

# Chemical Science

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## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 14(40) 10983–11284 (2023)



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**Inside cover**  
See Tsung-Che Chang, Katsunori Tanaka *et al.*, pp. 11033–11039. Image reproduced by permission of Katsunori Tanaka from *Chem. Sci.*, 2023, **14**, 11033.

## COMMENTARY

10994

### A focus on computer vision for non-contact monitoring of catalyst degradation and product formation kinetics

Niklaas J. Buurma and Scott W. Bagley

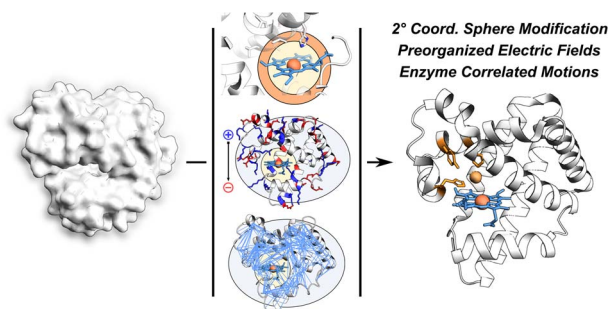


## PERSPECTIVE

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### From random to rational: improving enzyme design through electric fields, second coordination sphere interactions, and conformational dynamics

Shobhit S. Chaturvedi, Daniel Bim, Christo Z. Christov and Anastassia N. Alexandrova\*



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Chemical Science (electronic: ISSN 2041-6539) is published 48 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK.

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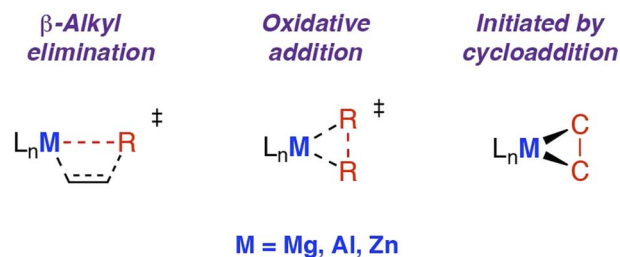


## REVIEW

11012

## Carbon–carbon bond activation by Mg, Al, and Zn complexes

Joseph M. Parr and Mark R. Crimmin\*

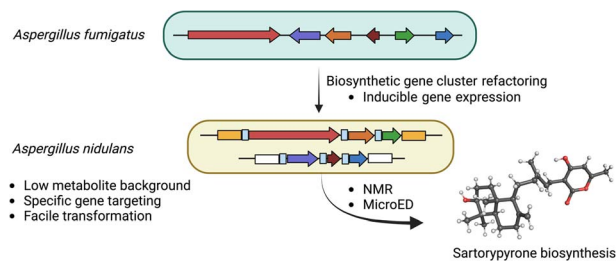


## EDGE ARTICLES

11022

A heterologous expression platform in *Aspergillus nidulans* for the elucidation of cryptic secondary metabolism biosynthetic gene clusters: discovery of the *Aspergillus fumigatus* sartorypyrone biosynthetic pathway

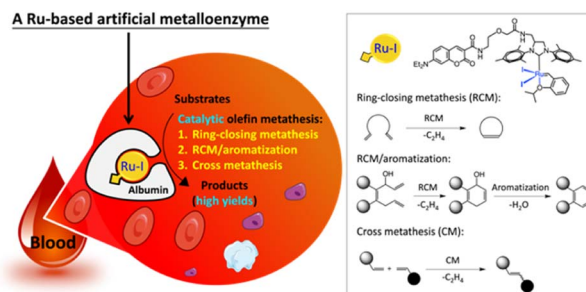
Shu-Yi Lin, C. Elizabeth Oakley, Cory B. Jenkinson, Yi-Ming Chiang, Ching-Kuo Lee, Christopher G. Jones, Paul M. Seidler, Hosea M. Nelson, Richard B. Todd, Clay C. Wang\* and Berl R. Oakley\*



11033

## Catalytic olefin metathesis in blood

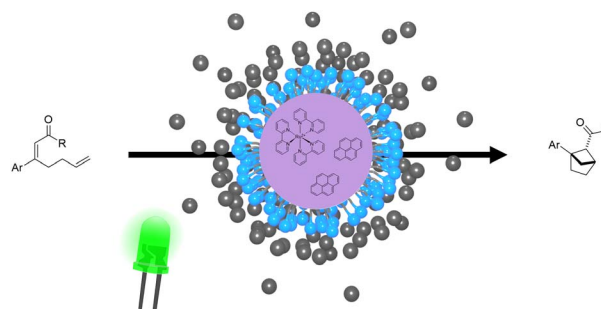
Igor Nasibullin, Hiromasa Yoshioka, Akari Mukaimine, Akiko Nakamura, Yuriko Kusakari, Tsung-Che Chang\* and Katsunori Tanaka\*



