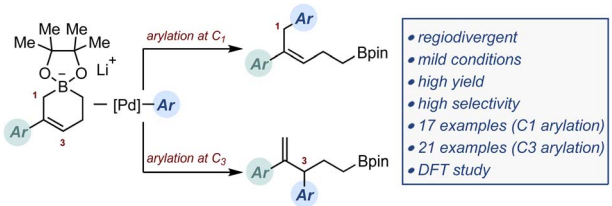
Ying Zhou, Shan Wang, Yi-Chuan Liu, Yan Liu, Fei Tan, Hongbo Dong and Jian Wang*




22656

**Pd-catalyzed regiodivergent arylation of cyclic allylboronates**

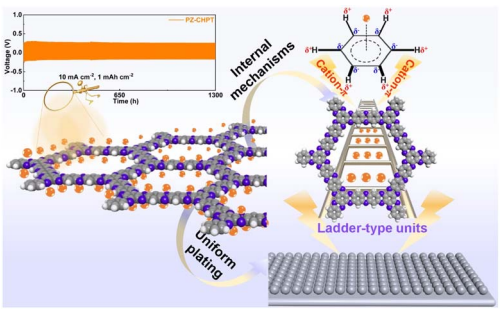
Cheng Zhang, Baptiste Leforestier, Céline Besnard and Clément Mazet*




22666

**Ladder-type phenazine-linked covalent organic polymers with synergistic cation–π interactions for highly stable lithium metal batteries**

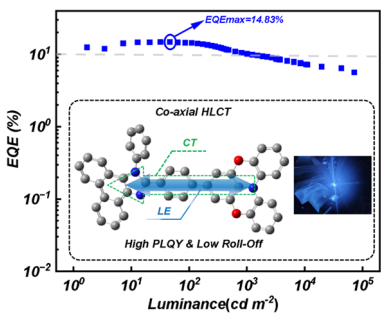
Xiao-Meng Lu, Haichao Wang, Yiwen Sun, Yi Xu, Yang Wu, Weiwei Sun, Chao Yang, Yifan Zhang and Yong Wang*




22679

**Realizing highly efficient electrofluorescence through a co-axial hybrid local and charge-transfer (HLCT) excited state**

Kuo Yu, Yingbo Lv, Yilong Li, Zirui Wang, Shi-Tong Zhang,* Jinbei Wei,* Shanfeng Xue,* Chenguang Wang and Bing Yang



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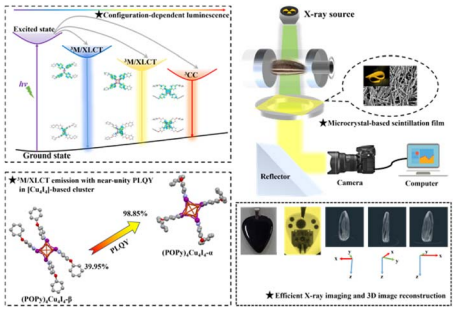
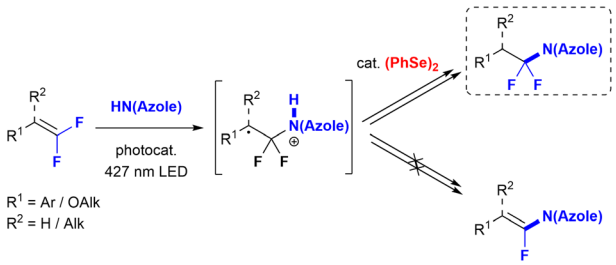
22690




## Regulating charge transfer of copper(I) coordination compounds *via* conformation engineering for highly efficient radioluminescence and 3D X-ray imaging

Yongkang Zhu, Yongjing Deng, Qianxi Li, Ning Ding, Yulong Wang, Mengzhu Wang, Kenneth Yin Zhang, Shujuan Liu* and Qiang Zhao*

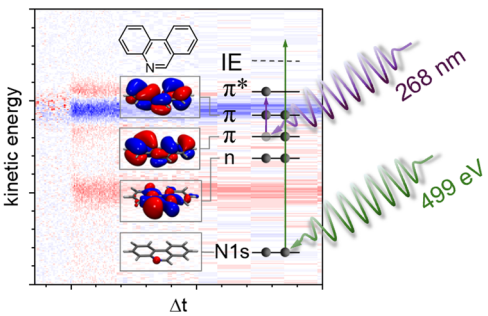
22701




## Diselenide-enabled photocatalytic hydroazolation of *gem*-difluoroalkenes

Mohammed K. Abd El-Gaber, Ryan M. Herrick, Pranaya Sudhakar, Ashutosh Rana, Brent A. Roach, Jeffrey E. Dick and Ryan A. Altman*

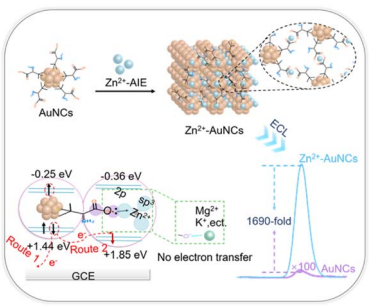
22711




## Time-resolved X-ray spectroscopy of phenanthridine: elucidating the photodynamics of a nitrogen-containing polycyclic aromatic hydrocarbon

