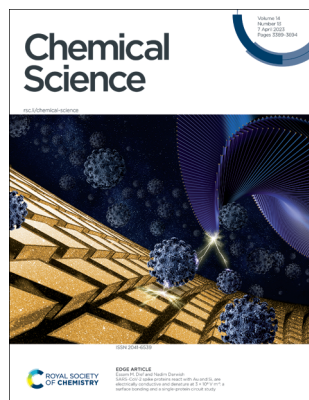


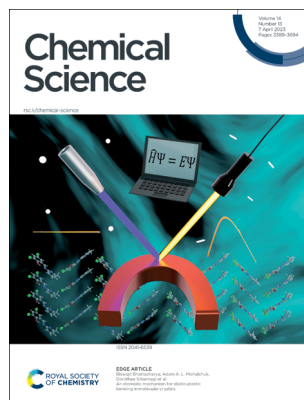
IN THIS ISSUE

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

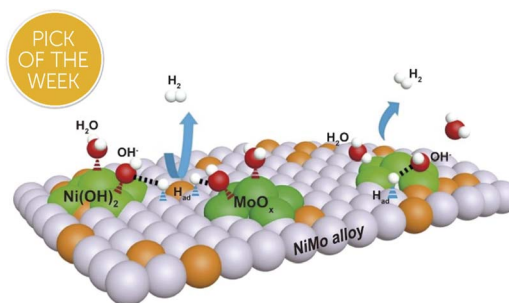
See Biswajit Bhattacharya, Adam A. L. Michalchuk, Dorothee Silbernagl *et al.*, pp. 3441–3450. Image reproduced by permission of Biswajit Bhattacharya from *Chem. Sci.*, 2023, 14, 3441.

PERSPECTIVES

3400

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

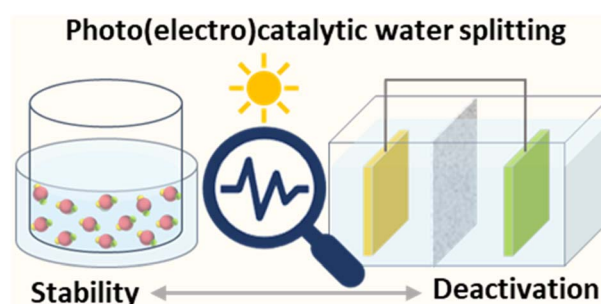
Min Luo, Jietian Yang, Xingang Li, Miهارu Eguchi, Yusuke Yamauchi and Zhong-Li Wang*



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 Copsey

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

For pre-submission queries please contact May Copsey, Executive Editor. E-mail 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 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

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

For marketing opportunities relating to this journal, contact marketing@rsc.org

Chemical Science

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
Mi Hee Lim, 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
Satoshi Maeda, Hokkaido University
Swadhin Mandal, IISER Kolkata
Ellen Matson, University of Rochester
Scott Miller, Yale University
Daniel Mindiola, 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

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 Martin
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

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.

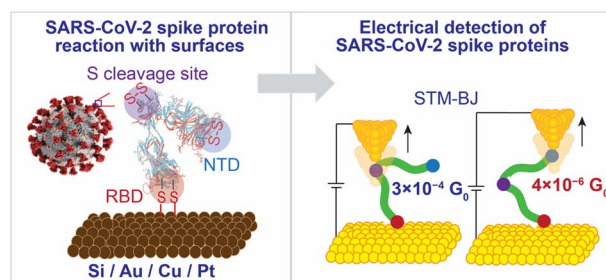
Registered charity number: 207890



3428

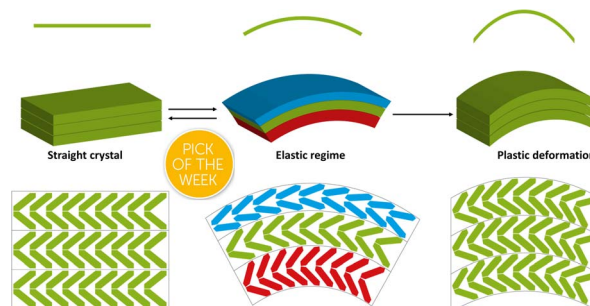
SARS-CoV-2 spike proteins react with Au and Si, are electrically conductive and denature at $3 \times 10^8 \text{ V m}^{-1}$: a surface bonding and a single-protein circuit study

