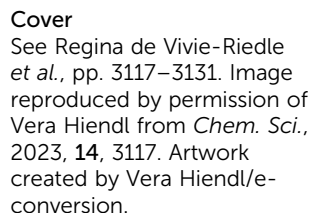
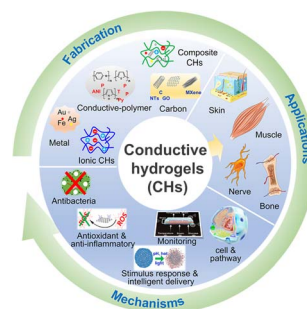


ISSN 2041-6539 CODEN CSHCBM 14(12) 3079–3388 (2023)

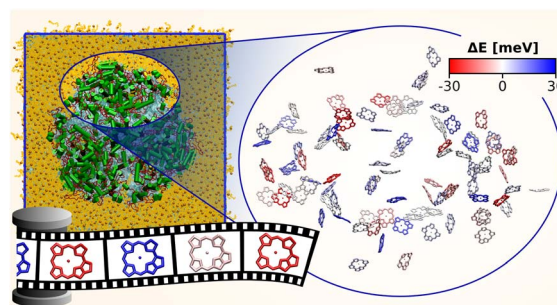


3091

Yongping Liang, Lipeng Qiao, Bowen Qiao
and Baolin Guo*



3117

Sebastian Reiter, Ferdinand L. Kiss, Jürgen Hauer
and Regina de Vivie-Riedle*

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
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.

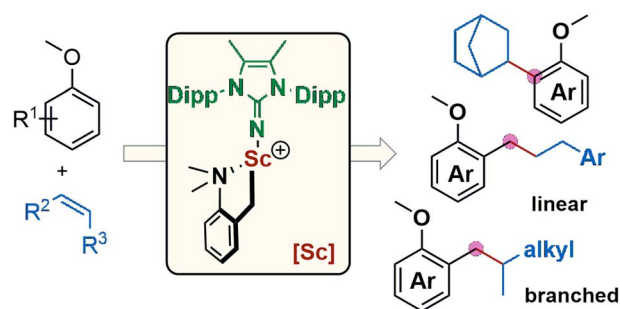
Registered charity number: 207890



3132

Regioselective C–H alkylation of anisoles with olefins by cationic imidazolin-2-iminato scandium(III) alkyl complexes

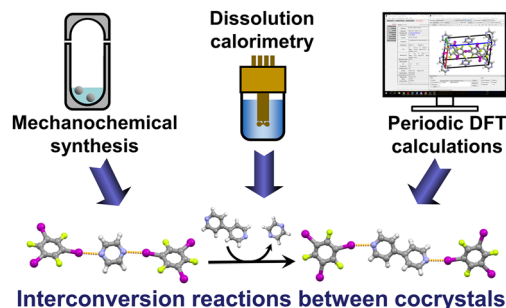
Shiyu Wang, Chenhao Zhu, Lichao Ning, Dawei Li, Xiaoming Feng and Shunxi Dong*



3140

Computational evaluation of halogen-bonded cocrystals enables prediction of their mechanochemical interconversion reactions

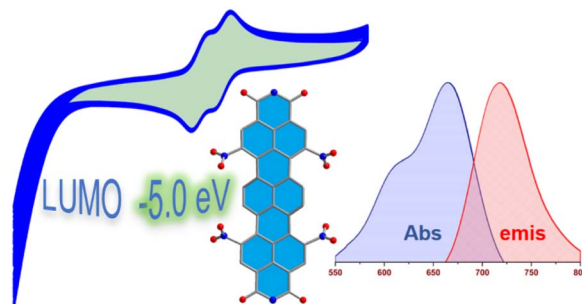
Lavanya Kumar, Katarina Leko, Vinko Nemec, Damian Trzybiński, Nikola Bregović, Dominik Cinčić and Mihails Arhangelkis*



3147

The deeper it goes, the brighter it glows: NIR emissive nitro-terrylene diimides with deep LUMOs

