

## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 6(3) 1593–2124 (2015)



### Cover

See Bo Wang, Ying-Wei Yang *et al.*, pp. 1640–1644.  
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### Inside cover

See Stuart L. James *et al.*, pp. 1645–1649.  
Image reproduced by permission of Stuart L. James from *Chem. Sci.*, 2015, 6, 1645.

## PERSPECTIVES

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### Experiences with a researcher-centric ELN

K. A. Badiola, C. Bird, W. S. Brocklesby, J. Casson, R. T. Chapman, S. J. Coles, J. R. Cronshaw, A. Fisher, J. G. Frey,\* D. Gloria, M. C. Grossel, D. B. Hibbert, N. Knight, L. K. Mapp, L. Marazzi, B. Matthews, A. Milsted, R. S. Minns, K. T. Mueller, K. Murphy, T. Parkinson, R. Quinnell, J. S. Robinson, M. N. Robertson, M. Robins, E. Springate, G. Tizzard, M. H. Todd, A. E. Williamson, C. Willoughby, E. Yang and P. M. Ylioja

Chemical scientists' experiences with LabTrove.

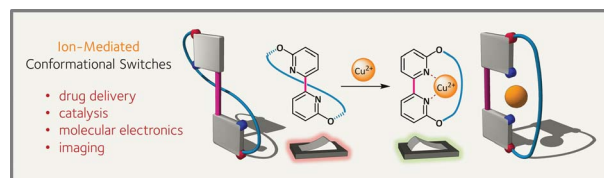


1630

### Ion-mediated conformational switches

Peter C. Knipe, Sam Thompson\* and Andrew D. Hamilton\*

The ability to control the conformation of a single molecule in a reversible and stimulus dependent manner holds great promise for fields as disparate as drug delivery and molecular electronics. Here we offer a perspective on recent developments in ion-mediated switching architectures and their ability to perform in a range of settings.



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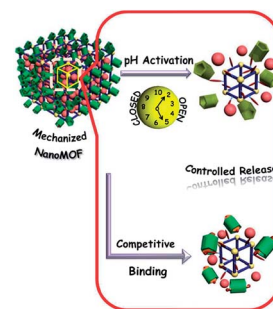


1640

### Stimuli-responsive metal–organic frameworks gated by pillar[5]arene supramolecular switches

Li-Li Tan, Haiwei Li, Yu-Chen Qiu, Dai-Xiong Chen, Xin Wang, Rui-Yi Pan, Yan Wang, Sean Xiao-An Zhang, Bo Wang\* and Ying-Wei Yang\*

Mechanized monodisperse nano metal–organic frameworks (NMOFs) gated by carboxylatopillar[5]arene (CP5) switches with bio-friendly pH-triggered release capabilities were constructed for the first time as a new stimuli-responsive theranostic hybrid platform.

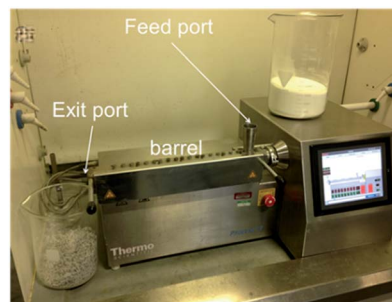


1645

### Synthesis by extrusion: continuous, large-scale preparation of MOFs using little or no solvent

Deborah Crawford, José Casaban, Robert Haydon, Nicola Giri, Tony McNally and Stuart L. James\*

Continuous flow mechanochemical and melt-phase synthesis at  $\text{kg h}^{-1}$  rates from solid reagents and either no solvent, or only minimal solvent, is reported.

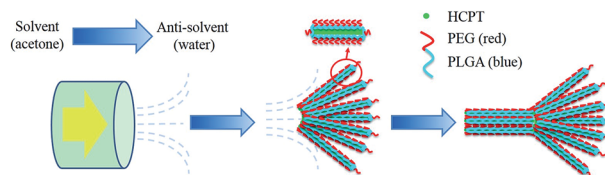


1650

### Integration of an anti-tumor drug into nanocrystalline assemblies for sustained drug release

Xiangrui Yang, Shichao Wu, Yang Li, Yu Huang, Jinyan Lin, Di Chang, Shefang Ye, Liya Xie, Yuan Jiang\* and Zhenqing Hou\*

A bio-inspired approach was used to integrate an anti-tumor drug into nanocrystalline assemblies for sustained drug release.

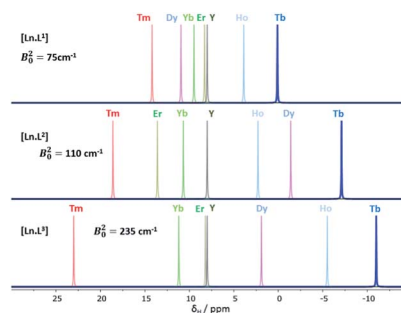


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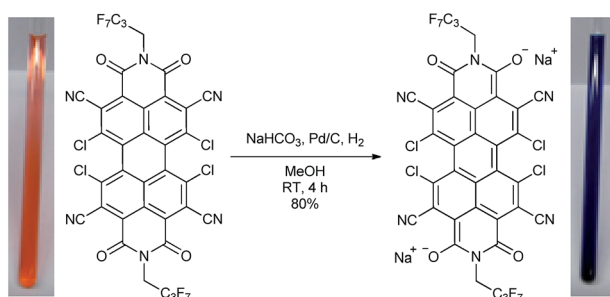
### Critical analysis of the limitations of Bleaney's theory of magnetic anisotropy in paramagnetic lanthanide coordination complexes

Alexander M. Funk, Katie-Louise N. A. Finney, Peter Harvey, Alan M. Kenwright, Emily R. Neil, Nicola J. Rogers, P. Kanthi Senanayake and David Parker\*

The origins of the breakdown of Bleaney's theory of magnetic anisotropy are described, based on an analysis of eleven different complexes of the second half of the 4f elements that form isostructural series.



1663

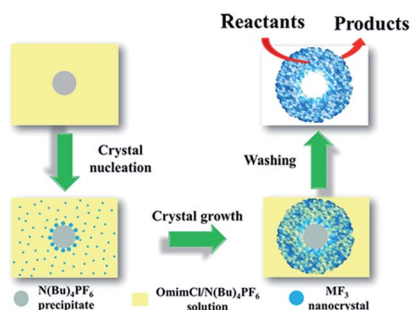


### An ambient stable core-substituted perylene bisimide dianion: isolation and single crystal structure analysis

Sabine Seifert, David Schmidt and Frank Würthner\*

The reduction of a highly electron deficient PBI afforded the corresponding dianion disodium salt that was characterized by single crystal structure analysis.

1668

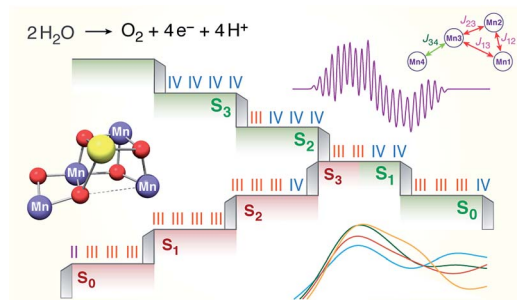


### Mesoporous inorganic salts with crystal defects: unusual catalysts and catalyst supports

Xinchen Kang, Wenting Shang, Qinggong Zhu, Jianling Zhang, Tao Jiang,\* Buxing Han,\* Zhonghua Wu, Zhihong Li and Xueqing Xing

Mesoporous LaF<sub>3</sub>, NdF<sub>3</sub>, and YF<sub>3</sub> particles with crystal defects, which are excellent catalysts and catalyst supports, have been synthesized successfully.

