

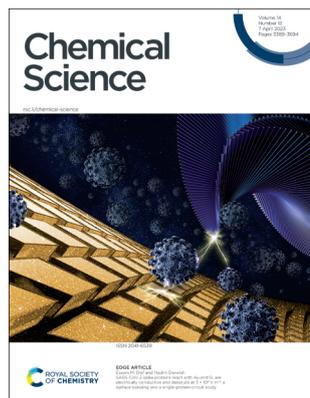
# Chemical Science

rsc.li/chemical-science

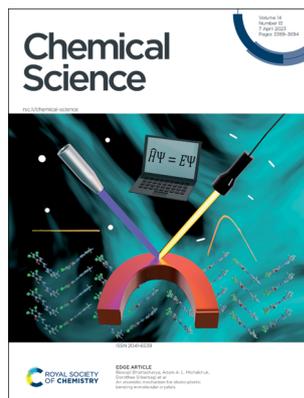
The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 14(13) 3389–3694 (2023)



**Cover**  
See Essam M. Dief and Nadim Darwish, pp. 3428–3440.  
Image reproduced by permission of Nadim Darwish from *Chem. Sci.*, 2023, 14, 3428.



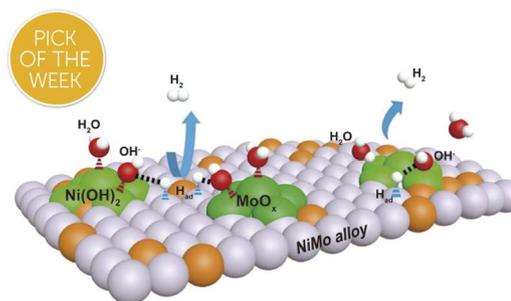
**Inside cover**  
See Biswajit Bhattacharya, Adam A. L. Michalchuk, Dorothee Silbernagl *et al.*, pp. 3441–3450. Image reproduced by permission of Biswajit Bhattacharya from *Chem. Sci.*, 2023, 14, 3441.

## PERSPECTIVES

3400

### Insights into alloy/oxide or hydroxide interfaces in Ni–Mo-based electrocatalysts for hydrogen evolution under alkaline conditions

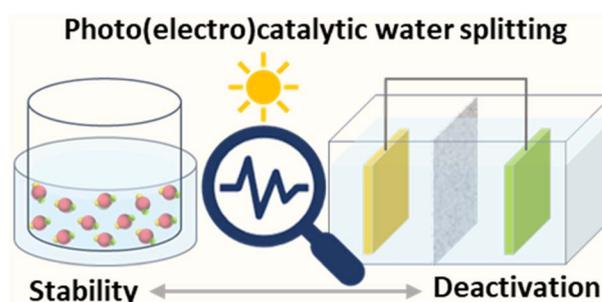
Min Luo, Jietian Yang, Xingang Li, Miharuru Eguchi, Yusuke Yamauchi and Zhong-Li Wang\*



3415

### Addressing the stability challenge of photo(electro)catalysts towards solar water splitting

Mu Xiao, Zhiliang Wang, Kazuhiko Maeda, Gang Liu and Lianzhou Wang\*



## Editorial Staff

### Executive Editor

May Copsy

### Deputy Editor

Samantha Apps

### Senior Editor

James Moore

### Scientific Editors

Ellis Crawford, Jingtao Huang, Esther Johnston, Sophie Orchard, Richard Thompson and Amy Welch

### Editorial Assistant

Karina Webster

### Publishing Assistant

David Bishop

For queries about submitted articles please contact James Moore, Senior Editor, in the first instance. E-mail [chemicalscience@rsc.org](mailto:chemicalscience@rsc.org)

For pre-submission queries please contact May Copsy, Executive Editor. E-mail [chemicalscience-rsc@rsc.org](mailto:chemicalscience-rsc@rsc.org)

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.

Chemical Science is a Gold Open Access journal and all articles from 2015 onwards are free to read.

