

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(40) 10983–11284 (2023)



Cover
See Clay C. C. Wang, Berl R. Oakley *et al.*, pp. 11022–11032. Image reproduced by permission of Clay C. C. Wang from *Chem. Sci.*, 2023, **14**, 11022. Artwork by Isaac Mora.



Inside cover
See Tsung-Che Chang, Katsunori Tanaka *et al.*, pp. 11033–11039. Image reproduced by permission of Katsunori Tanaka from *Chem. Sci.*, 2023, **14**, 11033.

COMMENTARY

10994

A focus on computer vision for non-contact monitoring of catalyst degradation and product formation kinetics

Niklaas J. Buurma and Scott W. Bagley

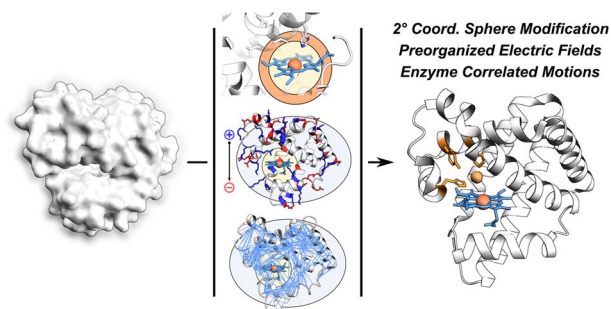


PERSPECTIVE

10997

From random to rational: improving enzyme design through electric fields, second coordination sphere interactions, and conformational dynamics

Shobhit S. Chaturvedi, Daniel Bim, Christo Z. Christov and Anastassia N. Alexandrova*



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
François Gabbai, Texas A&M University
Subi George, JNCASR
Ryan Gilmour, WWU Münster
Jinlong Gong, Tianjin University
Stephen Goldup, University of Birmingham
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

D. Adams, University of Glasgow
A. Ajayaghosh, NIIST
R. Amaro, UC San Diego
A. Anastasaki, ETH Zürich
U.-P. Apfel, Ruhr-University Bochum
K. Asmis, Leipzig University
X. Bao, DICP-CAS
Z. Bao, Stanford University
D. N. Beratan, Duke University
G. Bernardes, University of Cambridge
F. Biedermann, KIT
D. Blackmond, Scripps Research Institute
E. Blasco, Heidelberg University
J. Bode, ETH Zurich
J. S. Brodbelt, UT Austin
C. Chang, UC Berkeley
C.-M. Che, University of Hong Kong
J. Chen, Nankai University
M. Cohen, OHSU
C. Coley, MIT
J. Cornella, MPIK
L. Cronin, University of Glasgow
J. Crowley, University of Otago
C. C. Cummins, MIT
V. Däschlein-Gessner, Ruhr University Bochum
M. Delbianco, MPICI
J. Dempsey, UNC Chapel Hill
W. Dichtel, Northwestern University
K. Domen, University of Tokyo
H. Duan, Tsinghua University
X. Feng, TU Dresden
B. Feringa, University of Groningen
J. Figueroa, UC San Diego
N. Frank, University of Nevada
M. Freitag, Newcastle University
S. Gao, Peking University
J. Gassensmith, UT Dallas
G. Gasser, PSL University
E. Gibson, Newcastle University
F. Glorius, WWU Münster
L. González, University of Vienna
D. Graham, University of Strathclyde
V. Grassian, UC San Diego
A. Grimaud, Collège de France/CNRS
T. Gulder, Leipzig University
W. Gutkunst, Georgia Tech
C. Hackenberger, FMP Berlin
I. Hamachi, Kyoto University
G. Han, Brandeis University
B. Han, CAS
M. Hariharan, IISER-TVM