1676

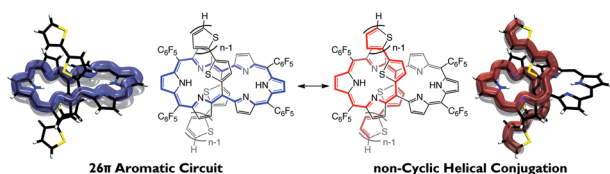


### Metal oxidation states in biological water splitting

Vera Krewald, Marius Retegan, Nicholas Cox, Johannes Messinger, Wolfgang Lubitz, Serena DeBeer, Frank Neese and Dimitrios A. Pantazis\*

A central question in biological water splitting concerns the oxidation states of the manganese ions that comprise the oxygen-evolving complex of photosystem II.

1696



### 5,20-Bis(α-oligothienyl)-substituted [26]hexaphyrins possessing electronic circuits strongly perturbed by meso-oligothienyl substituents

Hirotaka Mori, Masaaki Suzuki, Woojae Kim, Jong Min Lim, Dongho Kim\* and Atsuhiro Osuka\*

A series of [26]hexaphyrins(1.1.1.1.1.1) bearing two α-oligothienyl substituents at 5,20-positions have been synthesised and are shown to have a dumbbell hexaphyrin conformation, to which the α-oligothienyl groups are linked to form an acyclic helix-like conjugated network.



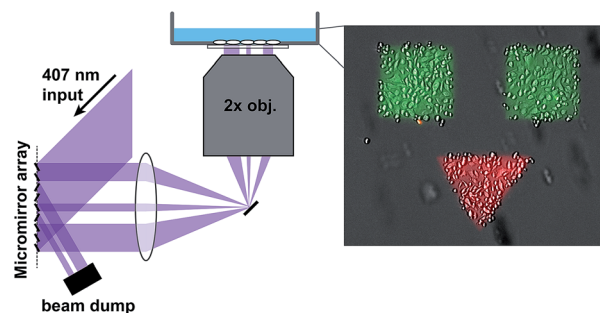


1701

### Photostick: a method for selective isolation of target cells from culture

Miao-Ping Chien, Christopher A. Werley, Samouil L. Farhi and Adam E. Cohen\*

A new method enables optical selection of one or more cells in culture *via* photochemical crosslinking to the culture dish.

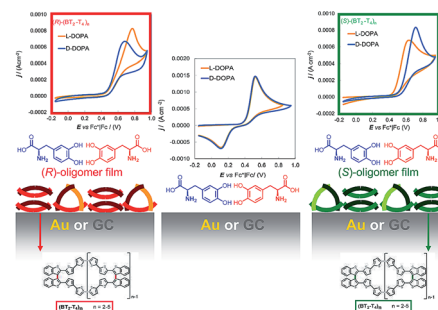


1706

### Inherently chiral electrodes: the tool for chiral voltammetry

Serena Arnaboldi,\* Tiziana Benincori, Roberto Cirilli, Włodzimierz Kutner, Mirko Magni, Patrizia Romana Mussini,\* Krzysztof Noworyta and Francesco Sannicolò\*

Artificial inherently chiral electrode surfaces perform clear enantiodiscrimination and enantiomeric ratio quantification, opening the way to chiral voltammetry.

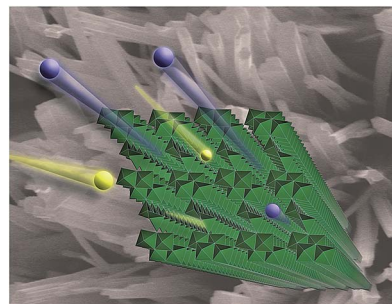


1712

### Emptying and filling a tunnel bronze

Peter M. Marley, Tesfaye A. Abtew, Katie E. Farley, Gregory A. Horrocks, Robert V. Dennis, Peihong Zhang and Sarbajit Banerjee\*

We report the synthesis of a new tunnel-structured polymorph of  $V_2O_5$  ( $\zeta$ - $V_2O_5$ ) synthesized by topotactic ion extraction.

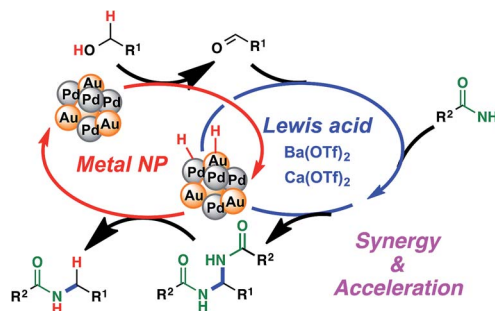


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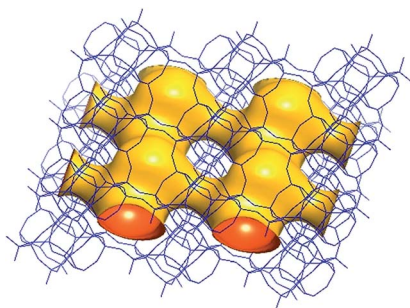
### Synergistic cascade catalysis by metal nanoparticles and Lewis acids in hydrogen autotransfer

Gerald C. Y. Choo, Hiroyuki Miyamura and Shū Kobayashi\*

Synergistic cascade catalysis of Au/Pd nanoparticles/Lewis acids achieved *N*-alkylation of primary amides to secondary amides with alcohols *via* hydrogen autotransfer.



1728

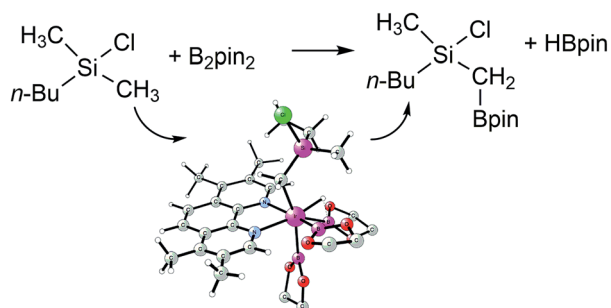


### CIT-7, a crystalline, molecular sieve with pores bounded by 8 and 10-membered rings

Joel E. Schmidt, Dan Xie, Thomas Rea and Mark E. Davis\*

CIT-7, a new microporous material that contains 8 and 10-membered rings prepared as a silicate, an aluminosilicate or titanosilicate.

1735

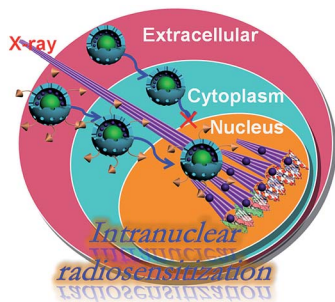


### Mechanism, reactivity, and selectivity of the iridium-catalyzed C(sp<sup>3</sup>)-H borylation of chlorosilanes

Genping Huang, Marcin Kalek, Rong-Zhen Liao and Fahmi Himo\*

DFT calculations are used to elucidate the reaction mechanism, the role of the chlorosilyl group, and primary vs. secondary and C(sp<sup>3</sup>)-H vs. C(sp<sup>2</sup>)-H selectivity of the iridium-catalyzed borylation of chlorosilanes.