Please email [orders@rsc.org](mailto:orders@rsc.org) to register your interest or contact Royal Society of Chemistry Order Department, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK

Tel +44 (0)1223 432398; E-mail [orders@rsc.org](mailto:orders@rsc.org)

Whilst this material has been produced with all due care, the Royal Society of Chemistry cannot be held responsible or liable for its accuracy and completeness, nor for any consequences arising from any errors or the use of the information contained in this publication. The publication of advertisements does not constitute any endorsement by the Royal Society of Chemistry or Authors of any products advertised. The views and opinions advanced by contributors do not necessarily reflect those of the Royal Society of Chemistry which shall not be liable for any resulting loss or damage arising as a result of reliance upon this material. The Royal Society of Chemistry is a charity, registered in England and Wales, Number 207890, and a company incorporated in England by Royal Charter (Registered No. RC000524), registered office: Burlington House, Piccadilly, London W1J 0BA, UK, Telephone: +44 (0) 207 4378 6556.

### Advertisement sales:

Tel +44 (0) 1223 432246; Fax +44 (0) 1223 426017; E-mail [advertising@rsc.org](mailto:advertising@rsc.org)

For marketing opportunities relating to this journal, contact [marketing@rsc.org](mailto:marketing@rsc.org)

# Chemical Science

[rsc.li/chemical-science](http://rsc.li/chemical-science)

## Editorial Board

### Editor-in-Chief

Andrew Cooper, University of Liverpool

### Associate Editors

Vincent Artero, CEA-Grenoble  
Luis M. Campos, Columbia University  
Michelle Chang, University of California, Berkeley  
Lin X. Chen, Northwestern University  
Graeme Day, University of Southampton  
Serena DeBeer, Max Planck Institute for Chemical Energy Conversion

Mircea Dincă, MIT

Vy Dong, University of California, Irvine  
François Gabbai, Texas A&M University  
Subi George, JNCASR  
Jinlong Gong, Tianjin University  
Stephen Goldup, University of Southampton  
Zaiping Guo, University of Adelaide  
Christopher A. Hunter, University of Cambridge  
Malika Jefferies-EL, Boston University  
Ning Jiao, Peking University  
Tanja Junkers, Monash University

Hemamala Karunadasa, Stanford University  
Maja Köhn, University of Freiburg  
Yi-Tao Long, Nanjing University  
Gabriel Merino, CINVESTAV Merida  
James K. McCusker, Michigan State University  
Thomas Meade, Northwestern University  
Paolo Melchiorre, University of Bologna  
Carsten Schultz, Oregon Health & Science University  
Dmitri Talapin, The University of Chicago  
Toshiharu Teranishi, Kyoto University  
Andrei Yudin, University of Toronto

## Advisory Board

Dave Adams, University of Glasgow  
Ayyappanpillai Ajayaghosh, NIIST  
Ulf-Peter Apfel, Ruhr-University Bochum  
Polly Arnold, University of California, Berkeley  
Xinhe Bao, Dalian Institute of Chemical Physics  
Zhenan Bao, Stanford University  
Gonçalo Bernardes, University of Cambridge  
Frank Biedermann, Karlsruhe Institute of Technology  
Donna Blackmond, Scripps Research Institute  
Jeffrey Bode, ETH Zurich  
Jennifer S. Brodbelt, University of Texas at Austin, USA  
Christopher Chang, University of California, Berkeley  
Chi-Ming Che, University of Hong Kong  
Jun Chen, Nankai University  
R. Graham Cooks, Purdue University  
Christophe Copéret, ETH Zurich  
Eugenio Coronado, University of Valencia  
Leroy Cronin, University of Glasgow  
James Crowley, University of Otago  
Christopher C. Cummins, Massachusetts Institute of Technology  
Ben Davis, University of Oxford  
Jillian Dempsey, University of North Carolina at Chapel Hill  
Kazunari Domen, University of Tokyo  
James Durrant, Imperial College London  
Xinlang Feng, TU Dresden  
Ben Feringa, University of Groningen  
Makoto Fujita, University of Tokyo  
Phillip Gale, University of Technology Sydney  
Song Gao, Peking University  
Jeremiah Gassensmith, University of Texas at Dallas  
Elizabeth Gibson, Newcastle University  
Ryan Gilmour, WWU Münster  
Hubert Girault, EPFL  
Frank Glorius, WWU Münster  
Leticia González, University of Vienna  
Duncan Graham, University of Strathclyde