C. Haynes, University of Minnesota
J. Heemstra, WUSTL
T. Heine, DTU
P. Holland, Yale University
K. E. Jelfs, Imperial College London
X. Jiang, Aramco
Y. Jung, KAIST
S. Kath-Schorr, University of Cologne
T. Kato, University of Tokyo
C. Kelly, Janssen Research/J&J
R. Klausen, Johns Hopkins University
Y. Krishnan, University of Chicago
M. Kuimova, Imperial College London
K. Lancaster, Cornell University
A.-L. Lee, Heriot-Watt University
D. Leonori, University of Manchester
X. Li, University of Washington
Y. Li, Jilin University
M. H. Lim, KAIST
J. Lloret-Fillol, ICIQ
B. Lotsch, Max Planck Institute
X. W. Lou, NTU
K. Maeda, Tokyo Tech
S. Maeda, Hokkaido University
D. Maiti, IIT Bombay
L. Malins, ANU
S. Mandal, IISER Kolkata
T. Martinez, Stanford University
C. Martinez-Huitle, UFRN
E. Matson, Rochester University
J. L. Medina-Franco, UNAM
V. Moliner, INAM, Jaume I University
W. Nam, Ewha Womans University
T. Noël, University of Amsterdam
A. Obermeyer, Columbia University
M. Oestreich, TU Berlin
D. O'Hagan, University of St Andrews
T. Ooi, Nagoya University
R. O'Reilly, University of Birmingham
S. Ott, Uppsala University
H. Ottosson, Uppsala University
Z. Ouyang, Tsinghua University
X. Pan, DICP-CAS
S. Patel, SSCU-IISC
E. Pentzer, Texas A&M University
S. Peter, JNCASR
W. Piers, University of Calgary
N. Plumeré, Ruhr-University Bochum
S. Qiao, University of Adelaide
V. Rai, IISER Bhopal
S. Rasmussen, North Dakota State University

J. Read de Alaniz, UC Santa Barbara
E. Reisner, University of Cambridge
A. Rentmeister, WWU Munster
J. Rinehart, UC San Diego
A. Rothberg, University of Florida
H. Sardon, UPV-EHU
R. Sarpong, UC Berkeley
G. Schatz, Northwestern University
D. Schultz, Merck
D. Seferos, University of Toronto
R. Sessoli, University of Florence
H. Shafaat, UCLA
M. Kumova, Imperial College London
M. Solà, University of Girona
G. Soler-Illia, UNSAM
D. Spring, University of Cambridge
B. Sumerlin, University of Florida
R. B. Sunoj, IIT Bombay
Y. Surendranath, MIT
M. Tada, Nagoya University
T. Tahara, RIKEN
Z. Tang, NCNST
S. Teichert, DESY
C. Thomas, Ohio State University
H. Tian, ECUST
Z.-Q. Tian, Xiamen University
A. Tkatchenko, University of Luxembourg
H. Tran, University of Toronto
T. Uemura, University of Tokyo
C. Vanderwal, UC Irvine
L. Venkataraman, Columbia University
G. Vilé, Politecnico di Milano
A. Wakamiya, Kyoto University
L.-S. Wang, Brown University
C. Wang, Peking University
E. Weerapana, Boston College
J. Weinstein, University of Sheffield
T. Welton, Imperial College London
A. Wendlandt, MIT
C. Williams, University of Oxford
V. Yam, University of Hong Kong
N. Yanai, Kyushu University
S. Q. Yao, National University of Singapore
A. Zharbin, UFPR
L. Zhang, ECNU
T. Zhang, TIPC-CAS
J. Zhang, University of Cambridge
Z.-J. Zhao, Tianjin University
B. Zhong Tang, CUHK-Shenzhen
Q.-L. Zhou, Nankai University