1747

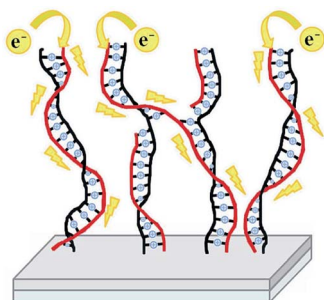


### Design of an intelligent sub-50 nm nuclear-targeting nanotheranostic system for imaging guided intranuclear radiosensitization

Wenpei Fan, Bo Shen, Wenbo Bu,\* Xiangpeng Zheng, Qianjun He, Zhaowen Cui, Kuaile Zhao, Shengjian Zhang and Jianlin Shi\*

MR/UCL bimodal imaging guided intranuclear radiosensitization was firstly achieved by an intelligent nuclear-targeting nanotheranostic system.

1754



### A facile route to electronically conductive polyelectrolyte brushes as platforms of molecular wires

Karol Wolski, Michał Szuwarzyński and Szczepan Zapotoczny\*

Conjugated polyelectrolyte brushes grafted from a conductive surface and forming a 1D macromolecular pathway for charge transport are synthesized.

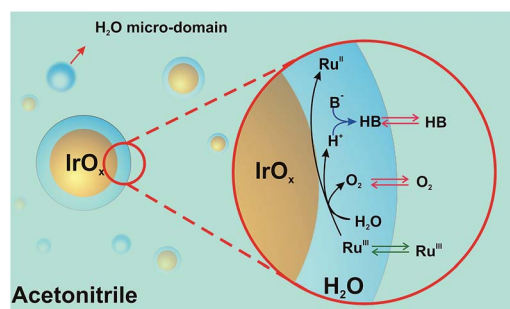


1761

### Catalysis of water oxidation in acetonitrile by iridium oxide nanoparticles

Jonnathan C. Hidalgo-Acosta, Manuel A. Méndez, Micheál D. Scanlon, Heron Vrabel, Véronique Amstutz, Wojciech Adamiak, Marcin Opallo and Hubert H. Girault\*

Micro-domains of water molecules surrounded by organic solvent exhibit enhanced reactivity towards oxidation compared to highly hydrogen-bonded bulk water molecules.

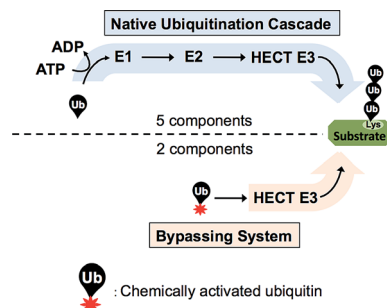


1770

### Protein ubiquitination and formation of polyubiquitin chains without ATP, E1 and E2 enzymes

Sungjin Park, David T. Krist and Alexander V. Statsyuk\*

Protein ubiquitination without ATP. This paper reports a chemical strategy to ubiquitinate proteins without ATP, E1, and E2 enzymes, offering new insights on the biochemical mechanism of E3s.

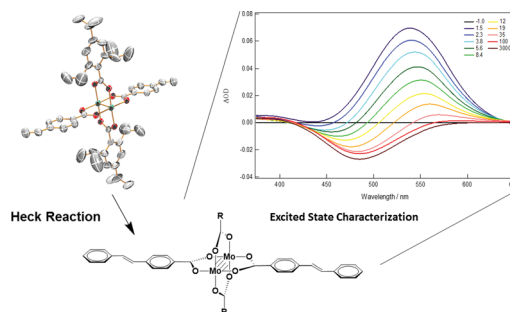


1780

### MM quadruply bonded complexes supported by vinylbenzoate ligands: synthesis, characterization, photophysical properties and application as synthons

Samantha E. Brown-Xu, Malcolm H. Chisholm,\* Christopher B. Durr, Thomas F. Spilker and Philip J. Young

MM complexes as potential synthons for the development of higher order extended structures via Heck coupling reactions, exhibiting interesting photophysical properties.

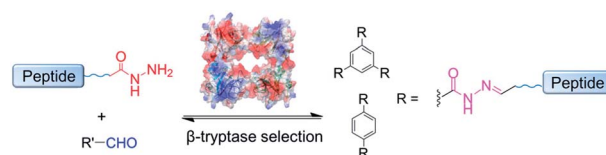


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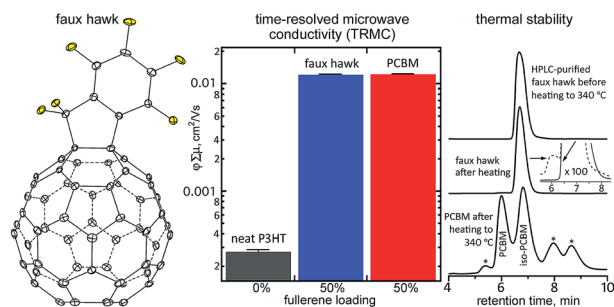
### Discovery of potent inhibitors of human $\beta$ -tryptase from pre-equilibrated dynamic combinatorial libraries

Qian-Qian Jiang, Wilhelm Sicking, Martin Ehlers and Carsten Schmuck\*

Pre-equilibrated combinatorial libraries based on multivalent peptide acyl hydrazones were used to find potent inhibitors of  $\beta$ -tryptase. The best inhibitors bind to the protein surface, and inhibit  $\beta$ -tryptase with nanomolar affinity ( $K_i$  ca. 10 nM) and high selectivity in a reversible and non-competitive way.



1801

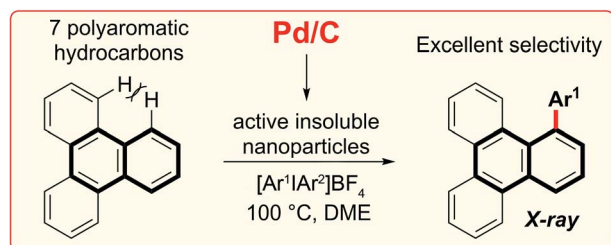


### A faux hawk fullerene with PCBM-like properties

Long K. San, Eric V. Bukovsky, Bryon W. Larson, James B. Whitaker, S. H. M. Deng, Nikos Kopidakis,<sup>\*</sup> Garry Rumbles,<sup>\*</sup> Alexey A. Popov,<sup>\*</sup> Yu-Sheng Chen,<sup>\*</sup> Xue-Bin Wang,<sup>\*</sup> Olga V. Boltalina<sup>\*</sup> and Steven H. Strauss<sup>\*</sup>

A fluorinated faux hawk fullerene with comparable OPV-relevant TRMC performance and far greater thermal stability than PCBM is reported.

1816

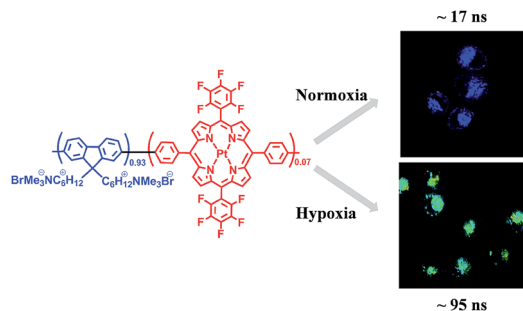


### C–H arylation of triphenylene, naphthalene and related arenes using Pd/C

Karl D. Collins, Roman Honeker, Suhelen Vásquez-Céspedes, Dan-Tam D. Tang and Frank Glorius<sup>\*</sup>

A highly selective arylation of a number of polyaromatic hydrocarbons (PAHs) with arylodonium salts and Pd/C as the only reagent is reported.