Essam M. Dief and Nadim Darwish*



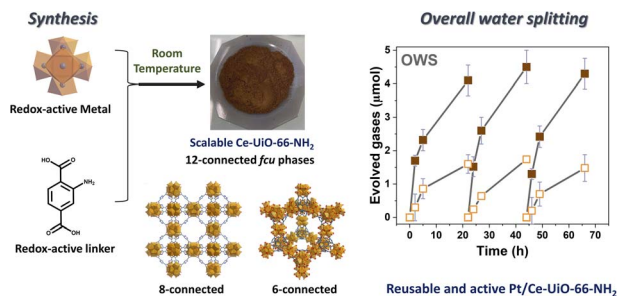
3441

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

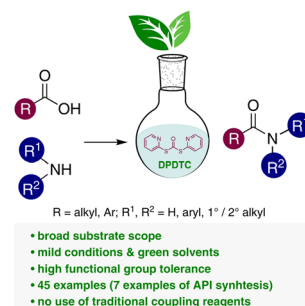
3451

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

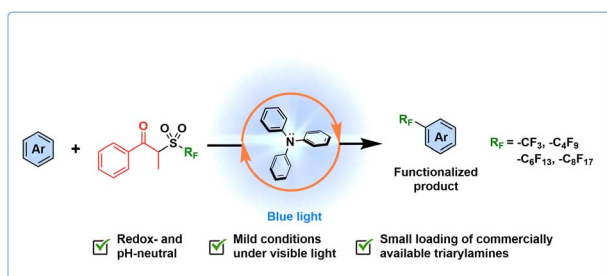
Shan Dai, Eva Montero-Lanzuela, Antoine Tissot,*
Herme G. Baldoví, Hermenegildo García, Sergio Navalón*
and Christian Serre*

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*

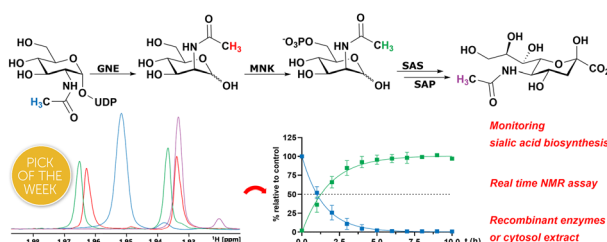
3470



Triarylamine 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*

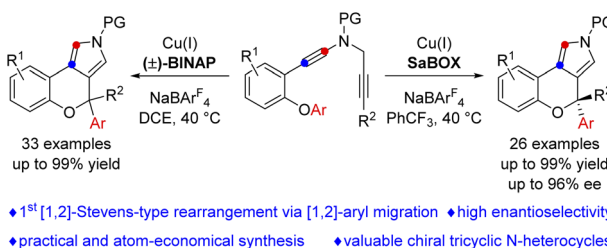
3482



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*

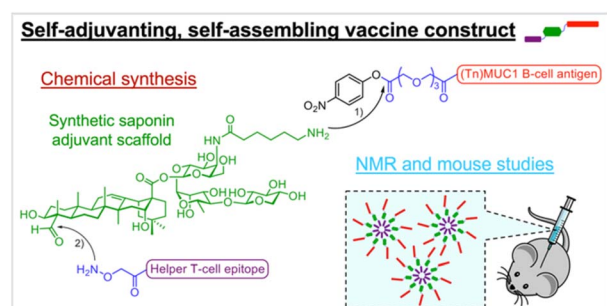
3493



Copper-catalyzed enantioselective diyne cyclization via C(sp²)–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-adjuvanting, and self-assembling anticancer vaccines based on a minimal saponin adjuvant and the tumor-associated MUC1 antigen

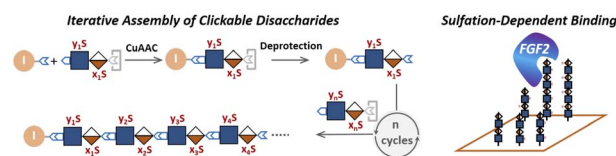
Carlo Pifferi, Leire Aguinagalde, Ane Ruiz-de-Angulo, Nagore Sacristán, Priscila Tonon Baschiroto, Ana Poveda, Jesús Jiménez-Barbero, Juan Anguita* and Alberto Fernández-Tejada*