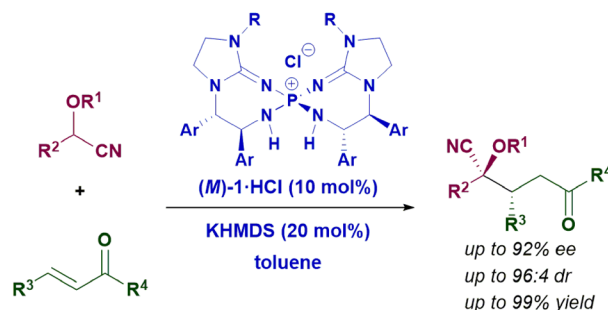
Kundan Singh Mehra, Shivangee Jha, Anila M. Menon, Deepak Chopra and Jeyaraman Sankar*



3154

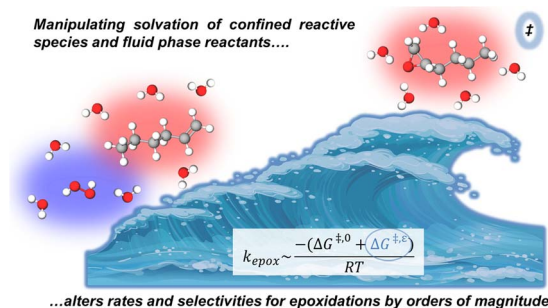
Enantioselective direct Michael addition of cyanohydrin ether derivatives to enones catalyzed by chiral bis(guanidino)iminophosphorane organosuperbase

Saikat Das, Azusa Kondoh* and Masahiro Terada*



3160

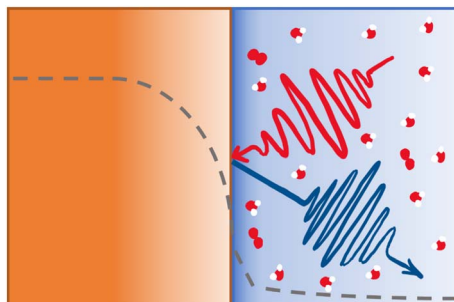
Manipulating solvation of confined reactive species and fluid phase reactants....



Engineering intraporous solvent environments: effects of aqueous-organic solvent mixtures on competition between zeolite-catalyzed epoxidation and H₂O₂ decomposition pathways

David S. Potts, Chris Torres, Ohsung Kwon and David W. Flaherty*

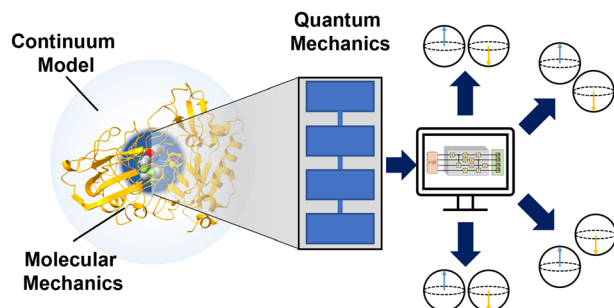
3182



Monitoring interfacial electric fields at a hematite electrode during water oxidation

Khezari H. Saeed, Dora-Alicia Garcia Osorio, Chao Li, Liam Banerji, Adrian M. Gardner and Alexander J. Cowan*

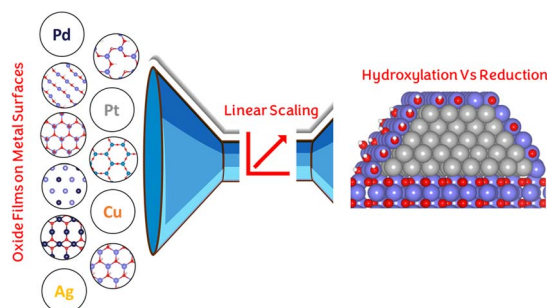
3190



Multiscale quantum algorithms for quantum chemistry

Huan Ma, Jie Liu,* Honghui Shang,* Yi Fan, Zhenyu Li and Jinlong Yang*

3206



Universal properties of metal-supported oxide films from linear scaling relationships: elucidation of mechanistic origins of strong metal-support interactions