1825

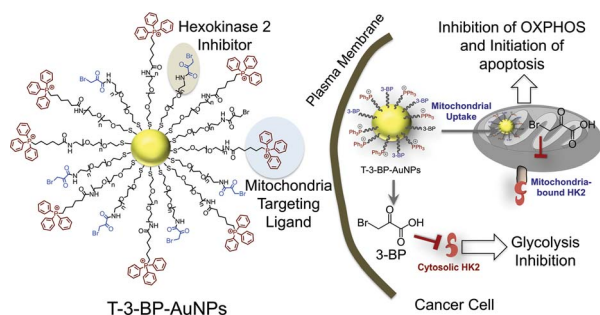


### Fluorescent/phosphorescent dual-emissive conjugated polymer dots for hypoxia bioimaging

Qiang Zhao,<sup>\*</sup> Xiaobo Zhou, Tianye Cao, Kenneth Yin Zhang, Lijuan Yang, Shujuan Liu, Hua Liang, Huiran Yang, Fuyou Li<sup>\*</sup> and Wei Huang<sup>\*</sup>

Fluorescent/phosphorescent dual-emissive conjugated polymer dots were designed and synthesized, which were used for tumor hypoxia sensing *via* ratiometric imaging and photoluminescence lifetime imaging.

1832



### The energy blocker inside the power house: mitochondria targeted delivery of 3-bromopyruvate

Sean Marrache and Shanta Dhar<sup>\*</sup>

Mitochondrial delivery of 3-bromopyruvate for metabolic reprogramming of cancer cells.



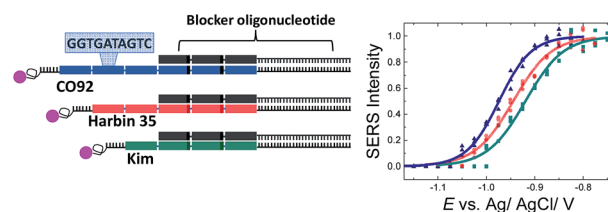


1846

### Strain discrimination of *Yersinia pestis* using a SERS-based electrochemically driven melting curve analysis of variable number tandem repeat sequences

E. Papadopoulou, N. Gale, S. A. Goodchild, D. W. Cleary, S. A. Weller, T. Brown and P. N. Bartlett\*

Variable number tandem repeats in DNA extracted from three bacterial *Y. pestis* strains have been differentiated using *E*-melting analysis monitored by SERS, combined with the use of a blocker oligonucleotide.

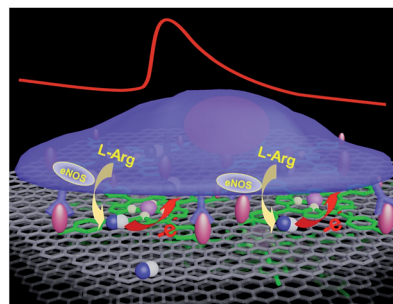


1853

### Functionalized graphene-based biomimetic microsensor interfacing with living cells to sensitively monitor nitric oxide release

Yan-Ling Liu, Xue-Ying Wang, Jia-Quan Xu, Chong Xiao, Yan-Hong Liu, Xin-Wei Zhang, Jun-Tao Liu and Wei-Hua Huang\*

We present a biomimetic and reusable microsensor with sub-nanomolar sensitivity by elaborate functionalizing graphene for monitoring NO release in real-time.

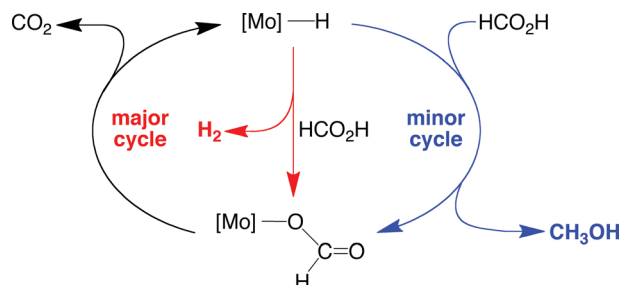


1859

### Dehydrogenation, disproportionation and transfer hydrogenation reactions of formic acid catalyzed by molybdenum hydride compounds

Michelle C. Neary and Gerard Parkin\*

Cyclopentadienyl molybdenum hydride compounds are catalysts for dehydrogenation, disproportionation and transfer hydrogenation reactions of formic acid, in which the latter provides a means to reduce aldehydes and ketones.

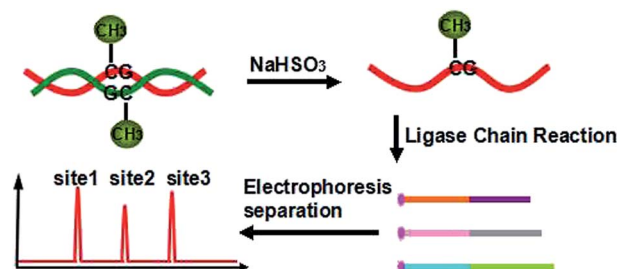


1866

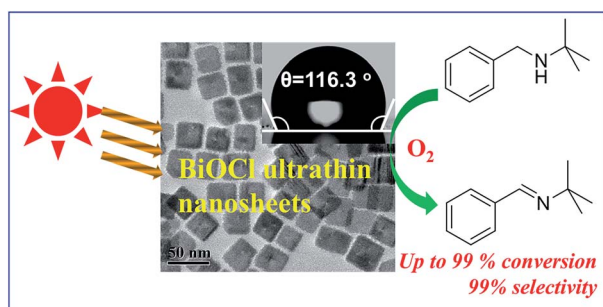
### Highly sensitive and multiplexed analysis of CpG methylation at single-base resolution with ligation-based exponential amplification

Fengxia Su, Limei Wang, Yueying Sun, Chenghui Liu, Xinrui Duan and Zhengping Li\*

Multiple CpG methylation can be accurately detected in one-tube ligase chain reaction (LCR) amplification with high sensitivity and specificity.



1873

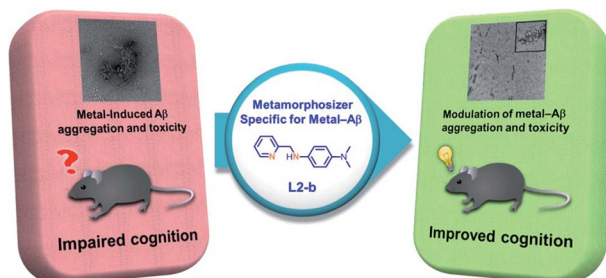


### Well-defined BiOCl colloidal ultrathin nanosheets: synthesis, characterization, and application in photocatalytic aerobic oxidation of secondary amines

Yihui Wu, Bo Yuan, Mingrun Li, Wen-Hua Zhang,\* Yan Liu\* and Can Li\*

Well-defined BiOCl ultrathin nanosheets were prepared by a facile colloidal route, and exhibit high photocatalytic performance toward the oxidation of secondary amines to corresponding imines under visible irradiation.