3514

Heparan sulfate glycomimetics via iterative assembly of "clickable" disaccharides

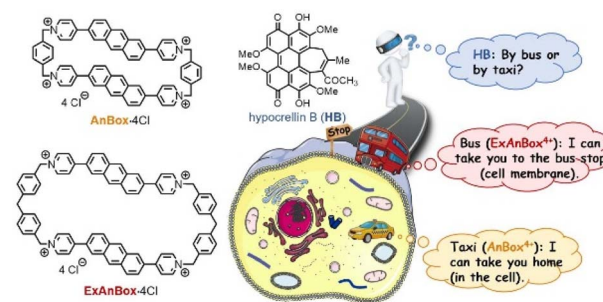
Cangjie Yang, Yu Deng, Yang Wang, Chaoshuang Xia, Akul Y. Mehta, Kelly J. Baker, Anuj Samal, Putthipong Booneimsri, Chanthakarn Lertmaneeang, Seung Hwang, James P. Flynn, Muqing Cao, Chao Liu, Alec C. Zhu, Richard D. Cummings, Cheng Lin, Udayan Mohanty* and Jia Niu*



3523

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

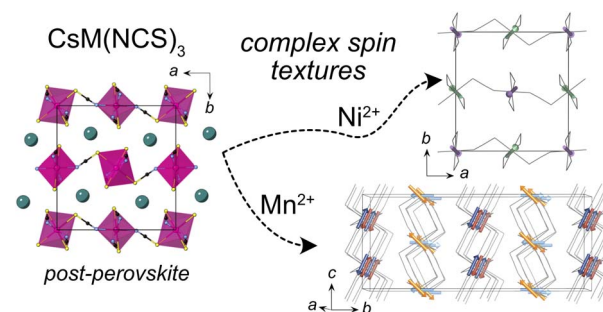
Xiuli Zheng, Sheng-Nan Lei, Zekun Gao, Xiangyu Dong, Hongyan Xiao, Weimin Liu,* Chen-Ho Tung, Li-Zhu Wu, Pengfei Wang* and Huan Cong*



3531

Non-collinear magnetism in the post-perovskite thiocyanate frameworks CsM(NCS)₃

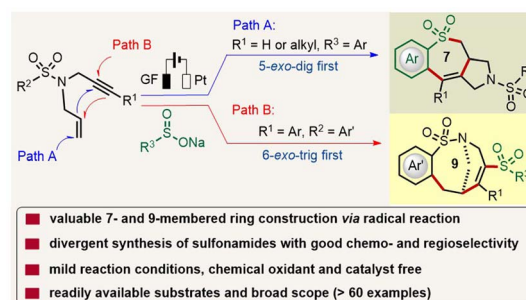
Madeleine Geers, Jie Yie Lee, Sanliang Ling, Oscar Fabelo, Laura Cañadillas-Delgado and Matthew J. Cliffe*



3541

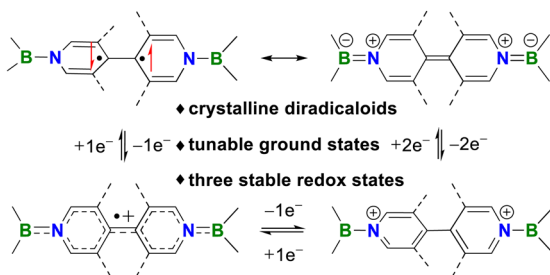
Electrosynthesis of bridged or fused sulfonamides through complex radical cascade reactions: divergence in medium-sized ring formation

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



3548

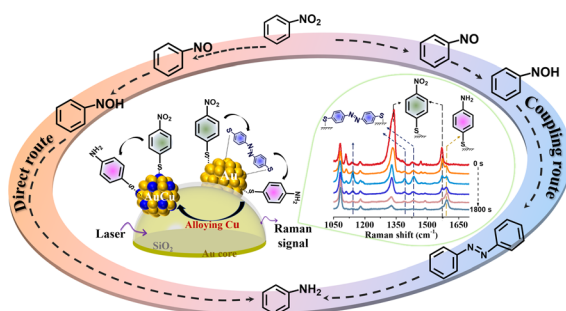
the Marriage of Vologens and Chichibabin's Hydrocarbon