Kaustubh J. Sawant, Zhenhua Zeng and Jeffrey P. Greeley*



3215

Reassessing CORM-A1: redox chemistry and idiosyncratic CO-releasing characteristics of the widely used carbon monoxide donor

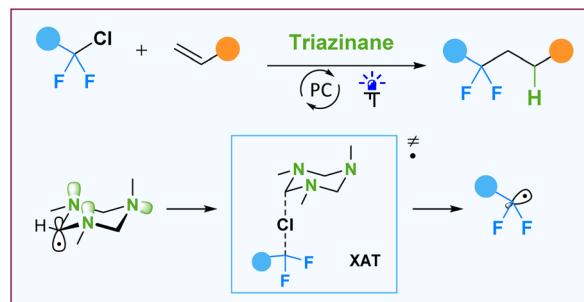
Nicola Bauer, Xiaoxiao Yang, Zhengnan Yuan and Binghe Wang*

	Variable or lack of CO production	CO-Independent Chemical Reactivity	CO-Independent Biological Activity
CORM-2	✓	✓	✓
CORM-3	✓	✓	✓
CORM-401	✓	✓	?
CORM-A1	✓	✓	?

3229

Aminals as powerful XAT-reagents: activation of fluorinated alkyl chlorides

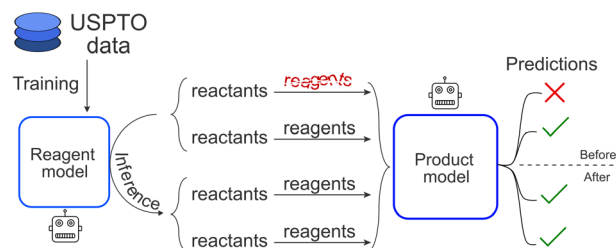
Vladislav S. Kostromitin, Artem O. Sorokin, Vitalij V. Levin and Alexander D. Dilman*



3235

Reagent prediction with a molecular transformer improves reaction data quality

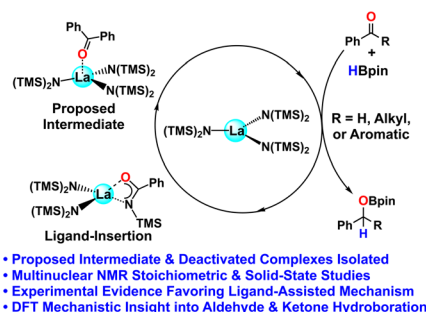
Mikhail Andronov,* Varvara Voinarovska, Natalia Andronova, Michael Wand, Djork-Arné Clevert and Jürgen Schmidhuber



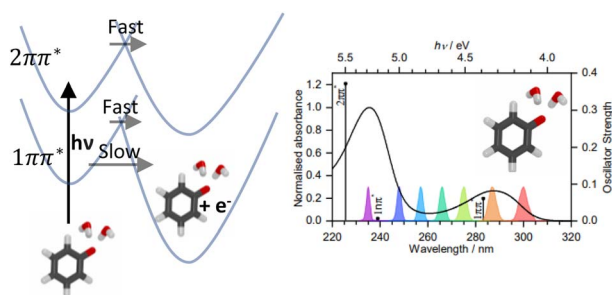
3247

Mechanistic study of homoleptic trisamidolanthanide-catalyzed aldehyde and ketone hydroboration. Chemically non-innocent ligand participation