1879

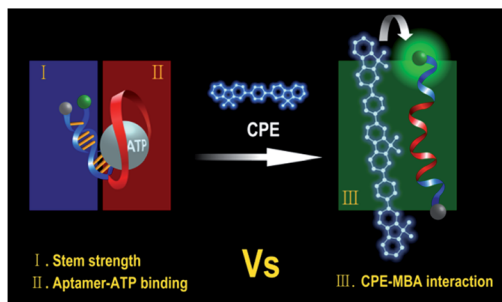


### A rationally designed small molecule for identifying an *in vivo* link between metal-amyloid- $\beta$ complexes and the pathogenesis of Alzheimer's disease

Michael W. Beck, Shin Bi Oh, Richard A. Kerr, Hyuck Jin Lee, So Hee Kim, Sujeong Kim, Milim Jang, Brandon T. Ruotolo,\* Joo-Yong Lee\* and Mi Hee Lim\*

An *in vivo* chemical tool designed to target metal-A $\beta$  complexes and modulate their activity was applied to the 5XFAD mouse model of Alzheimer's disease (AD) demonstrating the involvement of metal-A $\beta$  in AD pathology.

1887

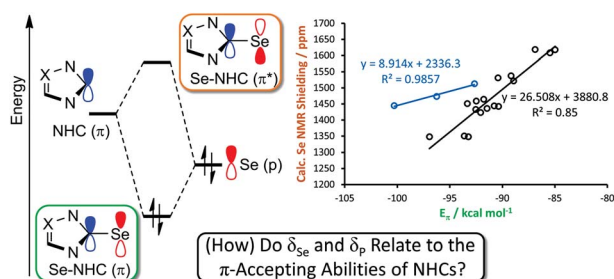


### Principal factors that determine the extension of detection range in molecular beacon aptamer/conjugated polyelectrolyte bioassays

Ji-Eun Jeong, Boram Kim, Shinjae Woo, Sungu Hwang, Guillermo C. Bazan\* and Han Young Woo\*

A new bioassay strategy based on the molecular beacon aptamer/conjugated polyelectrolyte demonstrates a fine-tuning of the detection range and limit of detection for weakly-binding targets.

1895



### What can NMR spectroscopy of selenoureas and phosphinidenes teach us about the $\pi$ -accepting abilities of *N*-heterocyclic carbenes?

Sai V. C. Vummaleti, David J. Nelson, Albert Poater, Adrián Gómez-Suárez, David B. Cordes, Alexandra M. Z. Slawin, Steven P. Nolan\* and Luigi Cavallo\*

The relationship between the NMR chemical shifts of phosphinidene and selenourea compounds and the  $\pi$ -accepting ability of the related carbene ligands has been investigated.

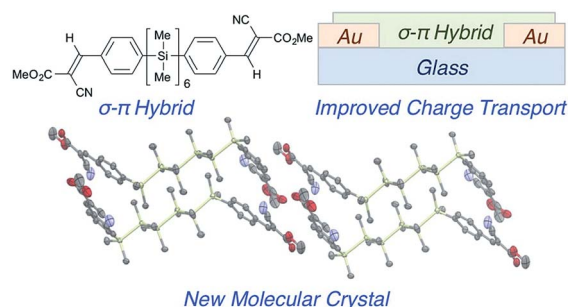


1905

### Increased carrier mobility in end-functionalized oligosilanes

S. Surampudi, M.-L. Yeh, M. A. Siegler, J. F. Martinez Hardigree, T. A. Kasl, H. E. Katz and R. S. Klausen\*

A class of hybrid oligosilane–arene materials outperforms the  $\sigma$ - and  $\pi$ -conjugated parent structures.

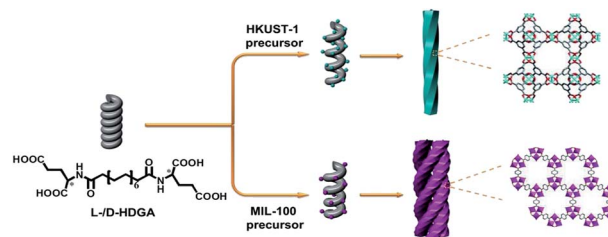


1910

### Helically structured metal–organic frameworks fabricated by using supramolecular assemblies as templates

Hui Wang, Wei Zhu, Jian Li, Tian Tian, Yue Lan, Ning Gao, Chen Wang, Meng Zhang, Charl F. J. Faul and Guangtao Li\*

Here we report on the use of a self-assembled organic object to template the first example of a nanoscale metal–organic framework (MOF) with a helical morphology.

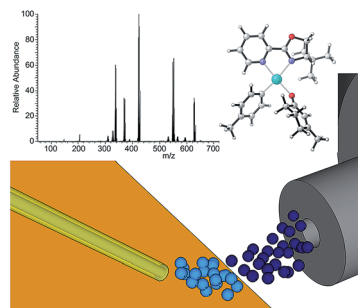


1917

### Mechanistic analysis of an asymmetric palladium-catalyzed conjugate addition of arylboronic acids to $\beta$ -substituted cyclic enones

Cornelia L. Boeser, Jeffrey C. Holder, Buck L. H. Taylor, K. N. Houk, Brian M. Stoltz and Richard N. Zare\*

Mechanistic insight into a Pd-catalyzed conjugate addition reaction was gained using desorption electrospray ionization coupled to mass spectrometry.

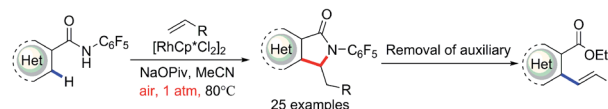


1923

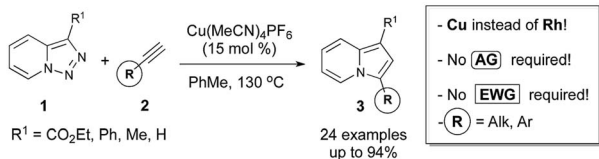
### Rh(III)-catalyzed C–H olefination of *N*-pentafluoroaryl benzamides using air as the sole oxidant

Yi Lu,\* Huai-Wei Wang, Jillian E. Spangler, Kai Chen, Pei-Pei Cui, Yue Zhao, Wei-Yin Sun\* and Jin-Quan Yu\*

Rhodium(III)-catalyzed C–H olefination reaction using air as the sole oxidant.



1928

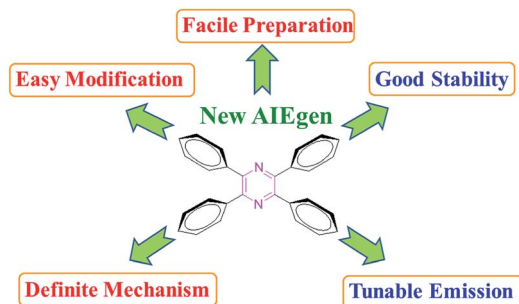
**This work:**

### Cu-catalyzed transannulation reaction of pyridotriazoles with terminal alkynes under aerobic conditions: efficient synthesis of indolizines

V. Helan, A. V. Gulevich and V. Gevorgyan\*

A Cu(I)-catalyzed denitrogenative transannulation reaction of pyridotriazoles with terminal alkynes en route to indolizines was developed.