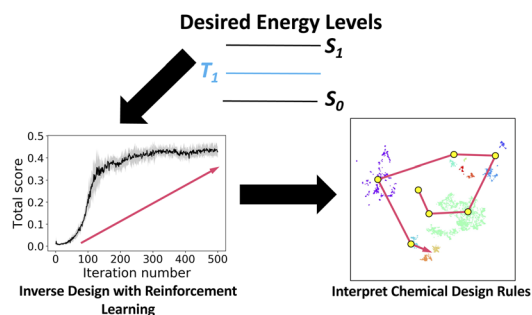
11040

## Photocyclization by a triplet–triplet annihilation upconversion pair in water – avoiding UV-light and oxygen removal

R. Jeyaseelan, M. Utikal, C. G. Daniliuc and L. Næsberg\*



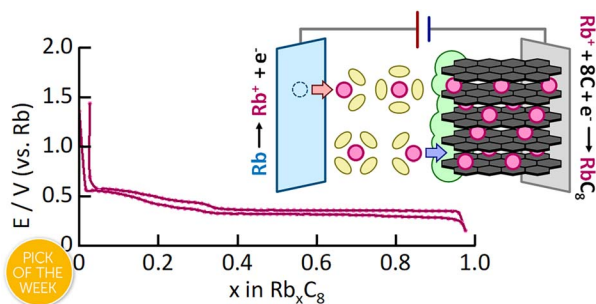
11045



### Generative organic electronic molecular design informed by quantum chemistry

Cheng-Han Li and Daniel P. Tabor\*

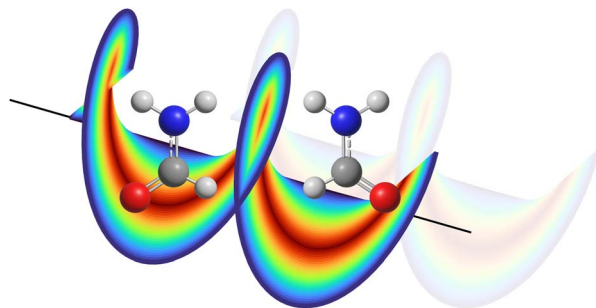
11056



### Electrochemical intercalation of rubidium into graphite, hard carbon, and soft carbon

Daisuke Igarashi, Ryoichi Tatara, Ryusei Fujimoto, Tomooki Hosaka and Shinichi Komaba\*

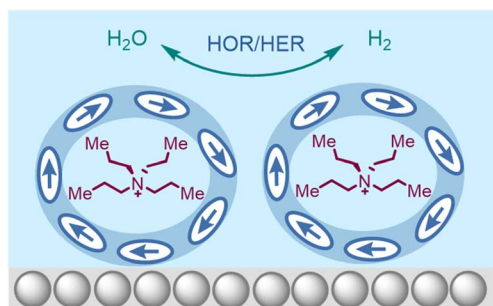
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### Time-resolved enantiomer-exchange probed by using the orbital angular momentum of X-ray light

Xiang Jiang,\* Yeonsig Nam, J r my R. Rouxel, Haiwang Yong and Shaul Mukamel\*

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### Action at a distance: organic cation induced long range organization of interfacial water enhances hydrogen evolution and oxidation kinetics

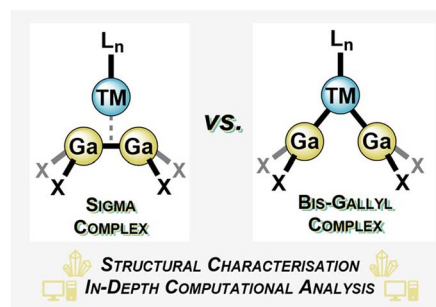
Kaiyue Zhao, Hao Yu, Haocheng Xiong, Qi Lu, Yi Qin Gao and Bingjun Xu\*



11088

### On the $\sigma$ -complex character of bis(gallyl)/digallane transition metal species

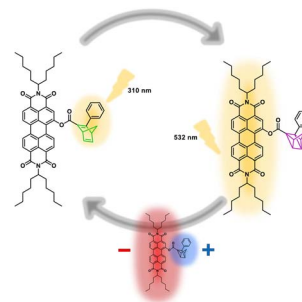
Till L. Kalkuhl, Lei Qin, Lili Zhao,\* Gernot Frenking\* and Terrance J. Hadlington\*



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### Driving the quadricyclane-to-norbornadiene isomerization by charge separation with perylenediimide as electron acceptor

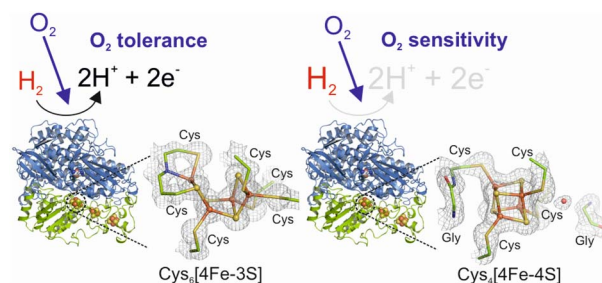
Wiebke Zika, Andreas Leng, René Weiß, Simone Pintér, Christoph M. Schüßlbauer, Timothy Clark, Andreas Hirsch and Dirk M. Guldi\*



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### Stepwise conversion of the Cys<sub>6</sub>[4Fe–3S] to a Cys<sub>4</sub>[4Fe–4S] cluster and its impact on the oxygen tolerance of [NiFe]-hydrogenase

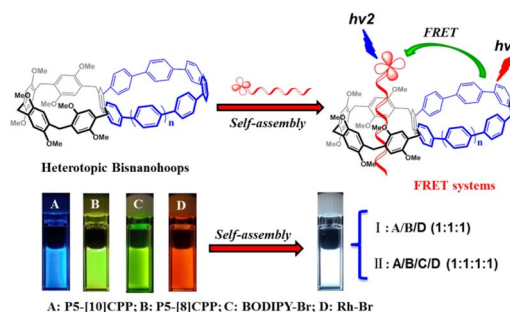
Andrea Schmidt, Jacqueline Kalms, Christian Lorent, Sagie Katz, Stefan Frielingsdorf, Rhiannon M. Evans, Johannes Fritsch, Elisabeth Siebert, Christian Teutloff, Fraser A. Armstrong, Ingo Zebger,\* Oliver Lenz\* and Patrick Scheerer\*



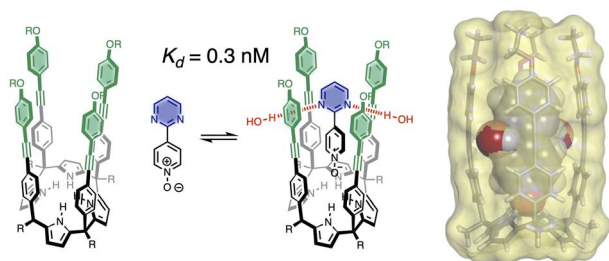
11121

### Efficient manipulation of Förster resonance energy transfer through host–guest interaction enables tunable white-light emission and devices in heterotopic bisnanohoops

Yanqing Fan, Shimin Fan, Lin Liu, Shengzhu Guo, Jing He, Xiaonan Li, Zhe Lian, Weijie Guo, Xuebo Chen, Ying Wang and Hua Jiang\*

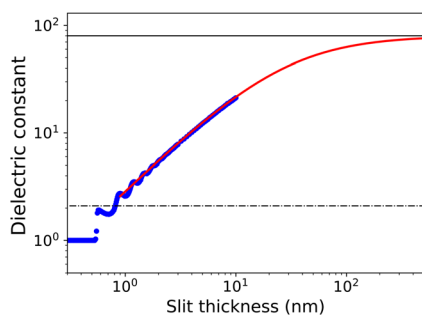


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**Aromatic interactions with heterocycles in water**

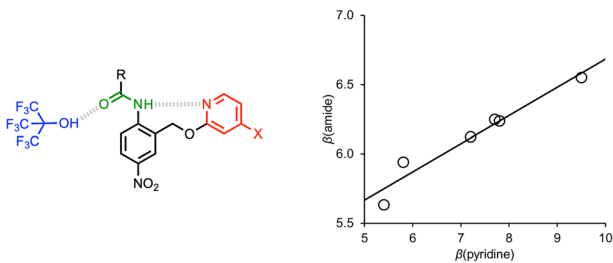
Gloria Tobajas-Curiel, Qingqing Sun, Jeremy K. M. Sanders, Pablo Ballester\* and Christopher A. Hunter\*

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**Dielectric response of confined water films from a classical density functional theory perspective**

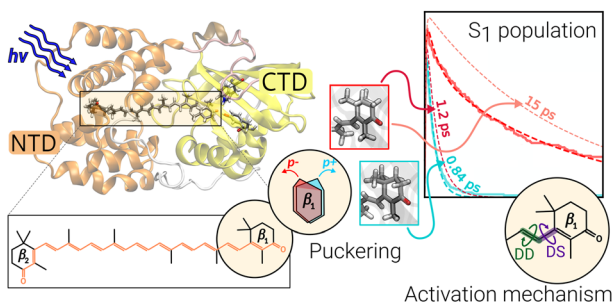
Daniel Borgis,\* Damien Laage, Luc Belloni and Guillaume Jeanmairet

11151

**Polarisation effects on the H-bond acceptor properties of secondary amides**

Fergal E. Hanna, Alexander J. Root and Christopher A. Hunter\*

11158

**How orange carotenoid protein controls the excited state dynamics of canthaxanthin**

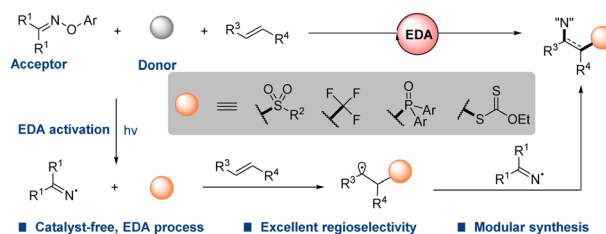
Amanda Arcidiacono, Davide Accomasso, Lorenzo Cupellini and Benedetta Mennucci\*



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### Photo-induced imino functionalizations of alkenes *via* intermolecular charge transfer

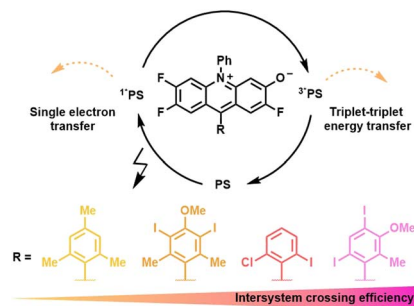
Xiang-Xin Zhang, Hao Zheng, Yong-Kang Mei, Yan Liu, Ying-Ying Liu, Ding-Wei Ji, Boshun Wan and Qing-An Chen\*



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### Isoacridone dyes with parallel reactivity from both singlet and triplet excited states for biphotonic catalysis and upconversion

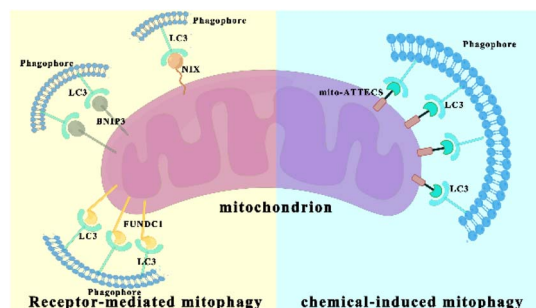
Björn Pfund, Valeriia Hutskalova, Christof Sparr\* and Oliver S. Wenger\*



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### Targeting mitochondrial degradation by chimeric autophagy-tethering compounds

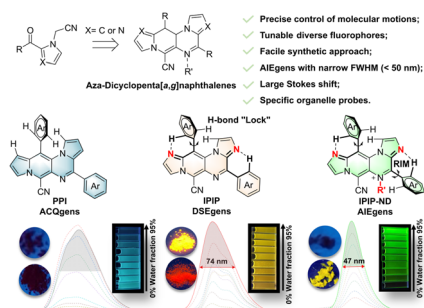
Zhenqi Liu, Geng Qin, Jie Yang, Wenjie Wang, Wenting Zhang, Boxun Lu,\* Jinsong Ren and Xiaogang Qu\*



11203

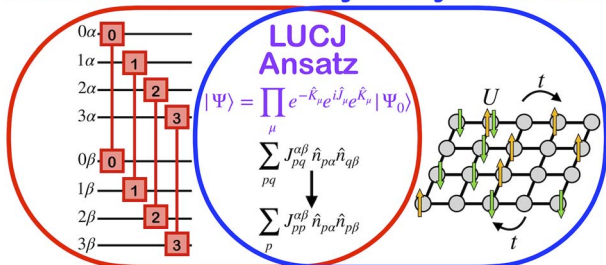
### Aza-dicyclopenta[*a,g*]naphthalenes: controllable seesaw-like emissive behavior and narrowband AIEgens

Jinbiao Li, Jiaxin Lao and Hongbin Zou\*



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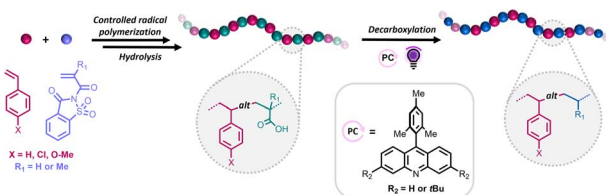
### Hardware-efficient Physically-motivated



### Bridging physical intuition and hardware efficiency for correlated electronic states: the local unitary cluster Jastrow ansatz for electronic structure

Mario Motta,\* Kevin J. Sung, K. Birgitta Whaley, Martin Head-Gordon and James Shee\*

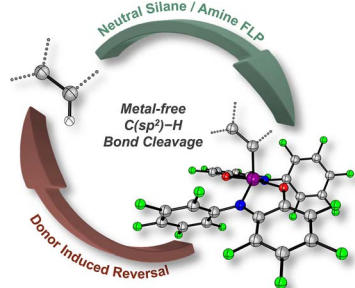
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### Alternating styrene-propylene and styrene-ethylene copolymers prepared by photocatalytic decarboxylation

Emmanuelle Schuë, Dillon R. L. Rickertsen, Angie B. Korpusik, Alafate Adili, Daniel Seidel\* and Brent S. Sumerlin\*

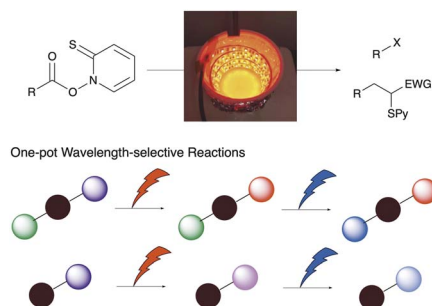
11237



### Reversible C–H bond silylation with a neutral silicon Lewis acid

Thaddäus Thorwart and Lutz Greb\*

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### Red-light-mediated Barton decarboxylation reaction and one-pot wavelength-selective transformations

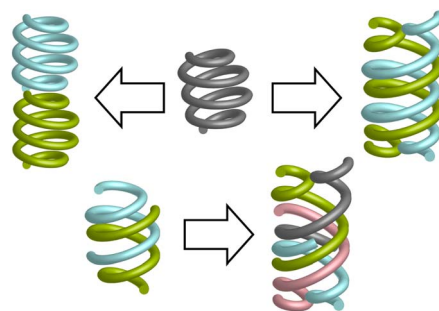
Hiroki Yamamoto, Kohei Yamaoka, Ann Shinohara, Kouhei Shibata, Ken-ichi Takao\* and Akihiro Ogura\*



11251

### Controlling aromatic helix dimerization in water by tuning charge repulsions

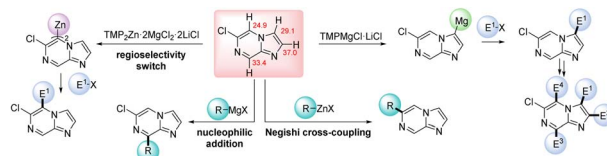
Binhao Teng, Pradeep K. Mandal, Lars Allmendinger, Céline Douat, Yann Ferrand and Ivan Huc\*



11261

### Calculation-assisted regioselective functionalization of the imidazo[1,2-a]pyrazine scaffold via zinc and magnesium organometallic intermediates

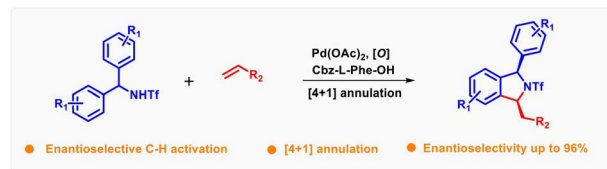
Agonist Kastrati, Alexander Kremsmair, Alisa S. Sunagatullina, Vasilii Korotenko, Yusuf C. Guersoy, Saroj K. Rout, Fabio Lima, Cara E. Brocklehurst, Konstantin Karaghiosoff, Hendrik Zipse\* and Paul Knochel\*



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### A palladium catalyzed asymmetric desymmetrization approach to enantioenriched 1,3-disubstituted isoindolines

Dattatraya H. Dethe,\* Vimlesh Kumar and Manmohan Shukla



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### Water-soluble polyphosphonate-based bottlebrush copolymers via aqueous ring-opening metathesis polymerization

Diego A. Resendiz-Lara, Suna Azhdari, Hubert Gojzewski, Andre H. Gröschel and Frederik R. Wurm\*

