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# Chemical Science

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## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 14(47) 13589–13990 (2023)

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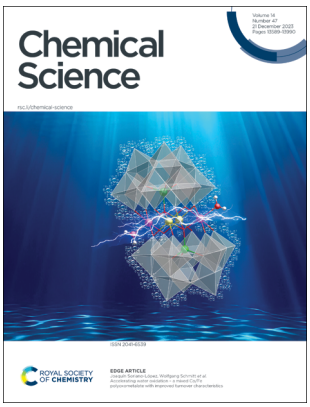


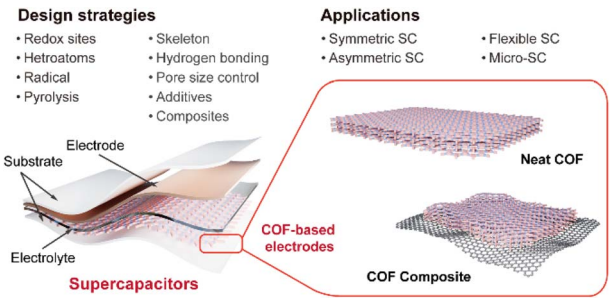

**Inside cover**
See Joaquín Soriano-López, Wolfgang Schmitt et al., pp. 13722–13733. Image reproduced by permission of Joaquín Soriano-López and Juan José Mufanó from *Chem. Sci.*, 2023, **14**, 13722.

## REVIEWS

13601

**Recent advances in the utilization of covalent organic frameworks (COFs) as electrode materials for supercapacitors**

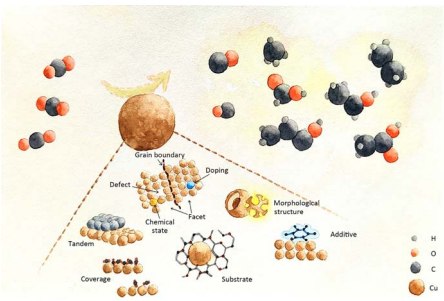
Shen Xu, Jinghang Wu, Xiang Wang and Qichun Zhang*




13629

**Cu-based catalyst designs in $CO_2$ electroreduction: precise modulation of reaction intermediates for high-value chemical generation**

Liangyiqun Xie, Yujing Jiang, Wenlei Zhu, Shichao Ding, Yang Zhou* and Jun-Jie Zhu*



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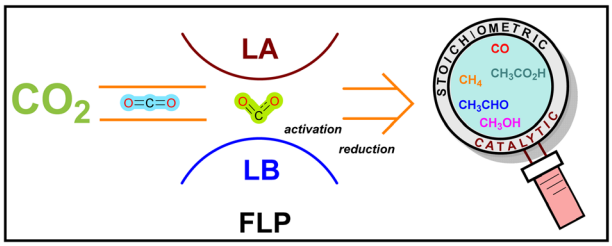
## REVIEWS

13661

**Advances in $CO_2$ activation by frustrated Lewis pairs: from stoichiometric to catalytic reactions**

Md. Nasim Khan, Yara van Ingen, Tribani Boruah, Adam McLauchlan, Thomas Wirth* and Rebecca L. Melen*

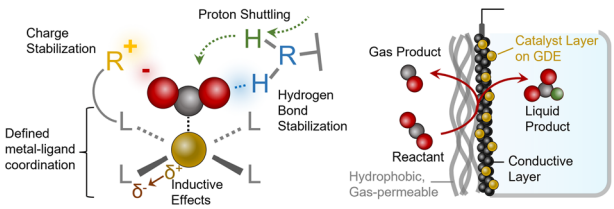



## PERSPECTIVE

13696

**Electrocatalysis with molecules and molecular assemblies within gas diffusion electrodes**

Hossein Bemana, Morgan McKee and Nikolay Kornienko*

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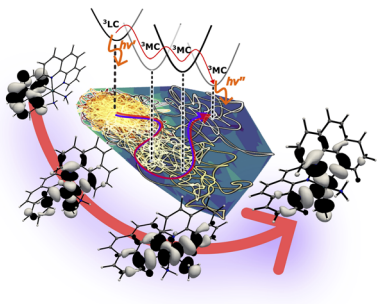
13713