1932

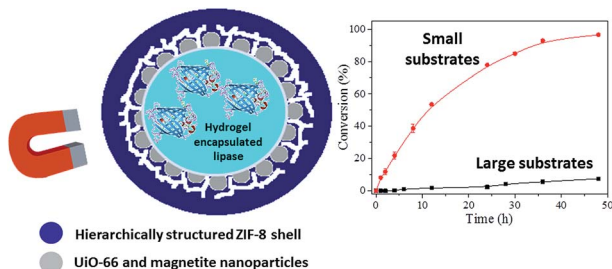


### Tetraphenylpyrazine-based AIEgens: facile preparation and tunable light emission

Ming Chen, Lingzhi Li, Han Nie, Jiaqi Tong, Lulin Yan, Bin Xu, Jing Zhi Sun, Wenjing Tian, Zujin Zhao, Anjun Qin\* and Ben Zhong Tang\*

Structurally new AIEgens with tunable emission based on tetraphenylpyrazine were rationally designed and readily prepared.

1938

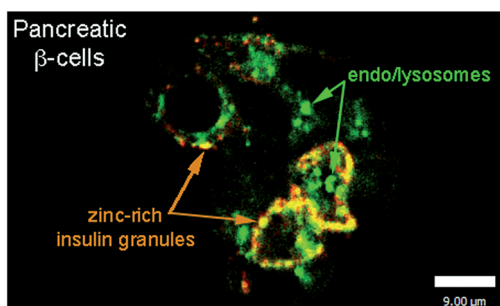


### Magnetic MOF microreactors for recyclable size-selective biocatalysis

Jia Huo, Jordi Aguilera-Sigalat, Samir El-Hankari and Darren Bradshaw\*

Highly porous magnetic MOF microreactors can be prepared around a Pickering-stabilized hydrogel core, providing a facile means for the encapsulation of enzymes for size-selective biocatalysis.

1944



### A far-red emitting probe for unambiguous detection of mobile zinc in acidic vesicles and deep tissue

Pablo Rivera-Fuentes, Alexandra T. Wrobel, Melissa L. Zastrow, Mustafa Khan, John Georgiou, Thomas T. Luyben, John C. Roder, Kenichi Okamoto and Stephen J. Lippard\*

A fluorescent sensor that is pH-insensitive and compatible with two-photon microscopy was developed and applied to live cell and deep tissue imaging.

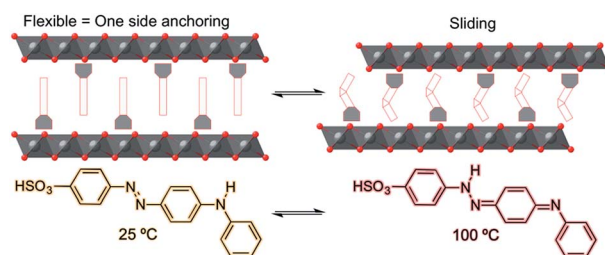


1949

### Stimuli-responsive hybrid materials: breathing in magnetic layered double hydroxides induced by a thermoresponsive molecule

Gonzalo Abellán, Jose Luis Jordá, Pedro Atienzar, María Varela, Miriam Jaafar, Julio Gómez-Herrero, Félix Zamora, Antonio Ribera, Hermenegildo García\* and Eugenio Coronado\*

A hybrid magnetic multilayer material consisting of CoAl-LDH ferromagnetic layers intercalated with thermoresponsive molecules diluted with a flexible surfactant has been obtained.

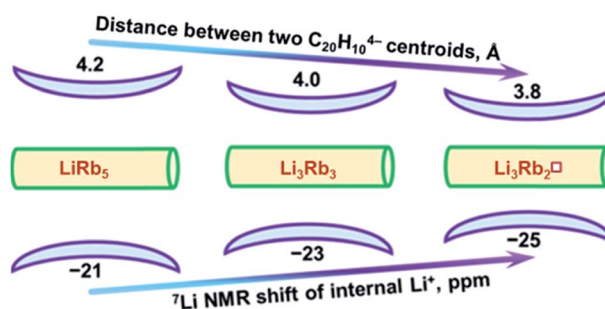


1959

### Self-assembly of tetra-reduced corannulene with mixed Li-Rb clusters: dynamic transformations, unique structures and record $^7\text{Li}$ NMR shifts

Alexander S. Filatov, Sarah N. Spisak, Alexander V. Zabula, James McNeely, Andrey Yu. Rogachev and Marina A. Petrukina\*

The record NMR shifts for the centrally encapsulated lithium ions are correlated with molecular and electronic structures of novel mixed alkali metal sandwiches.

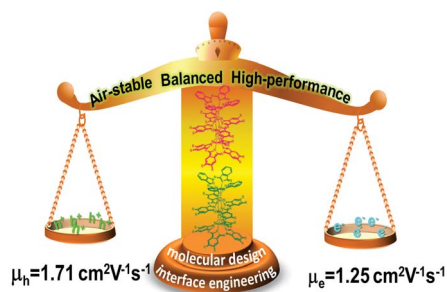


1967

### Air-stable ambipolar field-effect transistor based on a solution-processed octanaphthoxy-substituted tris(phthalocyaninato) europium semiconductor with high and balanced carrier mobilities

Xia Kong, Xia Zhang, Dameng Gao, Dongdong Qi, Yanli Chen\* and Jianzhuang Jiang\*

Simple solvent vapor annealing over QLS film-based OFET devices fabricated from  $(\text{Pc})\text{Eu}[\text{Pc}(\text{ONh})_8]\text{Eu}[\text{Pc}(\text{ONh})_8]$  led to a high and balanced ambipolar performance.

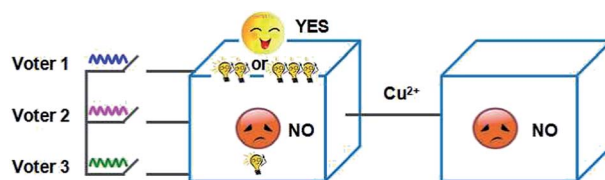


1973

### DNA-based visual majority logic gate with one-vote veto function

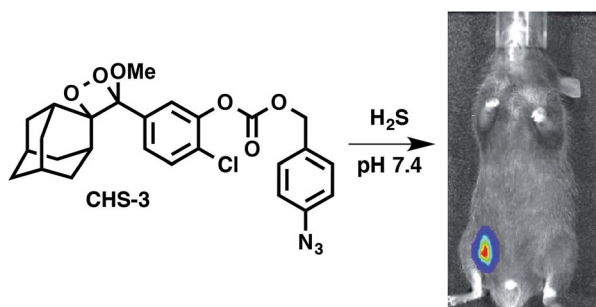
Daoqing Fan, Kun Wang, Jinbo Zhu, Yong Xia, Yanchao Han, Yaqing Liu\* and Erkang Wang\*

A label-free and enzyme-free three-input majority logic gate with one-vote veto function was developed for the first time.





1979

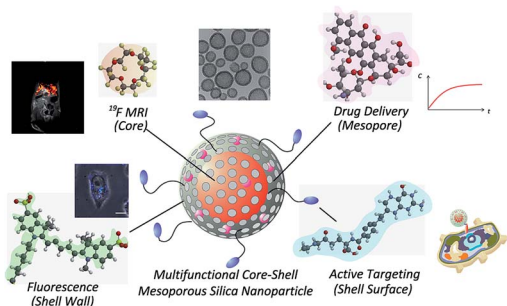


### Chemiluminescent probes for imaging H<sub>2</sub>S in living animals

J. Cao, R. Lopez, J. M. Thacker, J. Y. Moon, C. Jiang, S. N. S. Morris, J. H. Bauer, P. Tao, R. P. Mason and A. R. Lippert\*

Responsive 1,2-dioxetane chemiluminescent probes have been developed that display instantaneous, sensitive, and selective responses to H<sub>2</sub>S and are capable of imaging H<sub>2</sub>S in living mice.