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

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

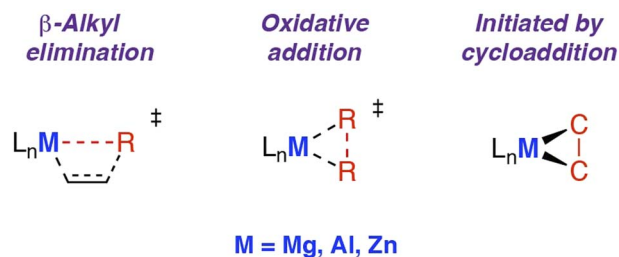


REVIEW

11012

Carbon–carbon bond activation by Mg, Al, and Zn complexes

Joseph M. Parr and Mark R. Crimmin*

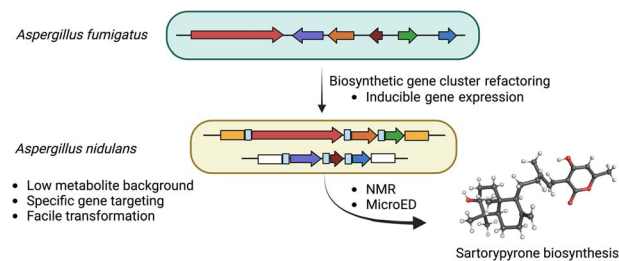


EDGE ARTICLES

11022

A heterologous expression platform in *Aspergillus nidulans* for the elucidation of cryptic secondary metabolism biosynthetic gene clusters: discovery of the *Aspergillus fumigatus* sartorypyrone biosynthetic pathway

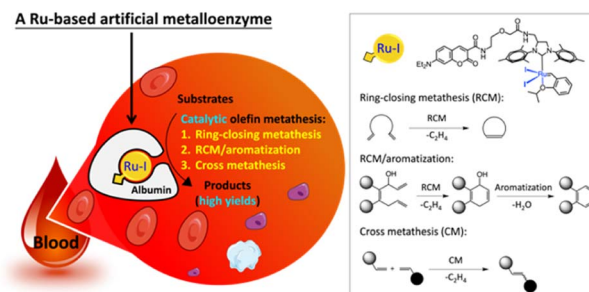
Shu-Yi Lin, C. Elizabeth Oakley, Cory B. Jenkinson, Yi-Ming Chiang, Ching-Kuo Lee, Christopher G. Jones, Paul M. Seidler, Hosea M. Nelson, Richard B. Todd, Clay C. Wang* and Berl R. Oakley*



11033

Catalytic olefin metathesis in blood

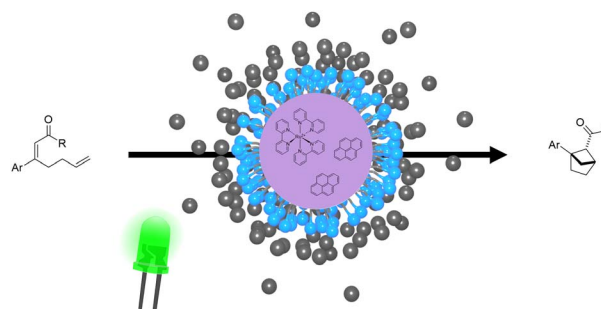
Igor Nasibullin, Hiromasa Yoshioka, Akari Mukaimine, Akiko Nakamura, Yuriko Kusakari, Tsung-Che Chang* and Katsunori Tanaka*



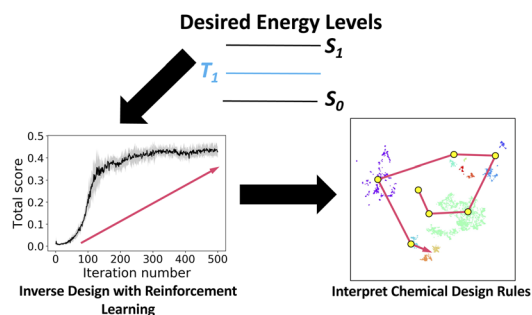
11040

Photocyclization by a triplet–triplet annihilation upconversion pair in water – avoiding UV-light and oxygen removal