Vicki Grassian, University of California, San Diego  
Alexis Grimaud, Boston College  
Christian Hackenberger, FMP Berlin  
Buxing Han, Chinese Academy of Sciences  
Christy Haynes, University of Minnesota  
Patrick Holland, Yale University  
Kim Jelfs, Imperial College London  
Yousung Jung, KAIST  
Stephanie Kath-Schorr, University of Cologne  
Takashi Kato, University of Tokyo  
Christopher Kelly, Janssen Research & Development  
Jérôme Lacour, University of Geneva  
Ai-Lan Lee, Heriot-Watt University  
Daniele Leonori, University of Manchester  
Chao-Jun Li, McGill University  
Yi Li, Jilin University  
R. Graham Cooks, KAIST  
Wenbin Lin, University of Chicago  
Kopin Liu, Academia Sinica  
Watson Loh, UNICAMP  
Bettina Lotsch, Max Planck Institute  
Xiong Wen (David) Lou, Nanyang Technological University  
Kazuhiko Maeda, Tokyo Institute of Technology  
Mi Hee Lim, KAIST  
Satoshi Maeda, Hokkaido University  
Swadhin Mandal, IISER Kolkata  
Ellen Matson, University of Rochester  
Scott Miller, Yale University  
Daniel Minciola, University of Pennsylvania  
Wonwoo Nam, Ewha Womans University  
Jonathan Nitschke, University of Cambridge  
Allie Obermeyer, Columbia University  
Martin Oestreich, Technical University of Berlin  
Takashi Ooi, Nagoya University  
Rachel O'Reilly, University of Birmingham  
Oleg Ozerov, Texas A&M University  
Xiulian Pan, Dalian Institute of Chemical Physics  
Nicolas Plummer, Technical University of

Munich  
Rasmita Raval, University of Liverpool  
Erwin Reisner, University of Cambridge  
Andrea Rentmeister, WWU Münster  
Jeffrey Rinehart, University of California, San Diego  
Stuart Rowan, University of Chicago  
Richmond Sarpong, University of California, Berkeley  
Danielle Schultz, Merck  
Dwight Seferos, University of Toronto  
Oliver Seitz, Humboldt University of Berlin  
Roberta Sessoli, University of Florence  
Kay Severin, Federal Polytechnic School of Lausanne  
Mikiko Sodeoka, RIKEN  
Galo Soler-Illia, Universidad Nacional de San Martín  
David Spring, University of Cambridge  
Brian Stoltz, California Institute of Technology  
Brent Sumerlin, University of Florida  
Raghavan B. Sunoj, IIT Bombay  
Yogesh Surendranath, MIT  
Mizuki Tada, Nagoya University  
Ben Zhong Tang, The Hong Kong University of Science and Technology  
Zhiyong Tang, National Center for Nanoscience and Nanotechnology  
Christine Thomas, Ohio State University  
He Tian, East China University of Science & Technology  
Zhong-Qun Tian, Xiamen University  
F. Dean Toste, University of California, Berkeley  
Takashi Uemura, University of Tokyo  
Jan van Hest, Radboud University  
Latha Venkataraman, Columbia University  
Chu Wang, Peking University  
Julia Weinstein, University of Sheffield  
Tom Welton, Imperial College London  
Charlotte Williams, University of Oxford  
Vivian Yam, University of Hong Kong  
Qi-Lin Zhou, Nankai University  
Jenny Zhang, University of Cambridge

## Information for Authors

Full details on how to submit material for publication in Chemical Science are given in the Instructions for Authors (available from <http://www.rsc.org/authors>). Submissions should be made via the journal's homepage: [rsc.li/chemical-science](http://rsc.li/chemical-science)

Authors may reproduce/republish portions of their published contribution without seeking permission from the Royal Society of Chemistry, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation)–Reproduced by permission of the Royal Society of Chemistry.

This journal is © The Royal Society of Chemistry 2023. Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

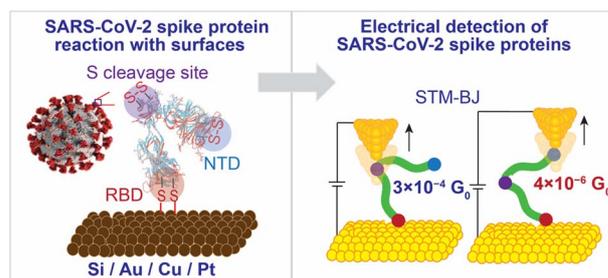
Registered charity number: 207890



3428

### SARS-CoV-2 spike proteins react with Au and Si, are electrically conductive and denature at $3 \times 10^8 \text{ V m}^{-1}$ : a surface bonding and a single-protein circuit study