1986

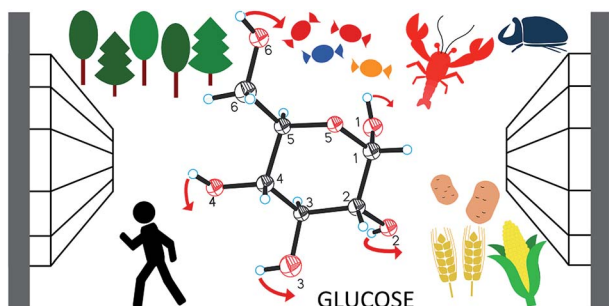


### Mesoporous silica nanoparticles for <sup>19</sup>F magnetic resonance imaging, fluorescence imaging, and drug delivery

Tatsuya Nakamura, Fuminori Sugihara, Hisashi Matsushita, Yoshichika Yoshioka, Shin Mizukami and Kazuya Kikuchi\*

We described perfluorocarbon encapsulated in mesoporous silica nanoparticles which enabled dual modal imaging (NIR/<sup>19</sup>F MRI) and drug delivery.

1991

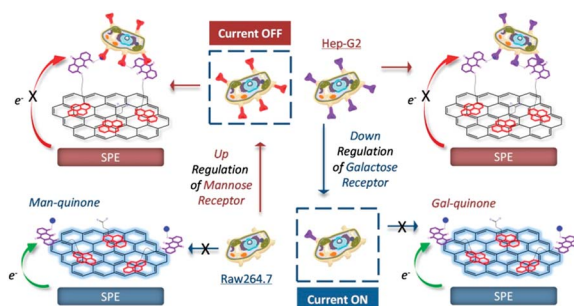


### Transformable H-bonds and conformation in compressed glucose

Ewa Patyk and Andrzej Katrusiak\*

Upon pressurisation above 5.4 GPa, α-D-glucose transforms into a new polymorph, with an altered molecular conformation and with intermolecular hydrogen bonds reshuffled.

1996



### Dynamic tracking of pathogenic receptor expression of live cells using pyrenyl glycoanthraquinone-decorated graphene electrodes

Xiao-Peng He,\* Bi-Wen Zhu, Yi Zang, Jia Li,\* Guo-Rong Chen, He Tian and Yi-Tao Long\*

Dynamic tracking of pathogenic receptor expression with live cells is made possible by pyrenyl glycoanthraquinones decorated on graphene electrodes.

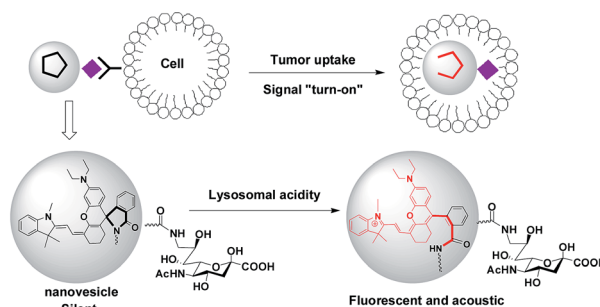


2002

### A carbohydrate-grafted nanovesicle with activatable optical and acoustic contrasts for dual modality high performance tumor imaging

Xuanjun Wu, Bijuan Lin, Mingzhu Yu, Liu Yang, Jiahuai Han and Shoufa Han\*

High-performance illumination of subcutaneous tumor and liver tumor foci was achieved with sialic acid-targeted acid-responsive nanovesicles which become fluorescent and photoacoustic upon internalization into tumor lysosomes.

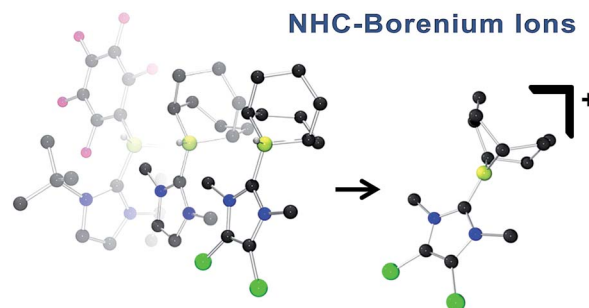


2010

### A family of N-heterocyclic carbene-stabilized borenium ions for metal-free imine hydrogenation catalysis

Jeffrey M. Farrell, Roy T. Posaratnanathan and Douglas W. Stephan\*

Room-temperature metal-free hydrogenation catalysis.

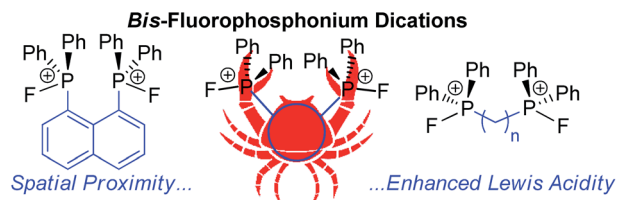


2016

### Electrophilic bis-fluorophosphonium dications: Lewis acid catalysts from diphosphines

Michael H. Holthausen, Rashi R. Hiranandani and Douglas W. Stephan\*

A series of electrophilic bis-fluorophosphonium dications derived from diphosphines with naphthalene- and (oligo)-methylene-linkers is presented. The resulting Lewis acidity is demonstrated to depend on the spatial proximity between the P moieties as evidenced in several Lewis acid catalyzed transformations.



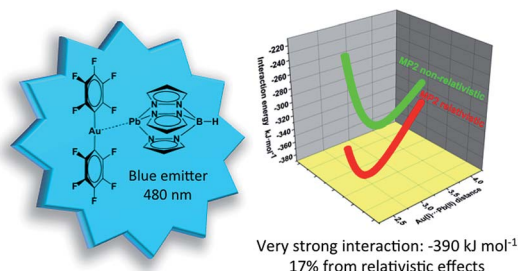
2022

### The gold(I)⋯lead(II) interaction: a relativistic connection

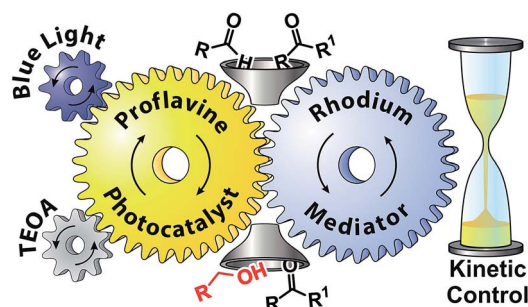
Raquel Echeverría, José M. López-de-Luzuriaga,\* Miguel Monge and M. Elena Olmos

The heteronuclear complex  $[\text{Pb}(\text{HB}(\text{pz})_3)\text{Au}(\text{C}_6\text{Cl}_5)_2]$  is a blue emitter in the solid state and displays an unprecedented and unsupported  $\text{Au}(\text{I})\cdots\text{Pb}(\text{II})$  contact. *Ab initio* calculations show a very strong metallophilic interaction that is greatly influenced by relativistic effects.