Jacob O. Rothbaum, Alessandro Motta,* Yosi Kratish* and Tobin J. Marks*



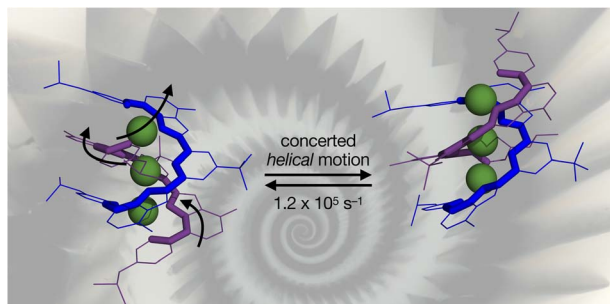
3257



Wavelength dependent mechanism of phenolate photooxidation in aqueous solution

Kate Robertson, William G. Fortune, Julia A. Davies, Anton N. Boichenko, Michael S. Scholz, Omri Tau, Anastasia V. Bochenkova and Helen H. Fielding*

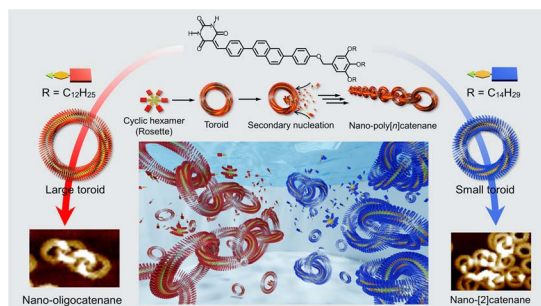
3265



Helical fluxionality: numerical frustration drives concerted low-barrier screw motions of a tricopper cluster

Heechan Kim, Juhwan Shin, Seyong Kim and Dongwhan Lee*

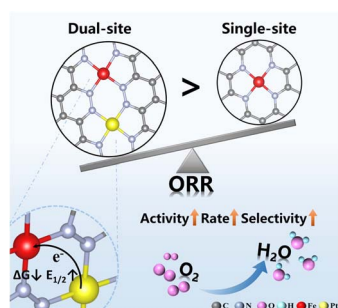
3270



Fine-tuning of the size of supramolecular nanotoroids suppresses the subsequent catenation of nano-[2]catenane

Hiroki Itabashi, Sougata Datta, Ryohei Tsukuda, Martin J. Hollamby and Shiki Yagai*

3277



Modulating the electronic structure of atomically dispersed Fe-Pt dual-site catalysts for efficient oxygen reduction reactions

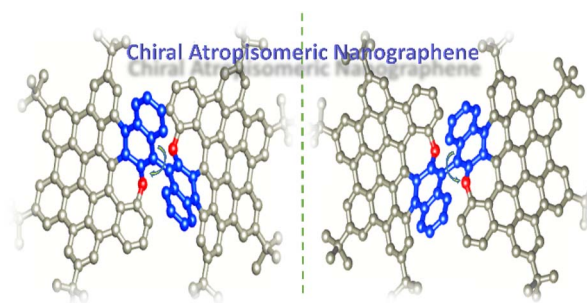
Wei-Shen Song, Mei Wang, Xiao Zhan, Yan-Jie Wang, Dong-Xu Cao, Xian-Meng Song, Zi-Ang Nan, Li Zhang* and Feng Ru Fan*



3286

BINOL-like atropisomeric chiral nanographene

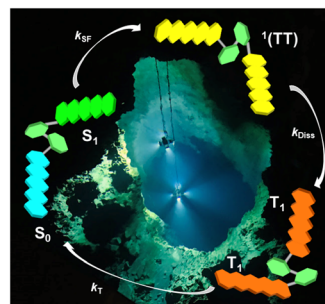
Shengtao Li, Ranran Li, Yi-Kang Zhang, Shutao Wang, Bin Ma, Bin Zhang and Peng An*



3293

Control of intramolecular singlet fission in a pentacene dimer by hydrostatic pressure