**Ligand-centered to metal-centered activation of a Rh(III) photosensitizer revealed by *ab initio* molecular dynamics simulations**

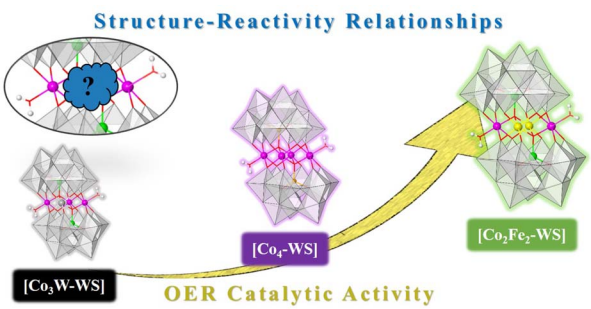
Iria Bolaño Losada and Petter Persson*



13722

**Accelerating water oxidation – a mixed Co/Fe polyoxometalate with improved turnover characteristics**

Joaquín Soriano-López,* Friedrich W. Steuber, Muhamed Mulahmetović, Maria Besora, Juan Modesto Clemente-Juan, Mariah O'Doherty, Nian-Yong Zhu, Craig L. Hill, Eugenio Coronado, Josep M. Poblet and Wolfgang Schmitt*



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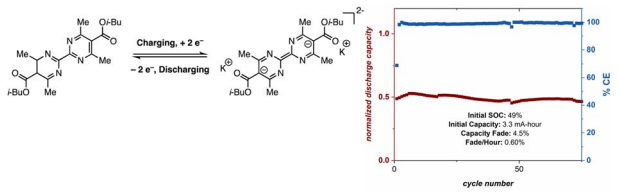
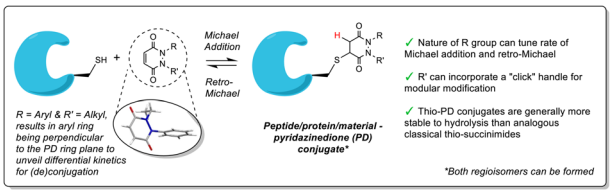



### Data science enabled discovery of a highly soluble 2,2′-bipyrimidine anolyte for application in a flow battery

Adam R. Pancoast, Sara L. McCormack, Shelby Galinat, Ryan Walser-Kuntz, Brianna M. Jett, Melanie S. Sanford and Matthew S. Sigman*

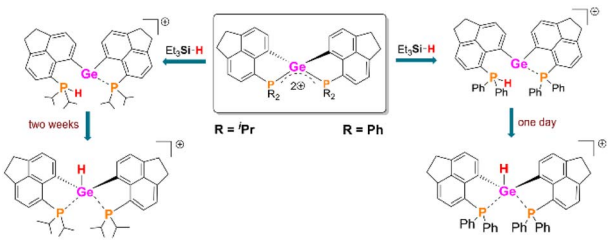
13743




### Use of pyridazinediones for tuneable and reversible covalent cysteine modification applied to peptides, proteins and hydrogels

Léa N. C. Rochet, Calise Bahou, Jonathan P. Wojciechowski, Ilias Koutsopetras, Phyllida Britton, Richard J. Spears, Ioanna A. Thanasi, Baihao Shao, Lisha Zhong, Dejan-Krešimir Bučar, Abil E. Aliev, Michael J. Porter, Molly M. Stevens, James R. Baker* and Vijay Chudasama*

13755




### Intramolecular donor-stabilized tetra-coordinated germanium(IV) di-cations and their Lewis acidic properties

Balakrishna Peddi, Souvik Khan, Rajesh G. Gonnade, Cem B. Yildiz* and Moumita Majumdar*