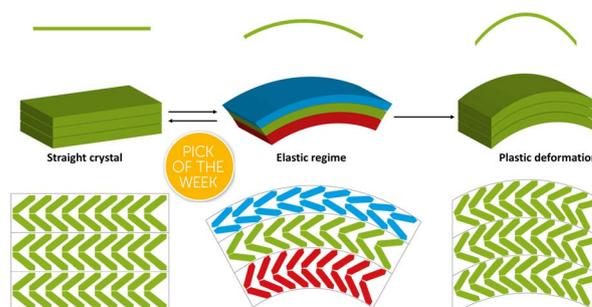
Essam M. Dief and Nadim Darwish\*



3441

### An atomistic mechanism for elasto-plastic bending in molecular crystals

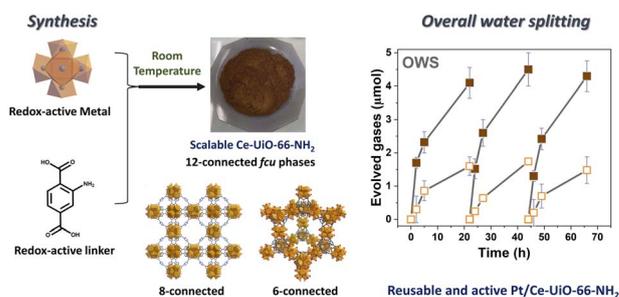
Biswajit Bhattacharya,\* Adam A. L. Michalchuk,\* Dorothee Silbernagl,\* Nobuhiro Yasuda, Torvid Feiler, Heinz Sturm and Franziska Emmerling



3451

### Room temperature design of Ce(IV)-MOFs: from photocatalytic HER and OER to overall water splitting under simulated sunlight irradiation

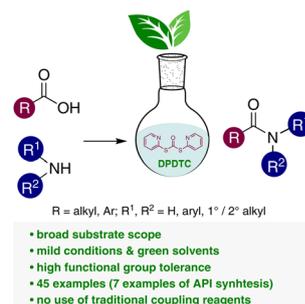
Shan Dai, Eva Montero-Lanzuela, Antoine Tissot,\* Herme G. Baldoví, Hermenegildo García, Sergio Navalón\* and Christian Serre\*



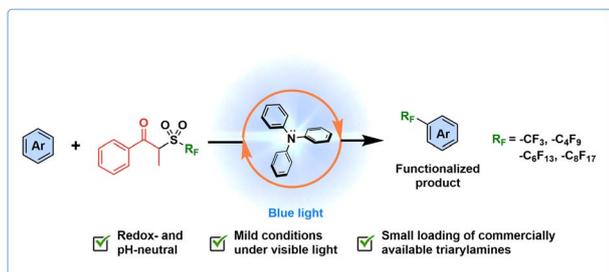
3462

### Direct formation of amide/peptide bonds from carboxylic acids: no traditional coupling reagents, 1-pot, and green

Kaitlyn M. Freiberg, Rahul D. Kavthe, Rohan M. Thomas, David M. Fialho, Paris Dee, Matthew Scurria and Bruce H. Lipshutz\*



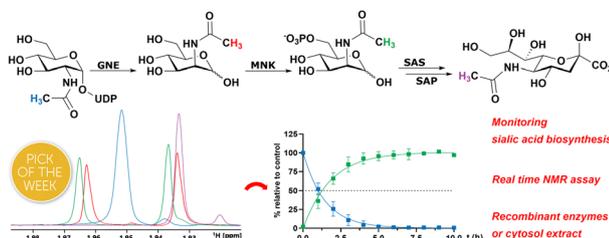
3470



### Triarylamines as catalytic donors in light-mediated electron donor–acceptor complexes

Durbis J. Castillo-Pazos, Juan D. Lasso, Ehsan Hamzehpoor, Jorge Ramos-Sánchez, Jan Michael Salgado, Gonzalo Cosa, Dmytro F. Perepichka and Chao-Jun Li\*