R. Jeyaseelan, M. Utikal, C. G. Daniliuc and L. Næsberg*



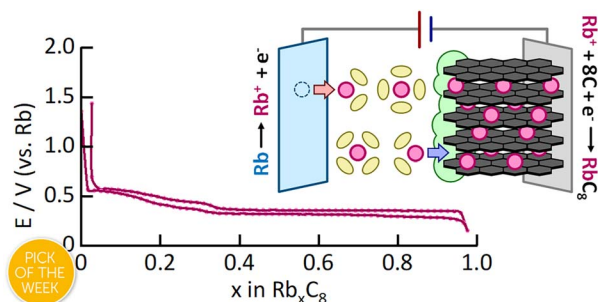
11045



Generative organic electronic molecular design informed by quantum chemistry

Cheng-Han Li and Daniel P. Tabor*

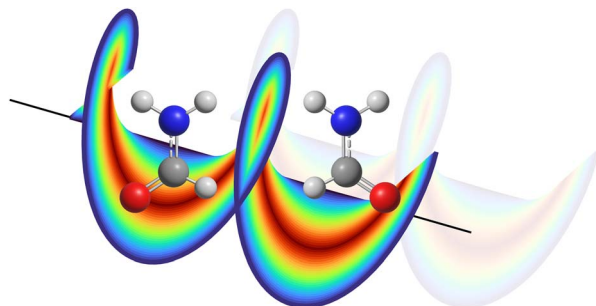
11056



Electrochemical intercalation of rubidium into graphite, hard carbon, and soft carbon

Daisuke Igarashi, Ryoichi Tatara, Ryusei Fujimoto, Tomooki Hosaka and Shinichi Komaba*

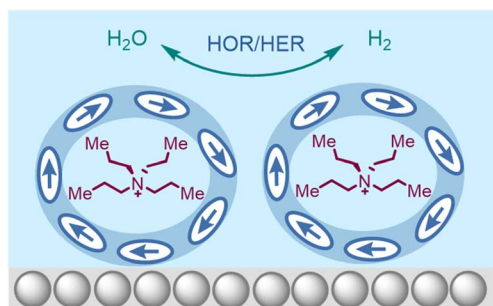
11067



Time-resolved enantiomer-exchange probed by using the orbital angular momentum of X-ray light

Xiang Jiang,* Yeonsig Nam, J r my R. Rouxel, Haiwang Yong and Shaul Mukamel*

11076



Action at a distance: organic cation induced long range organization of interfacial water enhances hydrogen evolution and oxidation kinetics

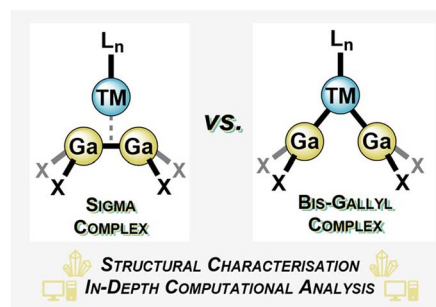
Kaiyue Zhao, Hao Yu, Haocheng Xiong, Qi Lu, Yi Qin Gao and Bingjun Xu*



11088

On the σ -complex character of bis(gallyl)/digallane transition metal species

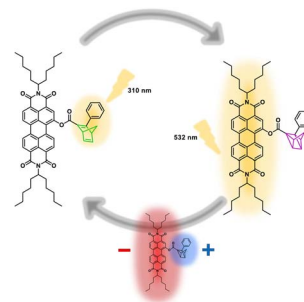
Till L. Kalkuhl, Lei Qin, Lili Zhao,* Gernot Frenking* and Terrance J. Hadlington*



11096

Driving the quadricyclane-to-norbornadiene isomerization by charge separation with perylenediimide as electron acceptor

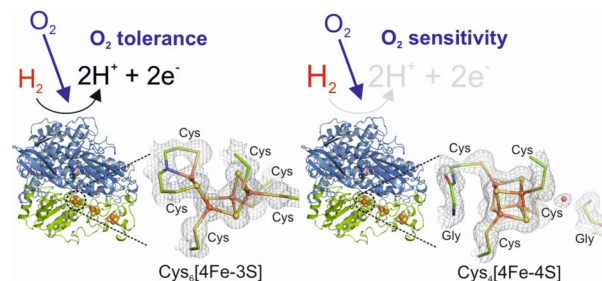
Wiebke Zika, Andreas Leng, René Weiß, Simone Pintér, Christoph M. Schüßlbauer, Timothy Clark, Andreas Hirsch and Dirk M. Guldi*



11105

Stepwise conversion of the Cys₆[4Fe–3S] to a Cys₄[4Fe–4S] cluster and its impact on the oxygen tolerance of [NiFe]-hydrogenase

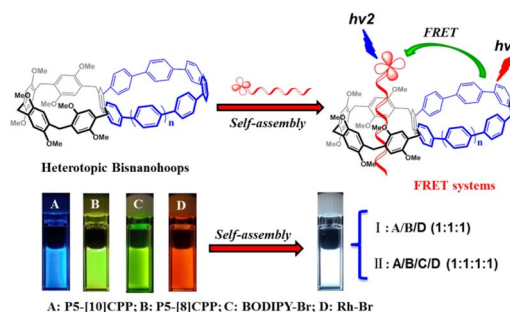
Andrea Schmidt, Jacqueline Kalms, Christian Lorent, Sagie Katz, Stefan Frielingsdorf, Rhiannon M. Evans, Johannes Fritsch, Elisabeth Siebert, Christian Teutloff, Fraser A. Armstrong, Ingo Zebger,* Oliver Lenz* and Patrick Scheerer*



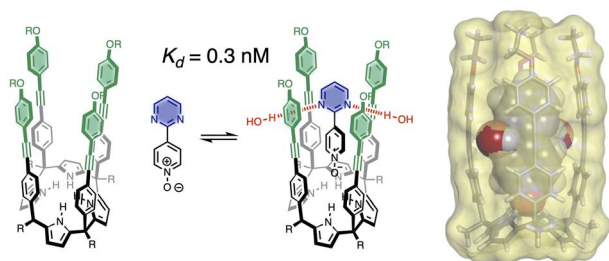
11121

Efficient manipulation of Förster resonance energy transfer through host–guest interaction enables tunable white-light emission and devices in heterotopic bisnanohoops

Yanqing Fan, Shimin Fan, Lin Liu, Shengzhu Guo, Jing He, Xiaonan Li, Zhe Lian, Weijie Guo, Xuebo Chen, Ying Wang and Hua Jiang*



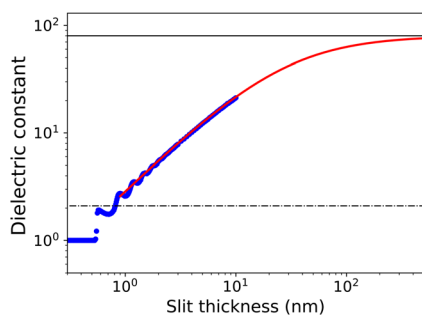
11131



Aromatic interactions with heterocycles in water

Gloria Tobajas-Curiel, Qingqing Sun, Jeremy K. M. Sanders, Pablo Ballester* and Christopher A. Hunter*

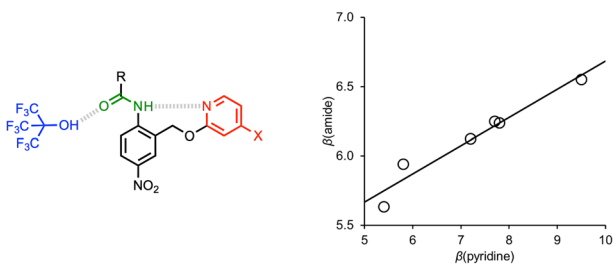
11141



Dielectric response of confined water films from a classical density functional theory perspective

Daniel Borgis,* Damien Laage, Luc Belloni and Guillaume Jeanmairet

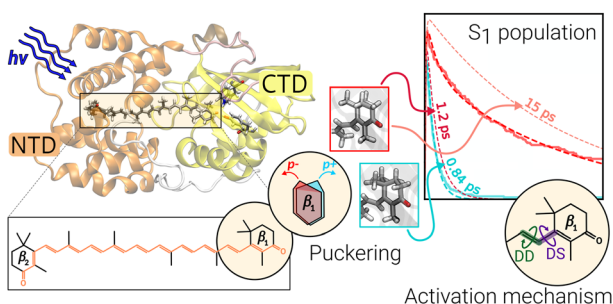
11151



Polarisation effects on the H-bond acceptor properties of secondary amides

Fergal E. Hanna, Alexander J. Root and Christopher A. Hunter*

11158



How orange carotenoid protein controls the excited state dynamics of canthaxanthin

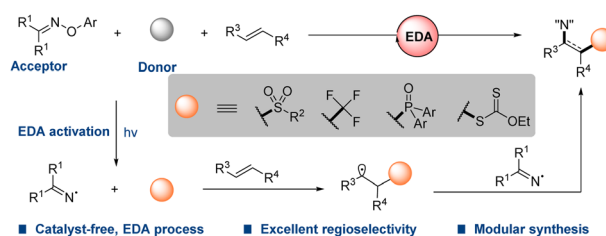
Amanda Arcidiacono, Davide Accomasso, Lorenzo Cupellini and Benedetta Mennucci*



11170

Photo-induced imino functionalizations of alkenes via intermolecular charge transfer

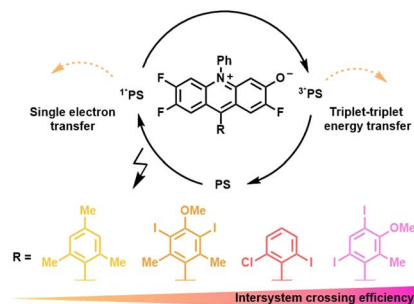
Xiang-Xin Zhang, Hao Zheng, Yong-Kang Mei, Yan Liu, Ying-Ying Liu, Ding-Wei Ji, Boshun Wan and Qing-An Chen*



11180

Isoacridone dyes with parallel reactivity from both singlet and triplet excited states for biphotonic catalysis and upconversion

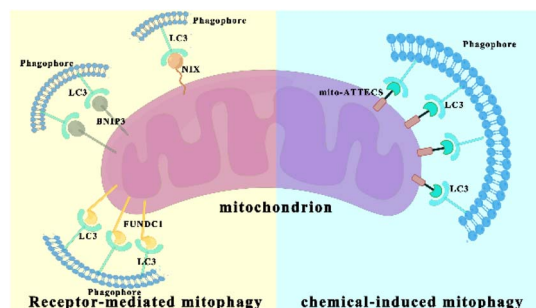
Björn Pfund, Valeriia Hutskalova, Christof Sparr* and Oliver S. Wenger*



11192

Targeting mitochondrial degradation by chimeric autophagy-tethering compounds

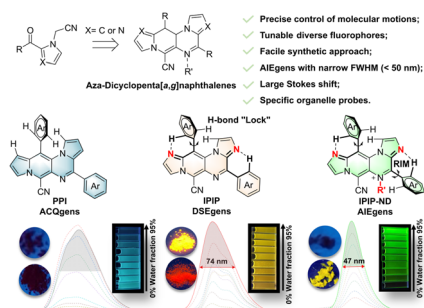
Zhenqi Liu, Geng Qin, Jie Yang, Wenjie Wang, Wenting Zhang, Boxun Lu,* Jinsong Ren and Xiaogang Qu*



11203

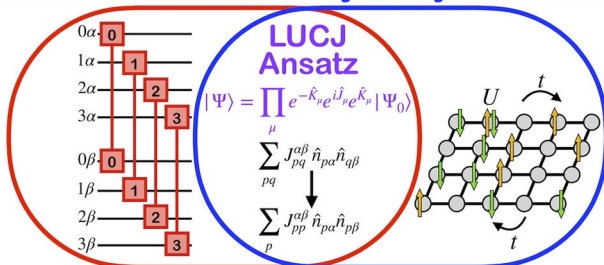
Aza-dicyclopenta[a,g]naphthalenes: controllable seesaw-like emissive behavior and narrowband AIEgens

Jinbiao Li, Jiixin Lao and Hongbin Zou*



11213

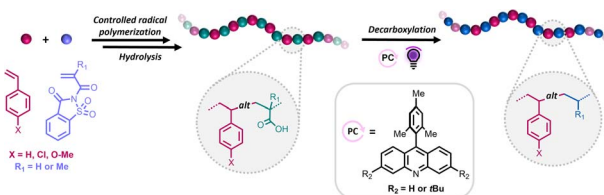
Hardware-efficient Physically-motivated



Bridging physical intuition and hardware efficiency for correlated electronic states: the local unitary cluster Jastrow ansatz for electronic structure

Mario Motta,* Kevin J. Sung, K. Birgitta Whaley, Martin Head-Gordon and James Shee*

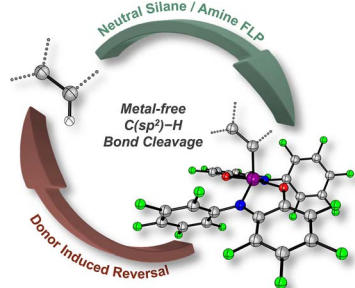
11228



Alternating styrene-propylene and styrene-ethylene copolymers prepared by photocatalytic decarboxylation

Emmanuelle Schu , Dillon R. L. Rickertsen, Angie B. Korpusik, Alafate Adili, Daniel Seidel* and Brent S. Sumerlin*

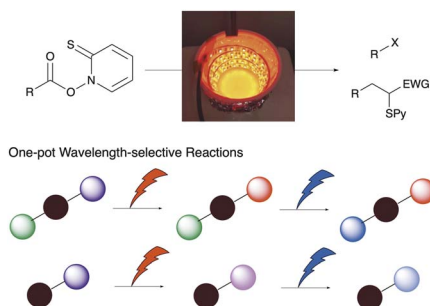
11237



Reversible C–H bond silylation with a neutral silicon Lewis acid

Thadd us Thorwart and Lutz Greb*

11243



Red-light-mediated Barton decarboxylation reaction and one-pot wavelength-selective transformations

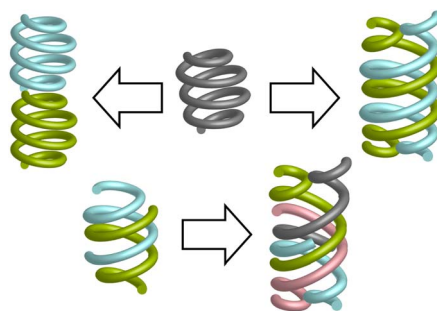
Hiroki Yamamoto, Kohei Yamaoka, Ann Shinohara, Kouhei Shibata, Ken-ichi Takao* and Akihiro Ogura*



11251

Controlling aromatic helix dimerization in water by tuning charge repulsions

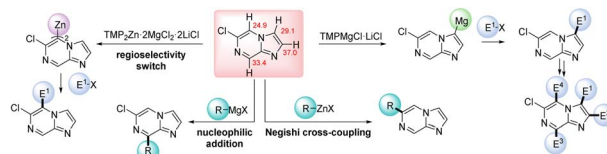
Binhao Teng, Pradeep K. Mandal, Lars Allmendinger, Céline Douat, Yann Ferrand and Ivan Huc*



11261

Calculation-assisted regioselective functionalization of the imidazo[1,2-a]pyrazine scaffold via zinc and magnesium organometallic intermediates

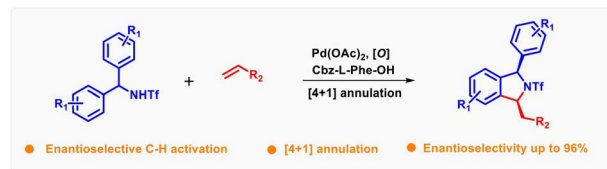
Agonist Kastrati, Alexander Kremsmair, Alisa S. Sunagatullina, Vasilii Korotenko, Yusuf C. Guersoy, Saroj K. Rout, Fabio Lima, Cara E. Brocklehurst, Konstantin Karaghiosoff, Hendrik Zipse* and Paul Knochel*



11267

A palladium catalyzed asymmetric desymmetrization approach to enantioenriched 1,3-disubstituted isoindolines

Dattatraya H. Dethe,* Vimlesh Kumar and Manmohan Shukla



11273

Water-soluble polyphosphonate-based bottlebrush copolymers via aqueous ring-opening metathesis polymerization

Diego A. Resendiz-Lara, Suna Azhdari, Hubert Gojzewski, Andre H. Gröschel and Frederik R. Wurm*