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

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

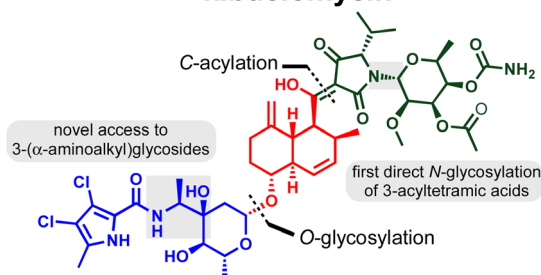
3554

*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

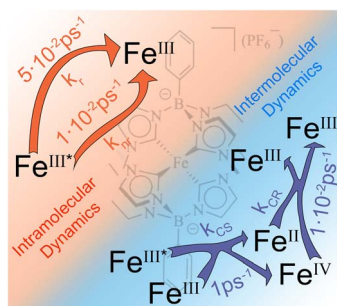
kibdelomycin



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

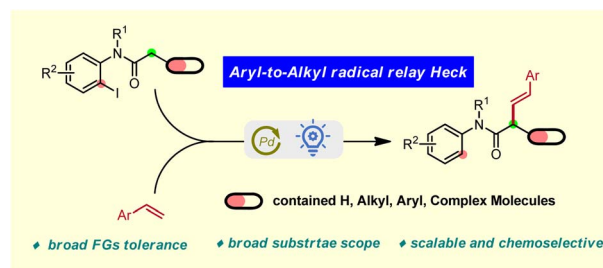
Nils W. Rosemann, Linnea Lindh, Iria Bolaño Losada, Simon Kaufhold, Om Prakash, Aleksandra Ilic, Jesper Schwarz, Kenneth Wärnmark, Pavel Chábera, Arkady Yartsev* and Petter Persson*



3580

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

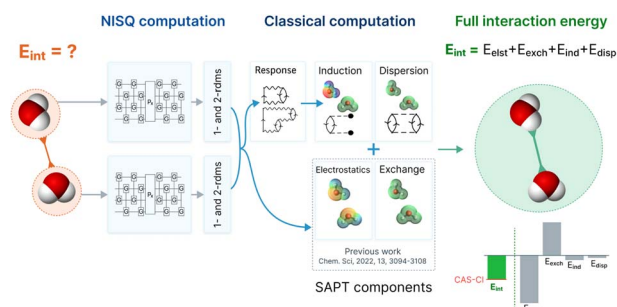
Yu-jia Du, Xia-xin Sheng, Jun-hua Li, Jia-ming Chen, Sen Yang* and Ming Chen*



3587

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

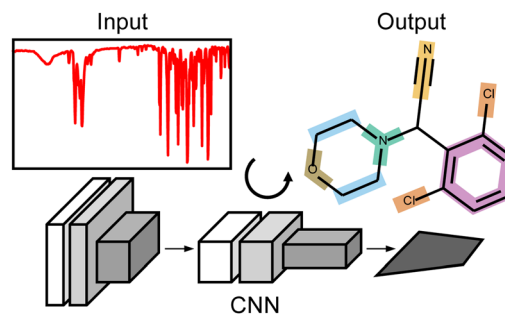
Matthias Loipersberger, Fionn D. Malone, Alicia R. Welden, Robert M. Parrish,* Thomas Fox, Matthias Degroote, Elica Kyoseva, Nikolaj Moll,* Raffaele Santagati and Michael Streif



3600

Automatic materials characterization from infrared spectra using convolutional neural networks

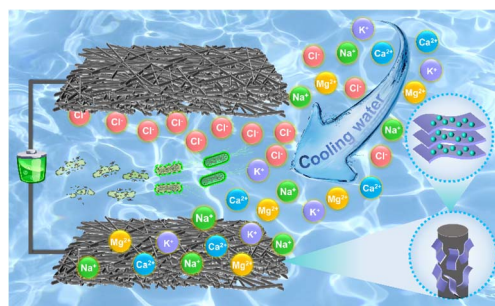
Guwon Jung, Son Gyo Jung and Jacqueline M. Cole*