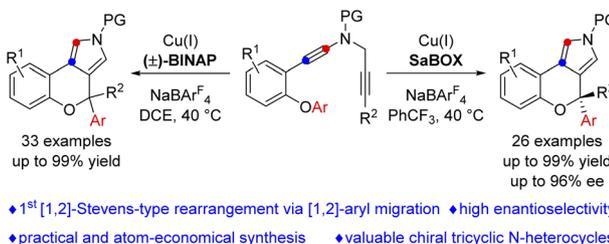
3482



### Real-time monitoring of the sialic acid biosynthesis pathway by NMR

Jacob L. Gorenflos López, Peter Schmieder, Kristin Kemnitz-Hassanin, Hatice Ceyda Asikoglu, Arif Celik, Christian E. Stieger, Dorothea Fiedler, Stephan Hinderlich\* and Christian P. R. Hackenberger\*

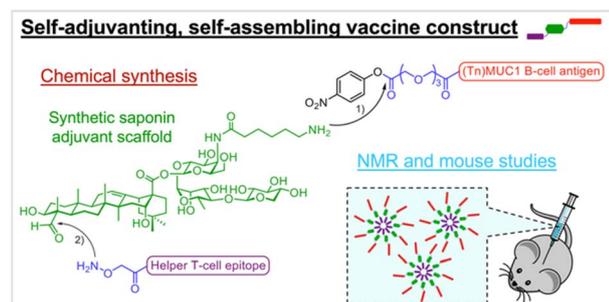
3493



### Copper-catalyzed enantioselective diyne cyclization via C(sp<sup>2</sup>)-O bond cleavage

Ji-Jia Zhou, Ya-Nan Meng, Li-Gao Liu, Yi-Xi Liu, Zhou Xu,\* Xin Lu,\* Bo Zhou and Long-Wu Ye\*

3501



### Development of synthetic, self-adjuvant, and self-assembling anticancer vaccines based on a minimal saponin adjuvant and the tumor-associated MUC1 antigen

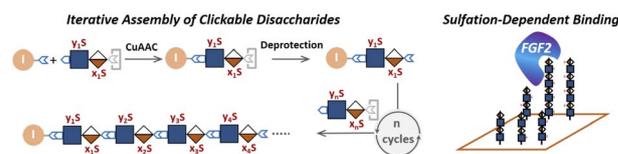
Carlo Pifferi, Leire Aguinagalde, Ane Ruiz-de-Angulo, Nagore Sacristán, Priscila Tonon Baschiroto, Ana Poveda, Jesús Jiménez-Barbero, Juan Anguita\* and Alberto Fernández-Tejada\*



3514

## Heparan sulfate glycomimetics via iterative assembly of "clickable" disaccharides

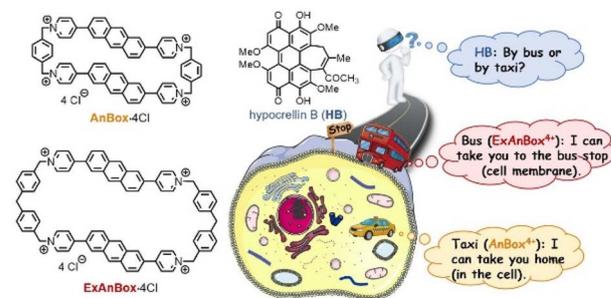
Cangjie Yang, Yu Deng, Yang Wang, Chaoshuang Xia, Akul Y. Mehta, Kelly J. Baker, Anuj Samal, Putthipong Booneimsri, Chanthakarn Lertmaneeang, Seung Hwang, James P. Flynn, Muqing Cao, Chao Liu, Alec C. Zhu, Richard D. Cummings, Cheng Lin, Udayan Mohanty\* and Jia Niu\*



3523

## Supramolecular photosensitizers using extended macrocyclic hosts for photodynamic therapy with distinct cellular delivery

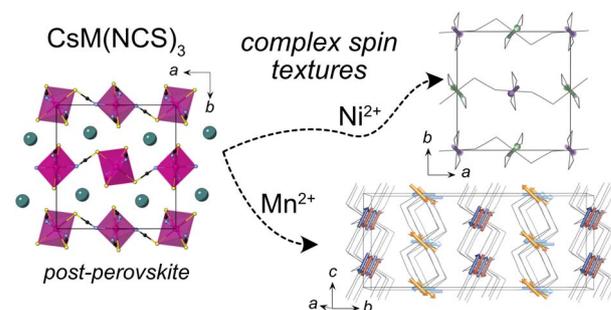
Xiuli Zheng, Sheng-Nan Lei, Zekun Gao, Xiangyu Dong, Hongyan Xiao, Weimin Liu,\* Chen-Ho Tung, Li-Zhu Wu, Pengfei Wang\* and Huan Cong\*