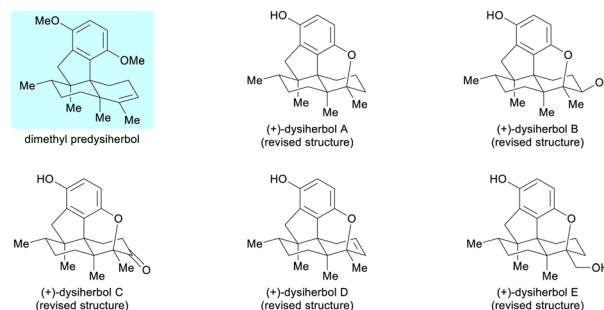
Tomokazu Kinoshita, Shunta Nakamura, Makoto Harada, Taku Hasobe* and Gaku Fukuhara*



3302

Divergent total synthesis of the revised structures of marine anti-cancer meroterpenoids (+)-dysiherbols A–E

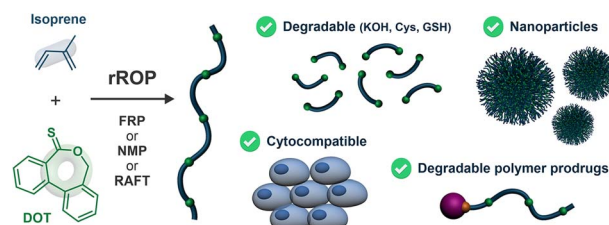
Chuanke Chong, Le Chang, Isabelle Grimm, Qunlong Zhang, Yang Kuang, Bingjian Wang, Jingyi Kang, Wenhui Liu, Julian Baars, Yuanqiang Guo, Hans-Günther Schmalz* and Zhaoyong Lu*



3311

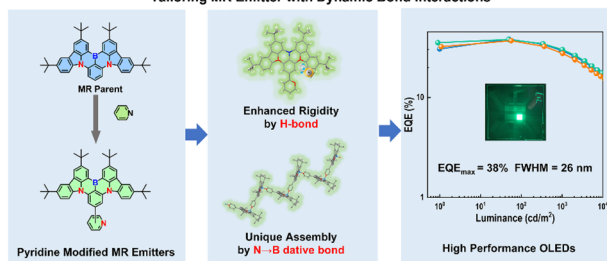
Degradable polyisoprene by radical ring-opening polymerization and application to polymer prodrug nanoparticles

Maëlle Lages, Théo Pesenti, Chen Zhu, Dao Le, Julie Mougin, Yohann Guillauneuf and Julien Nicolas*



3326

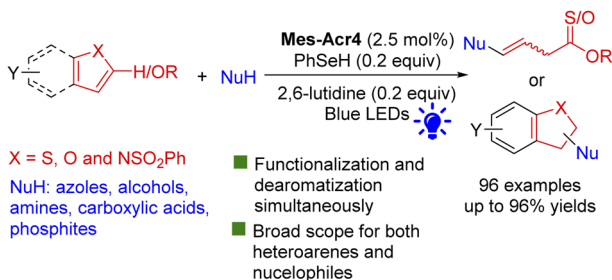
Tailoring MR Emitter with Dynamic Bond Interactions



Dynamic bond interactions fine-tune the properties of multiple resonance emitters towards highly efficient narrowband green OLEDs

Yang Zou, Mingxin Yu, Jingsheng Miao,* Taian Huang, Shuokun Liao, Xiaosong Cao and Chuluo Yang

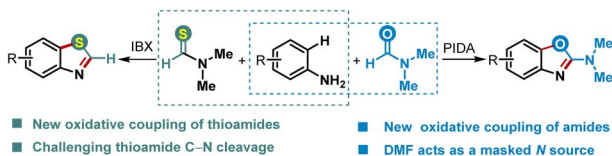
3332



Combining photoredox catalysis and hydrogen atom transfer for dearomative functionalization of electron rich heteroarenes

Peng Ji, Xiang Meng, Jing Chen, Feng Gao, Hang Xu and Wei Wang*

3338

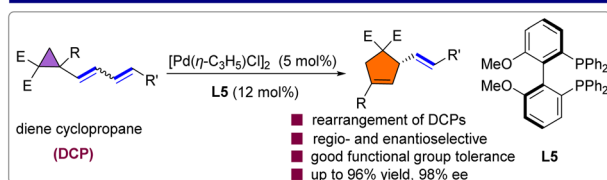


Hypervalent iodine-promoted twofold oxidative coupling of amines with amides and thioamides: chemoselective pathway to oxazoles and thiazoles