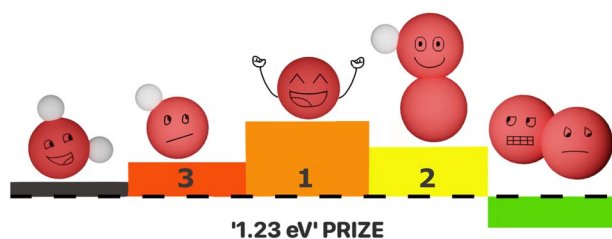
3610

Ti₃C₂T_x 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

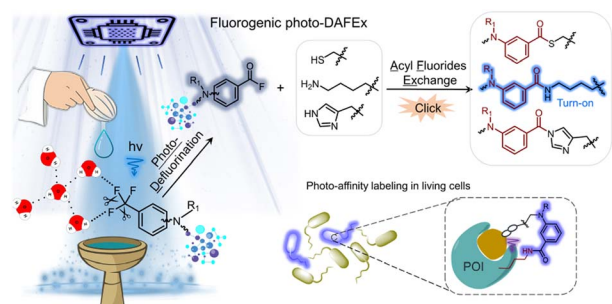
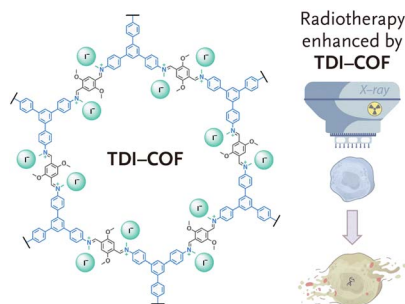


Photo-induced defluorination acyl fluoride exchange as a fluorogenic photo-click reaction for photo-affinity labeling

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

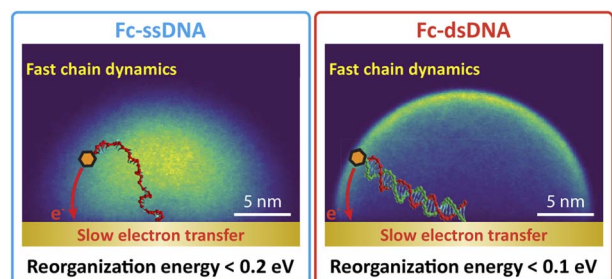
3642



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

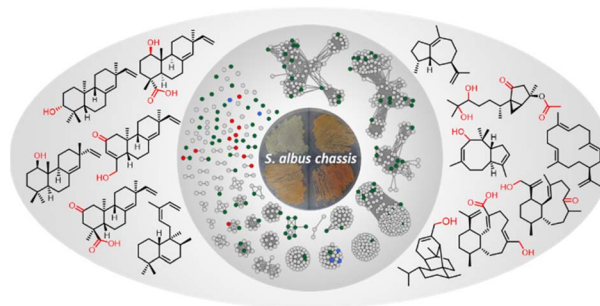
Zhiyong Zheng, Soo Hyeon Kim, Arnaud Chovin,
Nicolas Clement* and Christophe Demaille*



3661

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

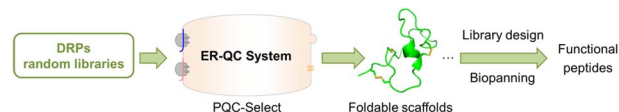
Yi Ling Hu, Qi Zhang, Shuang He Liu, Jia Li Sun, Fang Zhou Yin, Zi Ru Wang, Jing Shi, Rui Hua Jiao* and Hui Ming Ge*



3668

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

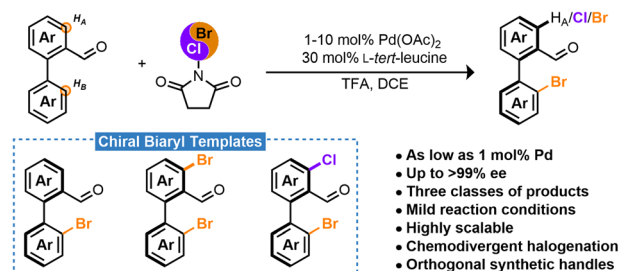
Xiaoting Meng, Chaoying Xu, Shihui Fan, Meng Dong, Jie Zhuang, Zengping Duan, Yibing Zhao and Chuanliu Wu*



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*