3531

## Non-collinear magnetism in the post-perovskite thiocyanate frameworks CsM(NCS)<sub>3</sub>

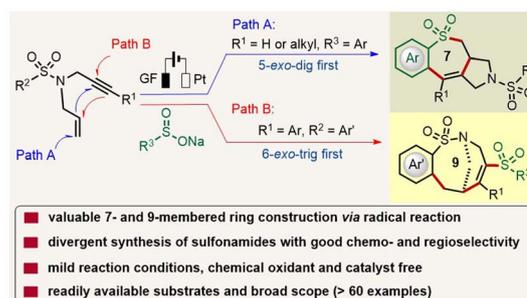
Madeleine Geers, Jie Yie Lee, Sanliang Ling, Oscar Fabelo, Laura Cañadillas-Delgado and Matthew J. Cliffe\*



3541

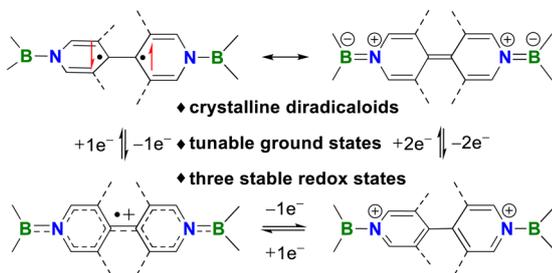
## Electrosynthesis of bridged or fused sulfonamides through complex radical cascade reactions: divergence in medium-sized ring formation

Yan Zhang,\* Zhenzhi Cai, Chunhang Zhao, Hanliang Zheng and Lutz Ackermann\*



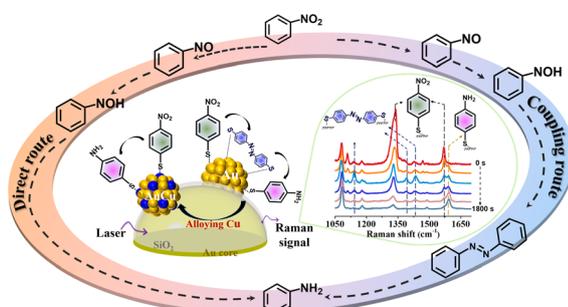
3548

## the Marriage of Viologens and Chichibabin's Hydrocarbon

Multiple stable redox states and tunable ground states *via* the marriage of viologens and Chichibabin's hydrocarbon

Yuyang Dai, Zhuofeng Xie, Manling Bao, Chunmeng Liu and Yuanting Su\*

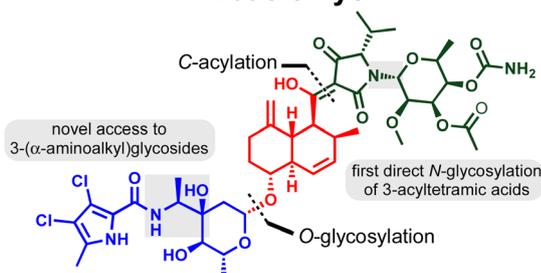
3554

*In situ* SERS reveals the route regulation mechanism mediated by bimetallic alloy nanocatalysts for the catalytic hydrogenation reaction

Xiaoxiao Li, Jinghua An, Ze Gao, Chang Xu, Yaoying Cheng, Simin Li, Lu Li\* and Bo Tang\*

3562

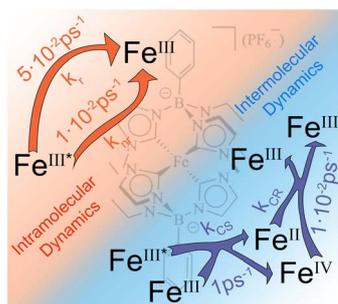
## kibdelomycin



## Formal synthesis of kibdelomycin and derivatisation of amycolose glycosides

Manuel G. Schriefer, Laura Treiber and Rainer Schobert\*

3569



## Competing dynamics of intramolecular deactivation and bimolecular charge transfer processes in luminescent Fe(III) N-heterocyclic carbene complexes