#### Unsupported $\text{Au}(\text{I})\cdots\text{Pb}(\text{II})$ closed-shell interaction



2027

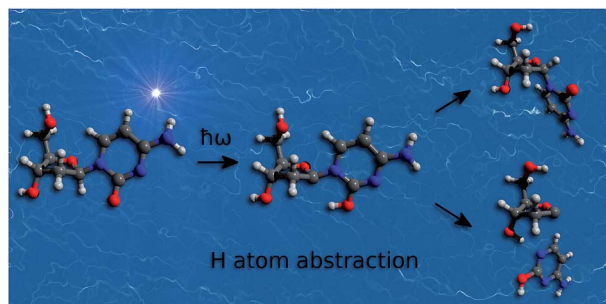


### Visible light photocatalytic reduction of aldehydes by Rh(III)-H: a detailed mechanistic study

T. Ghosh, T. Slanina and B. König\*

The slow visible light mediated generation of a rhodium hydride allows the chemoselective reduction of aldehydes in the presence of ketones. Electron transfer from the chromophore to the metal complex proceeds *via* a radical anion intermediate or a solvated electron as two competing reaction pathways.

2035

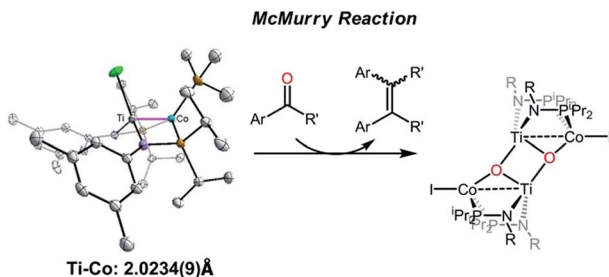


### Excited-state hydrogen atom abstraction initiates the photochemistry of $\beta$ -2'-deoxycytidine

Rafat Szabla,\* Jesús Campos, Judit E. Šponer, Jiří Šponer, Robert W. Góra\* and John D. Sutherland\*

H-D exchange experiments and quantum-chemical calculations elucidate the mechanism of photoinduced anomerisation and nucleobase loss reactions observed in  $\beta$ -2'-deoxycytidine.

2044

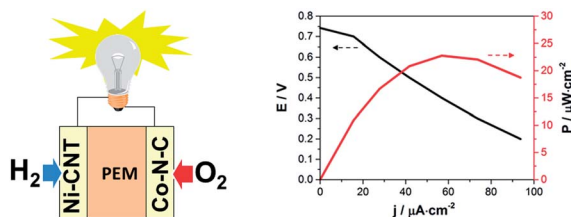


### A heterobimetallic complex featuring a Ti-Co multiple bond and its application to the reductive coupling of ketones to alkenes

Bing Wu, Mark W. Bezpalko, Bruce M. Foxman and Christine M. Thomas\*

A Ti/Co heterobimetallic complex featuring a very short metal-metal triple bond has been synthesized. This complex promotes the reductive coupling reaction of aryl ketones into alkenes.

2050



### A noble metal-free proton-exchange membrane fuel cell based on bio-inspired molecular catalysts

P. D. Tran, A. Morozan, S. Archambault, J. Heidkamp, P. Chenevier, H. Dau, M. Fontecave, A. Martinent,\* B. Joussetme\* and V. Artero\*

Bio-inspired chemistry allowed for the development of the first noble metal-free polymer electrolyte membrane hydrogen fuel cell (PEMFC). The device proved operational under technologically relevant conditions.

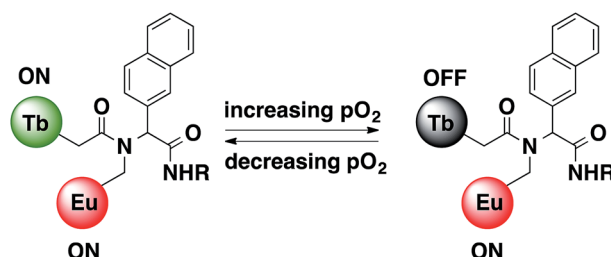


2054

### Bimetallic lanthanide complexes that display a ratiometric response to oxygen concentrations

Thomas Just Sørensen,<sup>\*</sup> Alan M. Kenwright<sup>\*</sup> and Stephen Faulkner<sup>\*</sup>

Heterometallic lanthanide complexes can display a ratiometric response to oxygen concentrations.

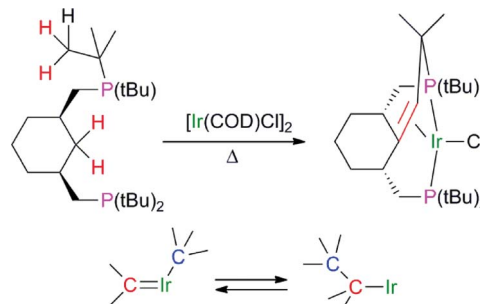


2060

### Formation of a C–C double bond from two aliphatic carbons. Multiple C–H activations in an iridium pincer complex

Alexey V. Polukeev, Rocío Marcos, Mårten S. G. Ahlquist and Ola F. Wendt<sup>\*</sup>

Iridium can mediate a reversible intramolecular coupling reaction involving up to four unactivated C<sub>sp</sub><sup>3</sup>–H bonds, to give a carbon–carbon double bond.

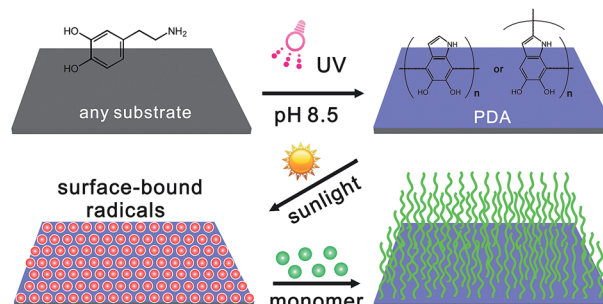


2068

### Brushing up from “anywhere” under sunlight: a universal surface-initiated polymerization from polydopamine-coated surfaces

Wenbo Sheng, Bin Li, Xiaolong Wang, Bin Dai, Bo Yu,<sup>\*</sup> Xin Jia<sup>\*</sup> and Feng Zhou<sup>\*</sup>

A generalized surface-initiated photografting procedure, which utilizes polydopamine as a photosensitive initiating layer, allows functionalization of almost any substrate with thin polymer films under sunlight.

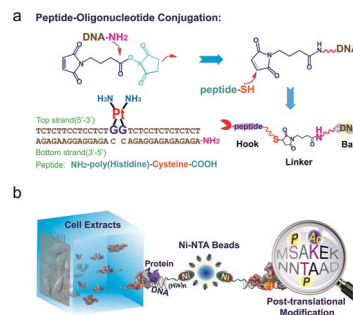


2074

### HMGB1 bound to cisplatin–DNA adducts undergoes extensive acetylation and phosphorylation *in vivo*

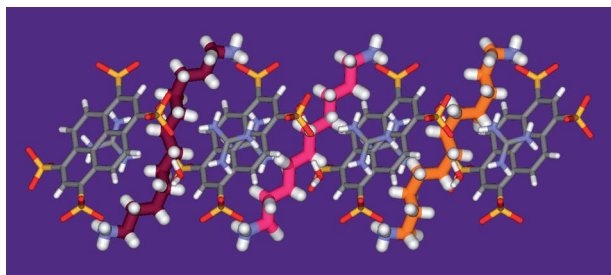
Yafeng He, Yin Ding, Dan Wang, Wanjun Zhang, Weizhong Chen, Xichun Liu, Weijie Qin, Xiaohong Qian, