

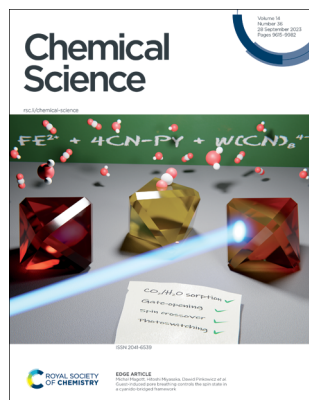
# Chemical Science

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## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 14(36) 9615–9982 (2023)



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### Inside cover

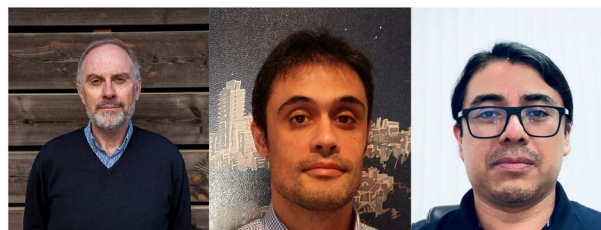
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Miquel Solà\*, Israel Fernández\* and Gabriel Merino\*

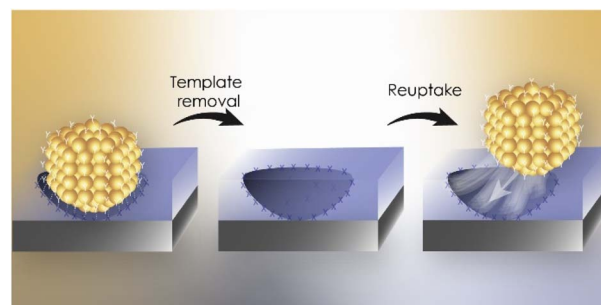


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Din Zelikovich, Linoy Dery, Hila Sagi-Cohen and Daniel Mandler\*



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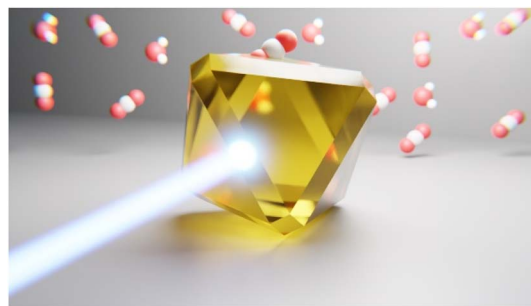
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### Guest-induced pore breathing controls the spin state in a cyanido-bridged framework

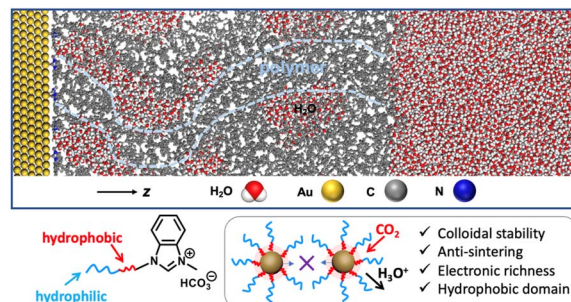
Michał Magott,\* Klaudia Płonka, Barbara Sieklucka, Katarzyna Dziedzic-Kocurek, Wataru Kosaka, Hitoshi Miyasaka\* and Dawid Pinkowicz\*



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### Why surface hydrophobicity promotes CO<sub>2</sub> electroreduction: a case study of hydrophobic polymer *N*-heterocyclic carbenes

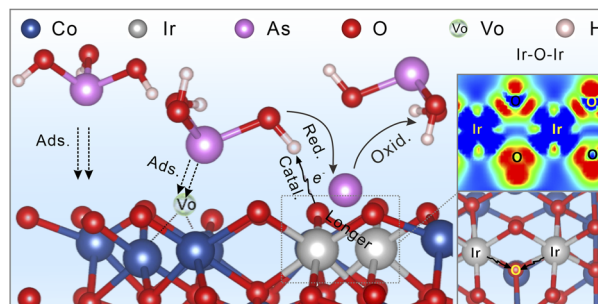
Qiang Luo, Hanyi Duan, Michael C. McLaughlin, Kecheng Wei, Joseph Tapia, Joseph A. Adewuyi, Seth Shuster, Maham Liaqat, Steven L. Suib, Gaël Ung, Peng Bai,\* Shouheng Sun\* and Jie He\*



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### Modulating paired Ir–O–Ir via electronic perturbations of correlated Ir single atoms to overcome catalytic selectivity

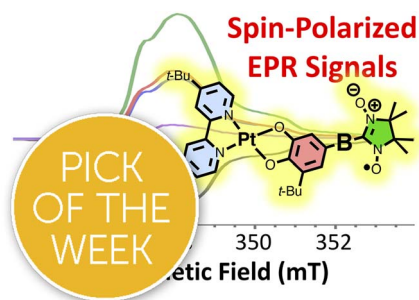
Shi-Hua Chen, Yuan-Fan Yang, Zong-Yin Song, Xiang-Yu Xiao, Cong-Cong Huang, Xin Cai, Pei-Hua Li, Meng Yang, Aicheng Chen, Wen-Qing Liu\* and Xing-Jiu Huang\*



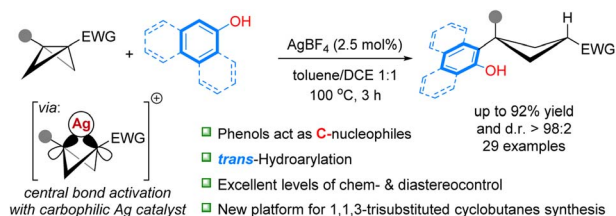
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### Competitive reversed quartet mechanisms for photogenerated ground state electron spin polarization

Martin L. Kirk,\* David A. Shultz,\* Patrick Hewitt, Anil Reddy Marri and Art van der Est\*



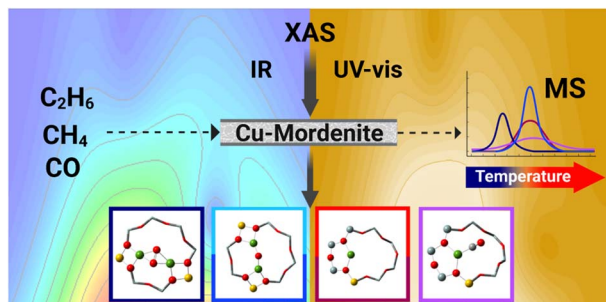
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### C(sp<sup>2</sup>)-H cyclobutylation of hydroxyarenes enabled by silver- $\pi$ -acid catalysis: diastereocontrolled synthesis of 1,3-difunctionalized cyclobutanes

Lei Tang, Qi-Nan Huang, Feng Wu, Yuanjiu Xiao, Jin-Lan Zhou, Tong-Tong Xu, Wen-Biao Wu,\* Shuanglin Qu\* and Jian-Jun Feng\*

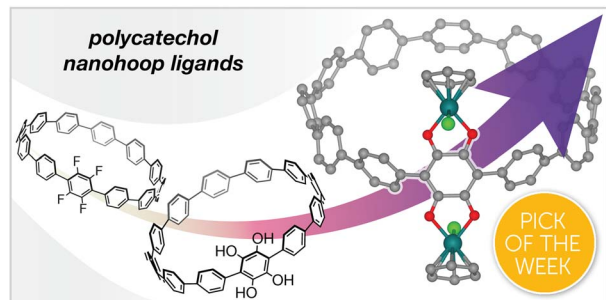
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### Understanding C-H activation in light alkanes over Cu-MOR zeolites by coupling advanced spectroscopy and temperature-programmed reduction experiments

Karoline Kvande, Beatrice Garetto, Gabriele Deplano, Matteo Signorile, Bjørn Gading Solemsli, Sebastian Proding, Unni Olsbye, Pablo Beato, Silvia Bordiga, Stian Svelle\* and Elisa Borfecchia\*

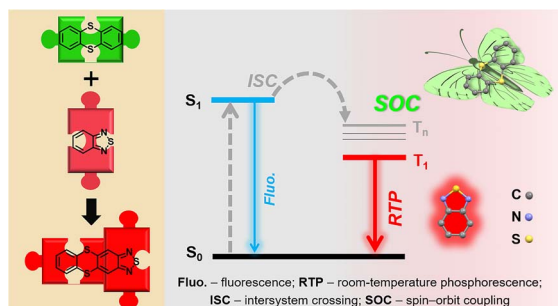
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### Synthesis and metalation of polycatechol nano hoops derived from fluorocycloparaphenylenes

Ashlyn A. Kamin, Tara D. Clayton, Claire E. Otteson, Paige M. Gannon, Sebastian Krajewski, Werner Kaminsky, Ramesh Jasti and Dianne J. Xiao\*

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### A functional unit combination strategy for enhancing red room-temperature phosphorescence

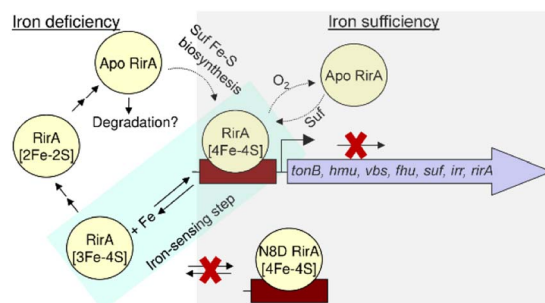
Shuaiqiang Zhao, Zhiqiang Yang, Xiangyu Zhang, Haichao Liu,\* Yingbo Lv, Shiyin Wang, Zhongzhao Yang, Shi-Tong Zhang and Bing Yang\*



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### Stabilisation of the RirA [4Fe–4S] cluster results in loss of iron-sensing function

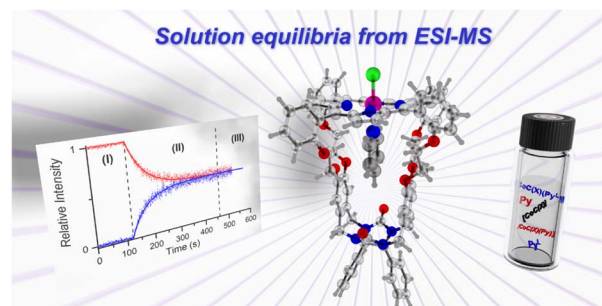
Elizabeth Gray, Melissa Y. Y. Stewart, Libby Hanwell, Jason C. Crack, Rebecca Devine, Clare E. M. Stevenson, Anne Volbeda, Andrew W. B. Johnston, Juan C. Fontecilla-Camps, Matthew I. Hutchings, Jonathan D. Todd and Nick E. Le Brun\*



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### Kinetics of ligand exchange in solution: a quantitative mass spectrometry approach

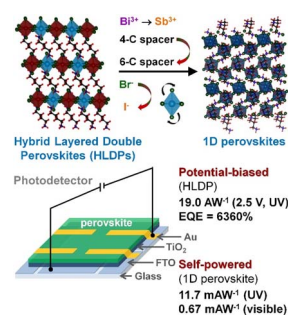
Quentin Duez,\* Paul Tinnemans, Johannes A. A. W. Elemans and Jana Roithová\*



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### Transition from Dion–Jacobson hybrid layered double perovskites to 1D perovskites for ultraviolet to visible photodetection

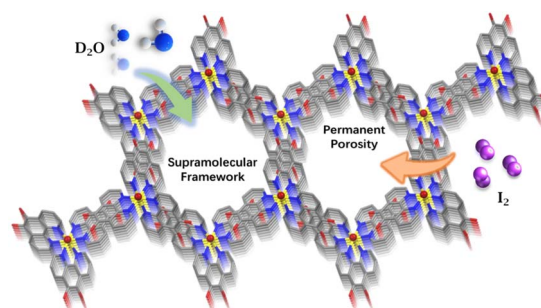
Arnab Mandal, Shresth Gupta, Supriti Dutta, Swapan K. Pati and Sayan Bhattacharyya\*



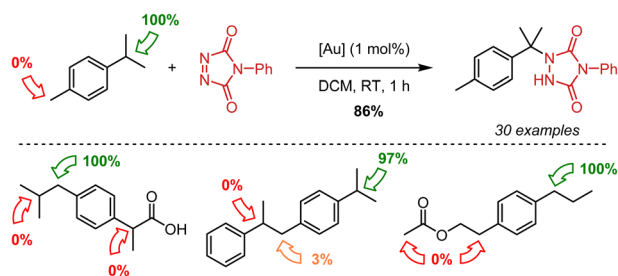
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### Modular metallotecton for engineering permanently porous frameworks: supernumerary role of ancillary ion

Deepak Gupta, Géraldine Chanteux, Gulshan Kumar, Koen Robeyns and Alexandru Vlad\*



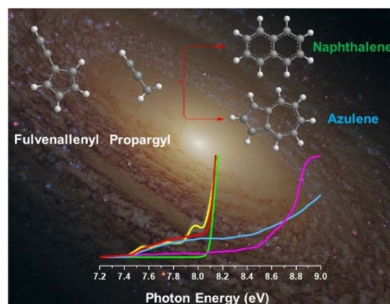
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### Site selective gold(I)-catalysed benzylic C–H amination via an intermolecular hydride transfer to triazolinediones

Kevin Bevernaege, Nikolaos V. Tzouras, Albert Poater, Luigi Cavallo, Steven P. Nolan,\* Fady Nahra\* and Johan M. Winne\*

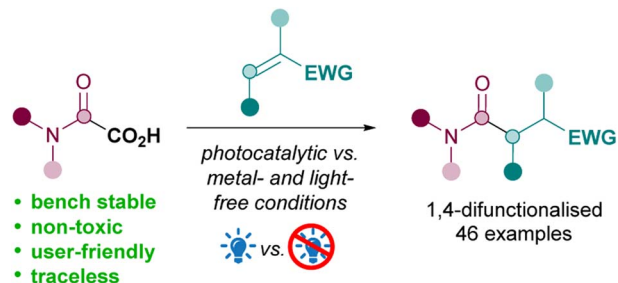
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Wang Li, Jiuzhong Yang, Long Zhao,\* David Couch, Myrsini San Marchi, Nils Hansen,\* Alexander N. Morozov, Alexander M. Mebel\* and Ralf I. Kaiser\*

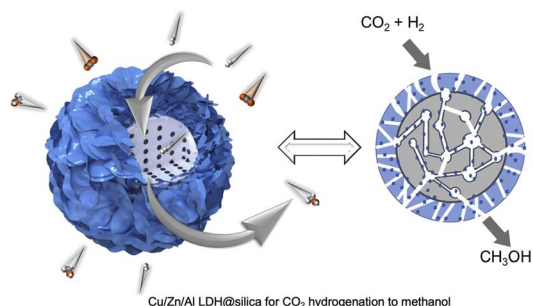
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### Direct decarboxylative Giese amidations: photocatalytic vs. metal- and light-free

David M. Kitcatt, Katie A. Scott, Elena Rongione, Simon Nicolle and Ai-Lan Lee\*

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### Core-shell silica@Cu<sub>x</sub>ZnAl LDH catalysts for efficient CO<sub>2</sub> hydrogenation to methanol

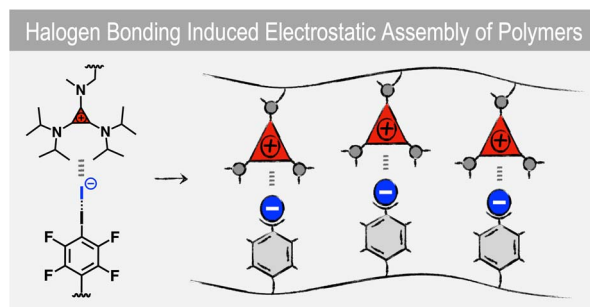
Meng Lyu, Jianwei Zheng, Claire Coulthard, Jing Ren, Yufei Zhao, Shik Chi Edman Tsang, Chunping Chen\* and Dermot O'Hare\*



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### Exploring the supramolecular chemistry of cyclopropeniums: halogen-bonding-induced electrostatic assembly of polymers

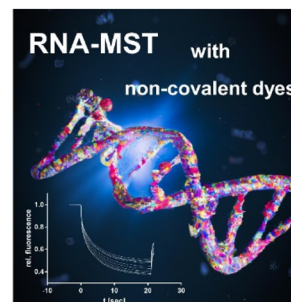
Shiwen Huang, Jianlin Zheng, Zihao Jiang, Jiaxiong Liu and Yiliu Liu\*



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### Non-covalent dyes in microscale thermophoresis for studying RNA ligand interactions and modifications

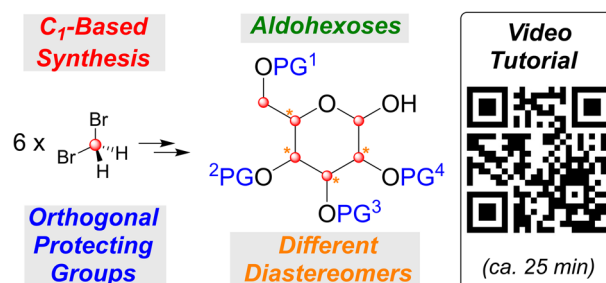
Elisabeth Kallert, Malte Behrendt, Ariane Frey, Christian Kersten and Fabian Barthels\*



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### A unified strategy for the synthesis of aldohexoses by boronate assisted assembly of $\text{CH}_2\text{X}_2$ derived $\text{C}_1$ -building blocks

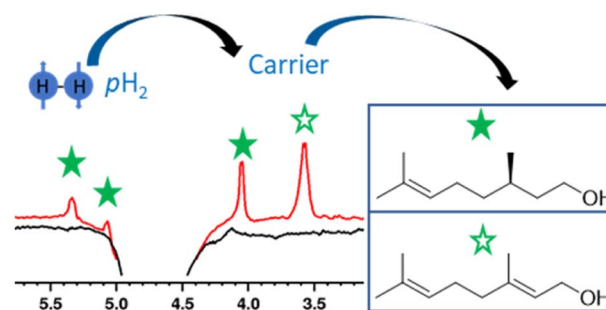
Sujenth Kirupakaran, Glib Arago and Christoph Hirschhäuser\*



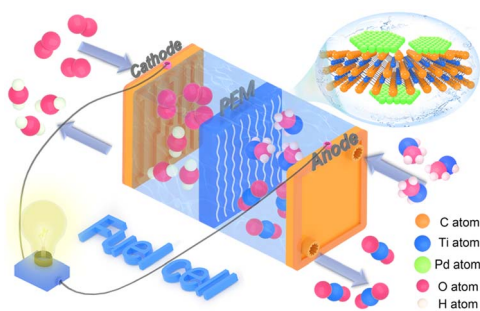
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### Enhancing the NMR signals of plant oil components using hyperpolarisation relayed *via* proton exchange

Adel Alshehri, Ben. J. Tickner, Wissam Iali and Simon B. Duckett\*



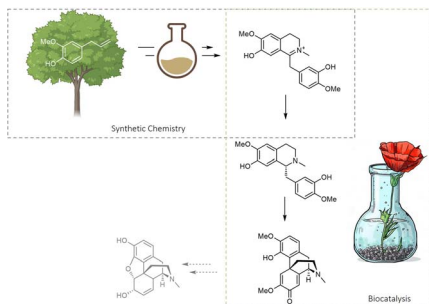
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### A 2D/2D heterojunction of ultrathin Pd nanosheet/MXene towards highly efficient methanol oxidation reaction: the significance of 2D material nanoarchitectonics

Huajie Huang, Di Xiao, Zihan Zhu, Chi Zhang, Lu Yang, Haiyan He, Jungmok You, Quanguo Jiang,\* Xingtao Xu\* and Yusuke Yamauchi\*

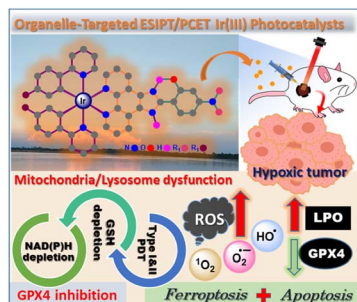
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### Concise synthesis of (*R*)-reticuline and (+)-salutaridin by combining early-stage organic synthesis and late-stage biocatalysis

Emmanuel Cigan, Jakob Pletz, Sarah A. Berger, Bettina Hierzberger, Michael Grilec-Zlamal, Alexander Steiner, Isabel Oroz-Guinea and Wolfgang Kroutil\*

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### Interrogating bioinspired ESIPT/PCET-based Ir(III)-complexes as organelle-targeted phototherapeutics: a redox-catalysis under hypoxia to evoke synergistic ferroptosis/apoptosis

Maniklal Shee, Dan Zhang, Moumita Banerjee, Samrat Roy, Bipul Pal, Anakuthil Anoop,\* Youyong Yuan\* and N. D. Pradeep Singh\*

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*ortho*-, *meta*-, and *polysubstituted* benzene bioisosteres  
new geometries outside aromatic chemical space

### Synthesis of polysubstituted bicyclo[2.1.1]hexanes enabling access to new chemical space

Marius Reinhold, Justin Steinebach, Christopher Golz and Johannes C. L. Walker\*

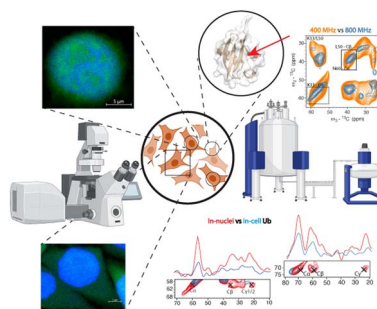




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## A high-field cellular DNP-supported solid-state NMR approach to study proteins with sub-cellular specificity

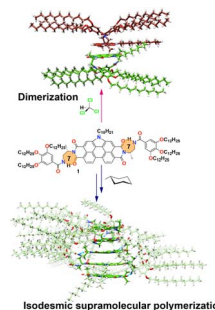
David Beriashvili, Ru Yao, Francesca D'Amico, Michaela Krafčiková, Andrei Gurinov, Adil Safeer, Xinyi Cai, Monique P. C. Mulder, Yangping Liu, Gert E. Folkers and Marc Baldus\*



9900

## Solvent-dependent self-assembly of *N*-annulated perylene diimides. From dimers to supramolecular polymers

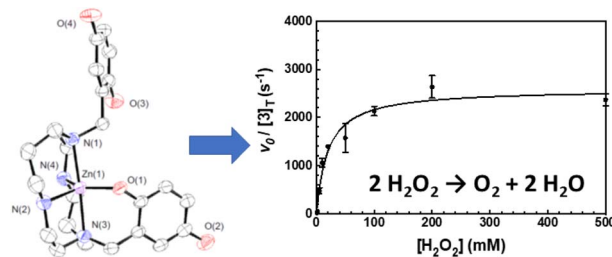
Cristina Naranjo, Azahara Doncel-Giménez, Rafael Gómez, Juan Aragón,\* Enrique Orti\* and Luis Sánchez\*



9910

## A macrocyclic quinol-containing ligand enables high catalase activity even with a redox-inactive metal at the expense of the ability to mimic superoxide dismutase

Sana Karbalaei, Alicja Franke, Julian Oppelt, Tarfi Aziz, Aubree Jordan, P. Raj Pokkuluri, Dean D. Schwartz, Ivana Ivanović-Burmazović\* and Christian R. Goldsmith\*

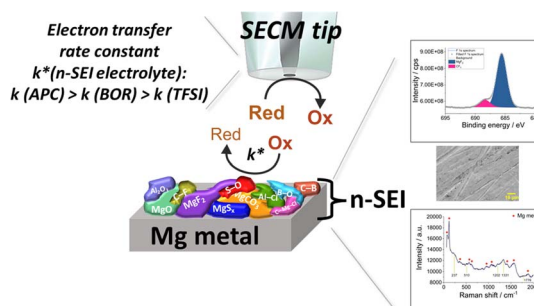


Rapid catalase activity without redox-active metals

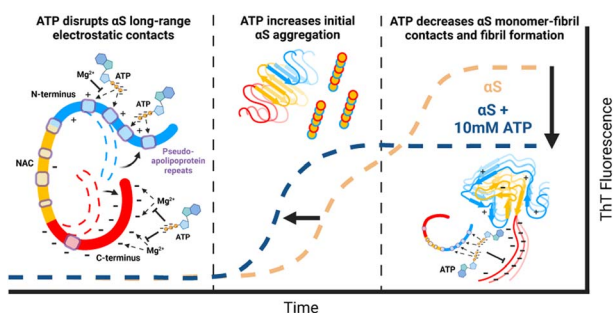
9923

## Unveiling the electronic properties of native solid electrolyte interphase layers on Mg metal electrodes using local electrochemistry

Carla Santana Santos, Martina Romio, Yuri Surace, Nicolas Eshraghi, Marco Amores, Andreas Mautner, Christiane Groher, Marcus Jahn, Edgar Ventosa and Wolfgang Schuhmann\*



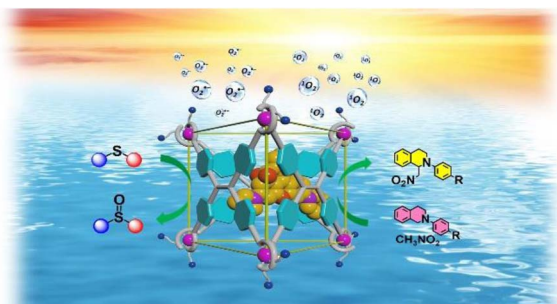
9933



### Toward a molecular mechanism for the interaction of ATP with alpha-synuclein

Evelyn Rose Kamski-Hennekam, Jinfeng Huang, Rashik Ahmed and Giuseppe Melacini\*

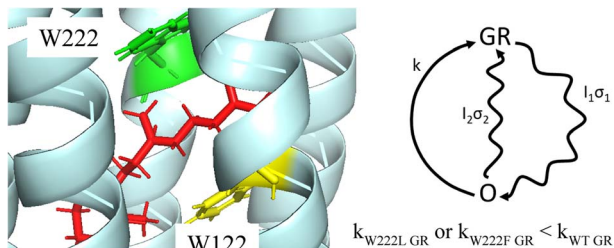
9943



### An artificial light-harvesting system constructed from a water-soluble metal–organic barrel for photocatalytic aerobic reactions in aqueous media

Danyang Li, Linlin Yang, Wangjian Fang, Xinmei Fu, Hechuan Li, Jianxu Li, Xuezhao Li and Cheng He\*

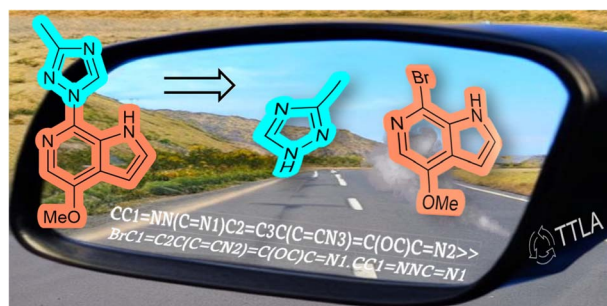
9951



### Impact of protein–chromophore interaction on the retinal excited state and photocycle of *Gloeobacter* rhodopsin: role of conserved tryptophan residues

Ramprasad Misra, Ishita Das, András Dér, Gábor Steinbach, Jin-gon Shim, Wayne Busse, Kwang-Hwan Jung, László Zimányi\* and Mordechai Sheves\*

9959



### Multistep retrosynthesis combining a disconnection aware triple transformer loop with a route penalty score guided tree search

David Kreutter and Jean-Louis Reymond\*



## EDGE ARTICLES

9970

**Continuous addition kinetic elucidation: catalyst and reactant order, rate constant, and poisoning from a single experiment**

Peter J. H. Williams, Charles Killeen, Ian C. Chagunda, Brett Henderson, Sofia Donnecke, Wil Munro, Jaspreet Sidhu, Denaisha Kraft, David A. Harrington\* and J. Scott McIndoe\*



## CORRECTIONS

9978

**Correction: Self-healing mixed matrix membranes containing metal–organic frameworks**

Prantik Mondal and Seth M. Cohen\*

9980

**Correction: Peptide epitope-imprinted polymer microarrays for selective protein recognition. Application for SARS-CoV-2 RBD protein**

Zsófia Bognár, Eszter Supala, Aysu Yarman, Xiaorong Zhang, Frank F. Bier, Frieder W. Scheller and Róbert E. Gyurcsányi\*