Jiang Nan,* Xin Ren, Qiang Yan, Shilei Liu, Jing Wang, Yangmin Ma and Michal Szostak*

3346

Palladium-catalyzed enantioselective rearrangement of diene cyclopropanes (DCPs)



Palladium-catalyzed enantioselective rearrangement of dienyl cyclopropanes

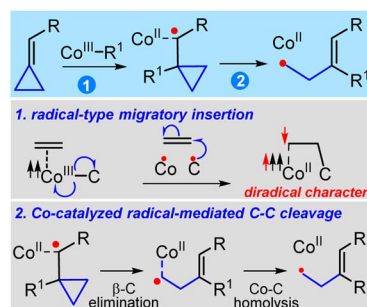
Qi Xu, Chuan-Jun Lu, Chang-Qiu Guo, Jia Feng and Ren-Rong Liu*



3352

Cobalt-catalyzed radical-mediated carbon–carbon scission *via* a radical-type migratory insertion

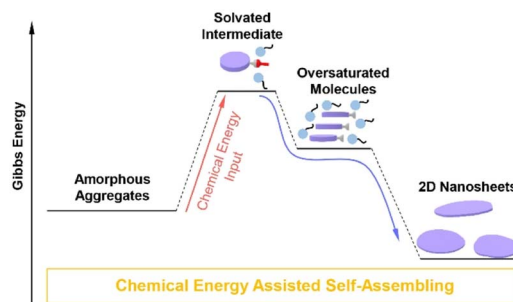
Jian-Biao Liu,* Xiao-Jun Liu, João C. A. Oliveira, De-Zhan Chen and Lutz Ackermann*



3363

Chemical energy assisted self-assembling of a porphyrin-substituted benzoic acid in complex environments

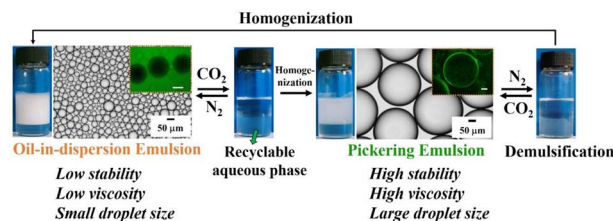
Bingxu Ma, Bowen Pang, Wang Zeng,* Huimin Fu, Yi Jiang, Shenglin Yao, Yida Yang, Kaisheng Zhu and Wei Zhang*



3370

CO₂-switchable emulsions with controllable size and viscosity

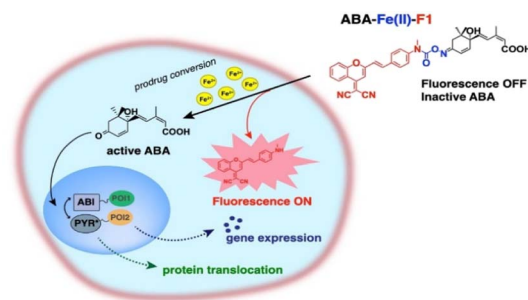
Jianzhong Jiang,* Huaixin Li and Yao Gu



3377

A theranostic abscisic acid-based molecular glue

Jing Chen, Huong T. X. Nguyen, Ming Yang, Fangxun Zeng, Hang Xu, Fu-Sen Liang* and Wei Wang*



CORRECTIONS

3385

Correction: Isolation of C1 through C4 derivatives from CO using heteroleptic uranium(III) metallocene aryloxide complexes

Robert J. Ward, Iker del Rosal, Steven P. Kelley, Laurent Maron* and Justin R. Walensky*

3386

Correction: Multi-stimuli programmable FRET based RGB absorbing antennae towards ratiometric temperature, pH and multiple metal ion sensing

Kavita Rani and Sanchita Sengupta*