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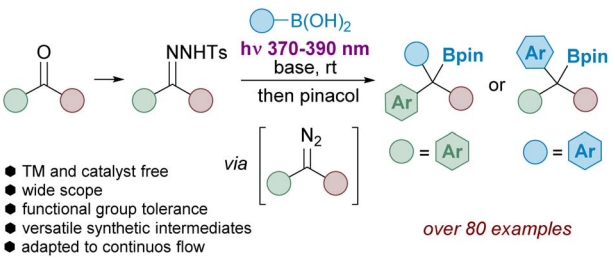


### Synthesis of substituted benzylboronates by light promoted homologation of boronic acids with *N*-sulfonylhydrazones

Álvaro Valdés-Maqueda, Lucía López, Manuel Plaza* and Carlos Valdés*


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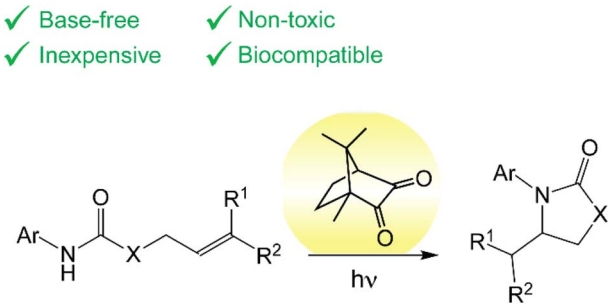
13776

**Chemoselective bond activation by unidirectional and asynchronous PCET using ketone photoredox catalysts**

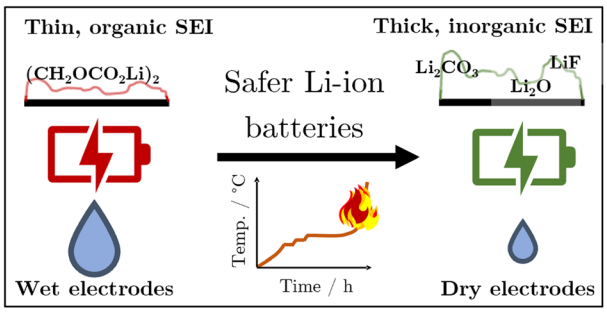
Rui Sun, Serge Ruccolo, Daniel L. Nascimento, Yangzhong Qin, Nathaniel Hibbert and Daniel G. Nocera*




13783

**Impact of electrolyte impurities and SEI composition on battery safety**

Florian Baakes, Daniel Witt and Ulrike Krewer*

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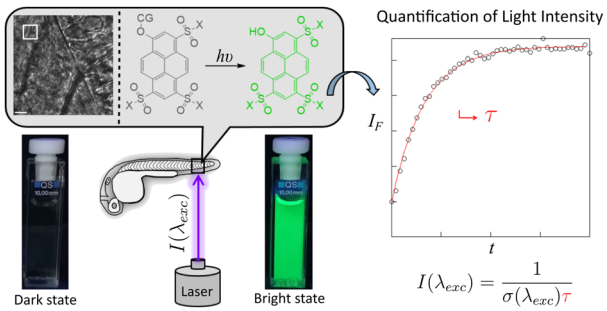
**A series of caged fluorophores for calibrating light intensity**

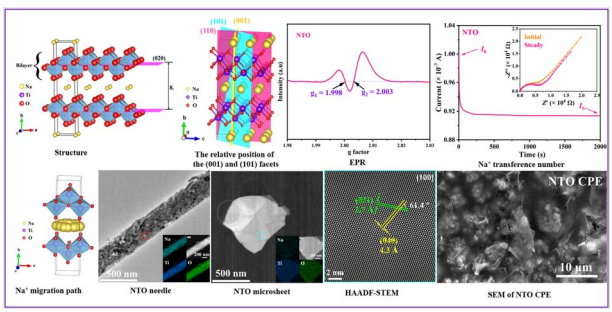
Mrinal Mandal, Hessam Sepasi Tehrani, Qianhua Mai, Emma Simon, Marie-Aude Plamont, Christine Rampon, Sophie Vriz, Isabelle Aujard,* Thomas Le Saux* and Ludovic Jullien*




13812

**Layered sodium titanate with a matched lattice: a single ion conductor in a solid-state sodium metal battery**

Xuanao Ma, Yang Liu, Yunhuai Zhang and Yun Gong*



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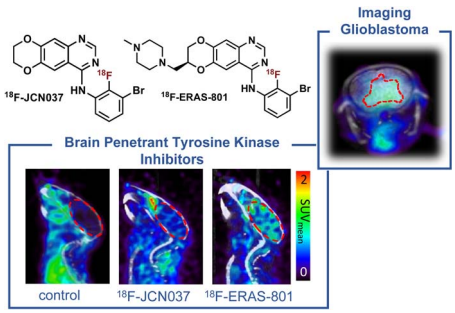


**$^{18}$F-Labeled brain-penetrant EGFR tyrosine kinase inhibitors for PET imaging of glioblastoma**

Maruthi Kumar Narayanam, Jonathan E. Tsang, Shili Xu, David A. Nathanson and Jennifer M. Murphy*

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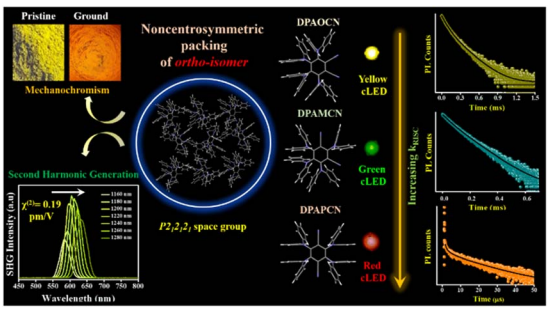


**Engineering TADF, mechanochromism, and second harmonic up-conversion properties in regioisomeric substitution space**

Abhijit Chatterjee, Joy Chatterjee, Subrahmanyam Sappati, Riteeka Tanwar, Madan D. Ambhore, Habibul Arfin, Rintu M. Umesh, Mayurika Lahiri, Pankaj Mandal and Partha Hazra*

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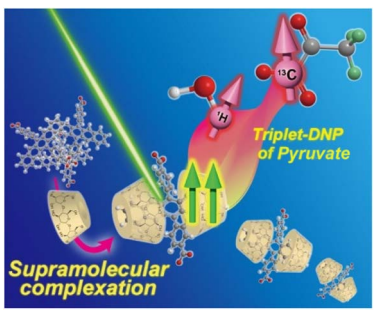
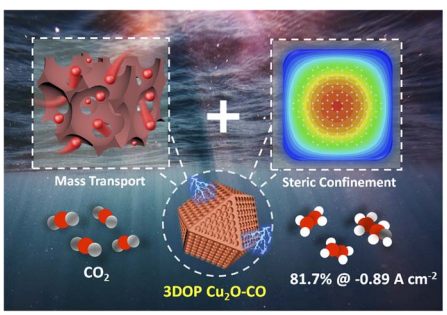



**Triplet dynamic nuclear polarization of pyruvate *via* supramolecular chemistry**

Tomoyuki Hamachi, Koki Nishimura, Keita Sakamoto, Yusuke Kawashima, Hironori Kouno, Shunsuke Sato, Go Watanabe, Kenichiro Tateishi, Tomohiro Uesaka and Nobuhiro Yanai*

13851




**Evoking $C_{2+}$ production from electrochemical $CO_2$ reduction by the steric confinement effect of ordered porous $Cu_2O$**

Longlong Fan, Qinghong Geng, Lian Ma, Chengming Wang, Jun-Xuan Li, Wei Zhu, Ruiwen Shao, Wei Li, Xiao Feng, Yusuke Yamauchi, Cuiling Li* and Lei Jiang



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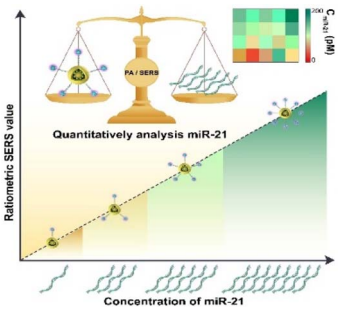
**Quantitative detection of microRNA-21 *in vivo* using *in situ* assembled photoacoustic and SERS nanoprobes**

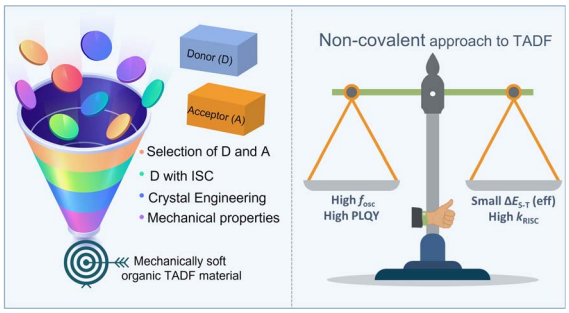
Liting Zheng, Qingqing Li, Ying Wu, Lichao Su, Wei Du, Jibin Song, Lanlan Chen* and Huanghao Yang*




13870

**Thermally activated delayed fluorescence in a mechanically soft charge-transfer complex: role of the locally excited state**

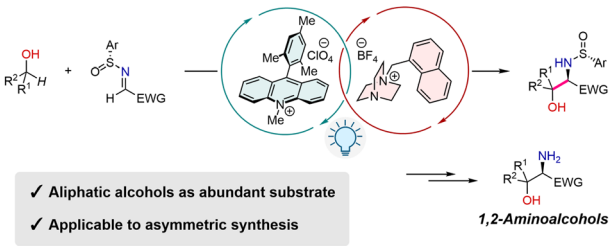
Kalyan Jyoti Kalita, Saikat Mondal, C. Malla Reddy* and Ratheesh K. Vijayaraghavan*




13879

**Facile synthesis of 1,2-aminoalcohols *via* α-C–H aminoalkylation of alcohols by photoinduced hydrogen-atom transfer catalysis**

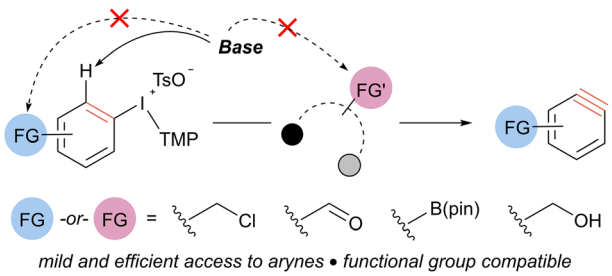
Joaquim Caner, Akira Matsumoto* and Keiji Maruoka*




13885

**An efficient and chemoselective method to generate arynes**

Bryan E. Metze, Riley A. Roberts, Aleksandra Nilova and David R. Stuart*



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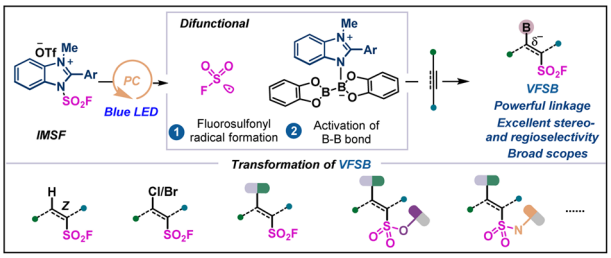
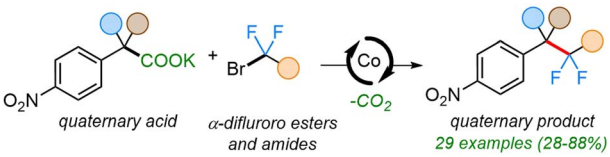
13893




## Photoredox-catalyzed stereo- and regioselective vicinal fluorosulfonyl-borylation of unsaturated hydrocarbons

Heyin Li, Mengjun Huang, Zhenlei Zou, Zhen Wang, Yifan Li, Chao Sun, Wangzhe Chen, Yi Pan, Weigang Zhang* and Yi Wang*

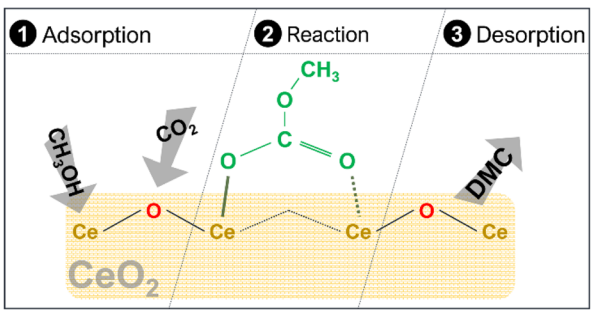
13902




## Cobalt-catalyzed decarboxylative difluoroalkylation of nitrophenylacetic acid salts

Ebbin Joseph, Ian Smith and Jon A. Tunge*

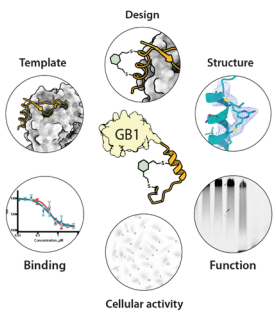
13908




## Dimethyl carbonate synthesis from $CO_2$ and methanol over $CeO_2$: elucidating the surface intermediates and oxygen vacancy-assisted reaction mechanism

Dragos Stoian, Toshiyuki Sugiyama, Atul Bansode, Francisco Medina, Wouter van Beek, Jun-ya Hasegawa, Akira Nakayama* and Atsushi Urakawa*

13915




## A recombinant approach for stapled peptide discovery yields inhibitors of the RAD51 recombinase

Teodors Pantelejevs,* Pedro Zuazua-Villar, Oliwia Koczy, Andrew J. Counsell, Stephen J. Walsh, Naomi S. Robertson, David R. Spring, Jessica A. Downs and Marko Hyvönen*

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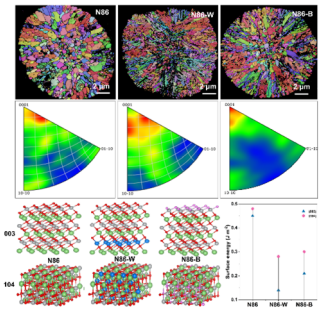
## EDGE ARTICLES

13924

**Manipulating the crystal plane angle within the primary particle arrangement for the radial ordered structure in a Ni-rich cathode**

Ting Chen, Chuyao Wen, Chen Wu, Lang Qiu, Zhenguo Wu,* Jiayang Li, Yanfang Zhu, Haoyu Li, Qingquan Kong, Yang Song, Fang Wan, Mingzhe Chen, Ismael Saadoune, Benhe Zhong, Shixue Dou, Yao Xiao* and Xiaodong Guo*



13934

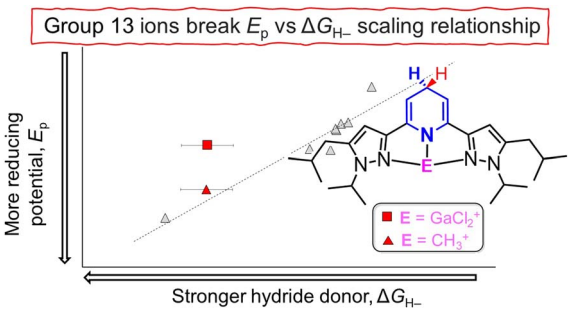
**Thermally activated delayed fluorescence in a deep red dinuclear iridium(III) complex: a hidden mechanism for short luminescence lifetimes**

Piotr Pander,* Andrey V. Zaytsev, Amit Sil, Glib V. Baryshnikov, Farhan Siddique, J. A. Gareth Williams,* Fernando B. Dias* and Valery N. Kozhevnikov*

13944

**Group 13 ion coordination to pyridyl breaks the reduction potential *vs.* hydricity scaling relationship for dihydropyridinates**

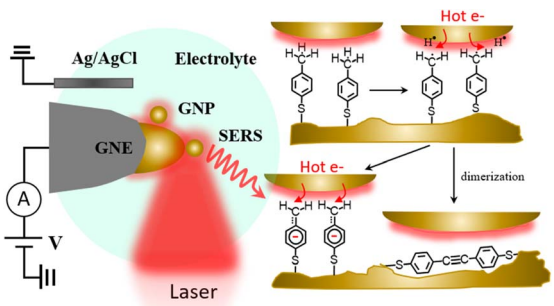
Leo W. T. Parsons, James C. Fettinger and Louise A. Berben*




13951

**Plasmon-mediated dehydrogenation of the aromatic methyl group and benzyl radical formation**

Jianghao Zhou, Jing Guo, Govinda Ghimire, Alexander M. Mebel, Shuai Chang* and Jin He*



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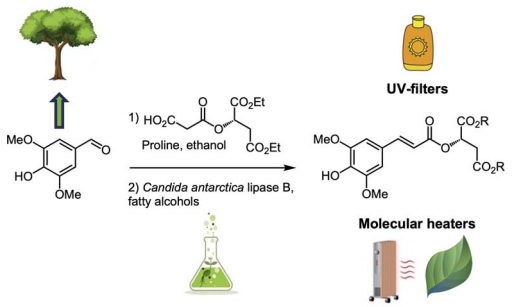
## EDGE ARTICLES

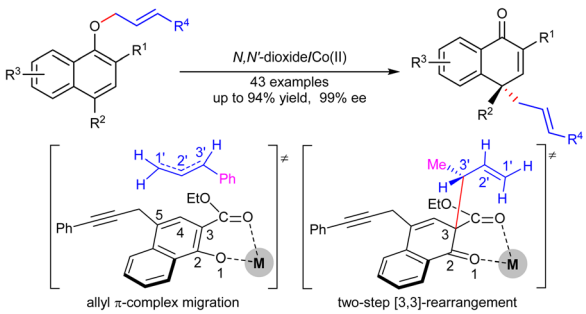
13962




### An expeditive and green chemo-enzymatic route to diester sinapoyl-L-malate analogues: sustainable bioinspired and biosourced UV filters and molecular heaters

Benjamin Rioux, Louis M. M. Mouterde, Jimmy Alarcan, Temitope T. Abiola, Matthias J. A. Vink, Jack M. Woolley, Aurélien A. M. Peru, Matthieu M. Mention, Fanny Brunissen, Giel Berden, Jos Oomens,* Albert Braeuning,* Vasilios G. Stavros* and Florent Allais*

13979




### Chiral cobalt(II) complex-promoted asymmetric *para*-Claisen rearrangement of allyl α-naphthol ethers

Hongkun Zeng, Lifeng Wang, Zhishan Su, Meijia Ying, Lili Lin* and Xiaoming Feng*

## CORRECTIONS

13986

### Correction: A non-sacrificial method for the quantification of poly(ethylene glycol) grafting density on gold nanoparticles for applications in nanomedicine

Jun Lu, Yao Xue, Rui Shi, Jing Kang, Chao-Yang Zhao, Ning-Ning Zhang, Chun-Yu Wang, Zhong-Yuan Lu* and Kun Liu*

13987

### Correction: The need for *operando* modelling of $^{27}$Al NMR in zeolites: the effect of temperature, topology and water

Chen Lei, Andreas Erlebach, Federico Brivio, Lukáš Grajciar, Zdeněk Tošner, Christopher J. Heard* and Petr Nachtigall

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