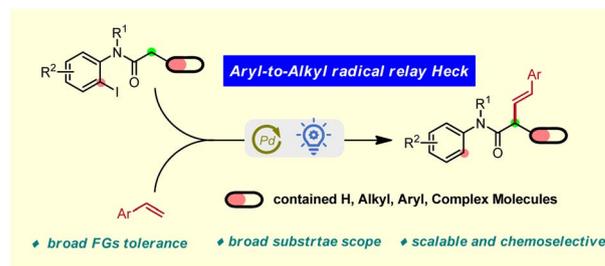
Nils W. Rosemann, Linnea Lindh, Iria Bolaño Losada, Simon Kaufhold, Om Prakash, Aleksandra Ilic, Jesper Schwarz, Kenneth Wärnmark, Pavel Chábera, Arkady Yartsev\* and Petter Persson\*



3580

### Aryl-to-alkyl radical relay Heck reaction of amides with vinyl arenes

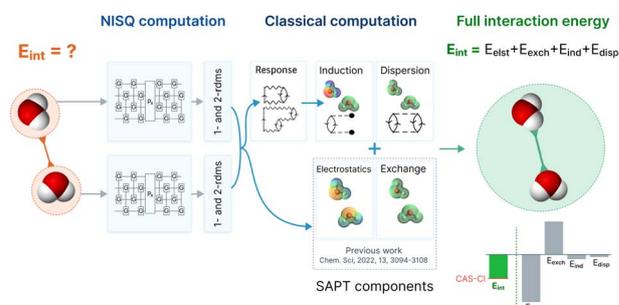
Yu-jia Du, Xia-xin Sheng, Jun-hua Li, Jia-ming Chen, Sen Yang\* and Ming Chen\*



3587

### Accurate non-covalent interaction energies on noisy intermediate-scale quantum computers via second-order symmetry-adapted perturbation theory

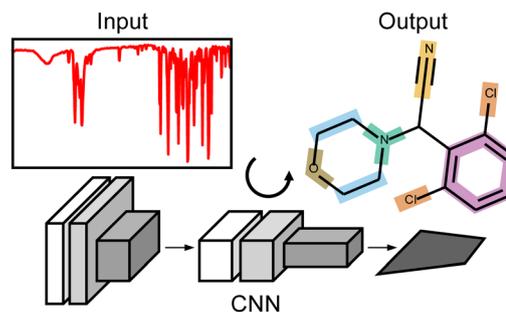
Matthias Loipersberger, Fionn D. Malone, Alicia R. Welden, Robert M. Parrish,\* Thomas Fox, Matthias Degroote, Elica Kyoseva, Nikolaj Moll,\* Raffaele Santagati and Michael Streif



3600

### Automatic materials characterization from infrared spectra using convolutional neural networks

Guwon Jung, Son Gyo Jung and Jacqueline M. Cole\*



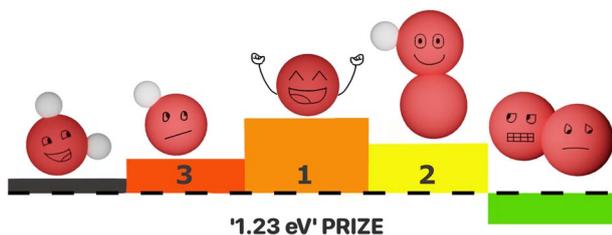
3610

### Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene/carbon nanofiber multifunctional electrode for electrode ionization with antifouling activity

Jingjing Lei, Fei Yu, Haijiao Xie and Jie Ma\*



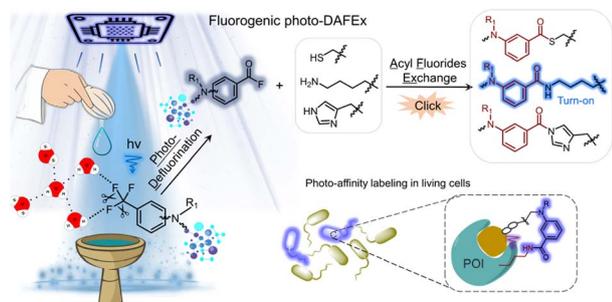
3622



### A general but still unknown characteristic of active oxygen evolution electrocatalysts

Eleonora Romeo, Francesc Illas\* and Federico Calle-Vallejo\*

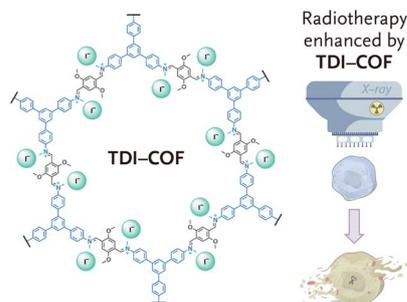
3630



### Photo-induced defluorination acyl fluoride exchange as a fluorogenic photo-click reaction for photo-affinity labeling