Dorothee Schaffner, Kira Diemer, Xincheng Miao, Emil Karaev, Marco Flock, Katharina Theil, Constant Schouder, Audrey Scognamiglio, Lou Barreau, Lionel Poisson, Dennis Mayer, Andre Al Haddad, Antoine Sarracini, Gregor Knopp, Xinhua Xie, Patrick Hemberger, Kirsten Schnorr, Roland Mitric* and Ingo Fischer*

22723




## 1690-Fold enhanced electrochemiluminescence of gold nanoclusters *via* $Zn^{2+}$ induced aggregation

Yujiao Wang, Xuwen Gao, Qinqing Zhang, Xiaoxuan Ren and Guizheng Zou*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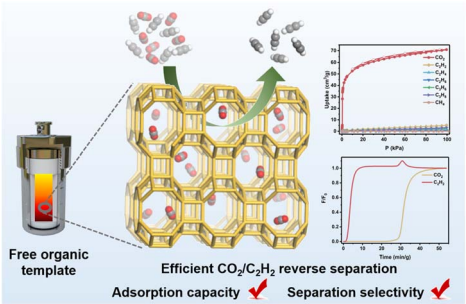
## EDGE ARTICLES

22732

**A cation gating–breathing synergetic mechanism in K-MER-2.0 zeolite enables unprecedented selective $CO_2$ separation from hydrocarbon gas streams**

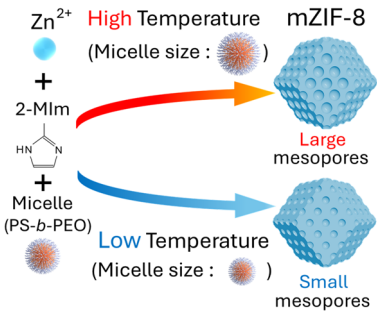
Renhao Li, Chenxu Liu, Wenli Bao, Lin Li, Jingfeng Han, Xiaoxin Zou, Xiaowei Song,* Donghai Mei* and Zhiqiang Liang*




22742

**Gradient mesoporosity in hierarchical ZIF-8 by temperature-modulated soft-templating**

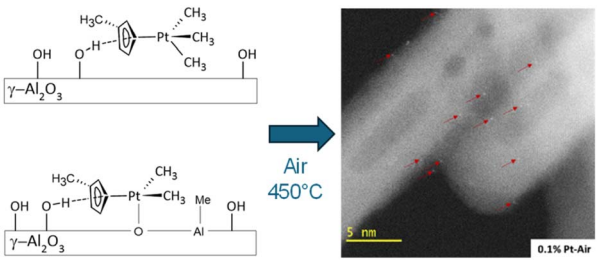
Keisuke Shirasaki, Yingji Zhao,* Norman C.-R. Chen, Xiangyang Liu, Yusuke Asakura, Kevin C.-W. Wu and Yusuke Yamauchi*




22748

**Tuning cluster size down to single atoms on Pt/γ-$Al_2O_3$ catalysts *via* surface organometallic chemistry**

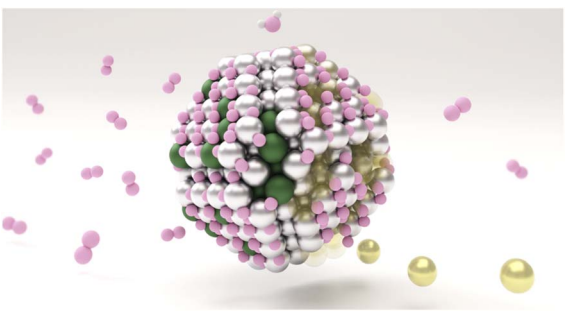
Martin Cotoni, Mickaël Rivallan,* Isabelle Clémençon, Virgile Rouchon, Anne-Lise Taleb, Julie Poulizac, Amandine Cabiac, Christophe Bouchy, Christophe Copéret* and Céline Chizallet*




22757

**Effect of metal substitution on the intrinsic activity of iridium-based oxides for the oxygen evolution reaction**

Yinghao Xu, Yi-Hsuan Wu, Paula M. Abdala, Connor Sherwin, Veronica Celorrio, Diana Piankova, Payal Chaudhary, Vitaly Alexandrov, Agnieszka Kierzkowska, Denis A. Kuznetsov* and Christoph R. Müller*



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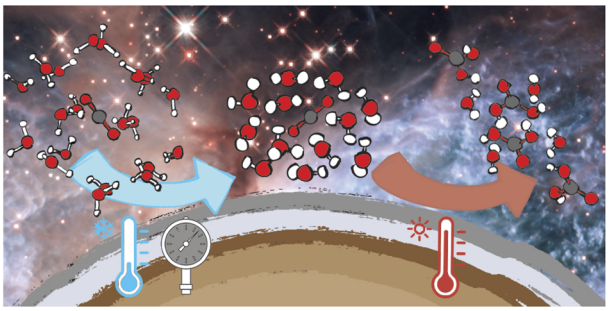

## Understanding the formation mechanism of crystalline hydrated polymorphs of carbonic acid from $CO_2$ clathrate hydrate

Selene Berni, Demetrio Scelta,* Sebastiano Romi, Samuele Fanetti, Frederico Alabarse, Bjorn Wehinger and Roberto Bini*

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