Lijun Deng, Cefei Zhang, Baolin Li, Jieli Fu, Zhong Zhang, Sitong Li, Xiaohu Zhao, Zhishan Su, Changwei Hu\* and Zhipeng Yu\*

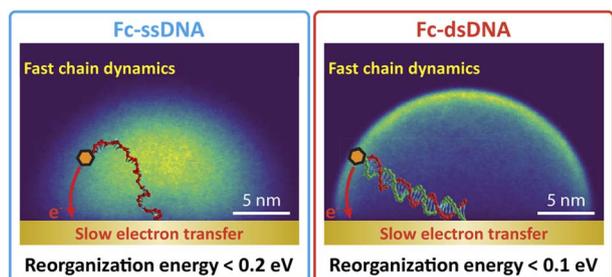
3642



### An iodide-containing covalent organic framework for enhanced radiotherapy

Le-Le Zhou, Qun Guan, Wei Zhou, Jing-Lan Kan and Yu-Bin Dong\*

3652



### Electrochemical response of surface-attached redox DNA governed by low activation energy electron transfer kinetics

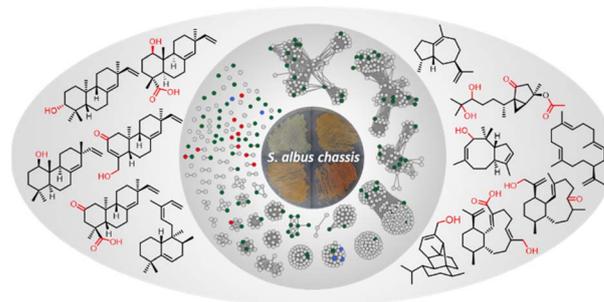
Zhiyong Zheng, Soo Hyeon Kim, Arnaud Chovin, Nicolas Clement\* and Christophe Demaille\*



3661

### Building *Streptomyces albus* as a chassis for synthesis of bacterial terpenoids

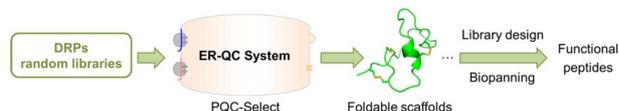
Yi Ling Hu, Qi Zhang, Shuang He Liu, Jia Li Sun, Fang Zhou Yin, Zi Ru Wang, Jing Shi, Rui Hua Jiao\* and Hui Ming Ge\*



3668

### Selection and evolution of disulfide-rich peptides via cellular protein quality control

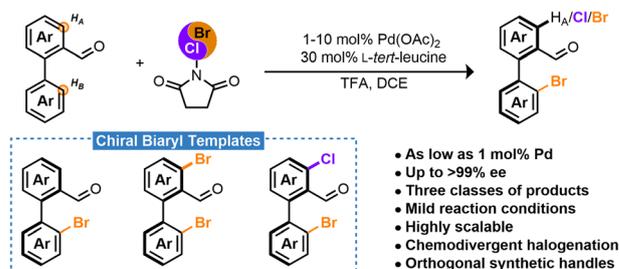
Xiaoting Meng, Chaoying Xu, Shihui Fan, Meng Dong, Jie Zhuang, Zengping Duan, Yibing Zhao and Chuanliu Wu\*



3676

### Atroposelective brominations to access chiral biaryl scaffolds using high-valent Pd-catalysis

Sif T. Linde, Vasco Corti, Vibeke H. Lauridsen, Johannes N. Lamhauge, Karl Anker Jørgensen and Nomaan M. Rezayee\*



3682

### Redox tuning of the H-cluster by second coordination sphere amino acids in the sensory [FeFe] hydrogenase from *Thermotoga maritima*

Nipa Chongdar,\* Patricia Rodríguez-Maciá, Edward J. Reijerse, Wolfgang Lubitz, Hideaki Ogata\* and James A. Birrell\*

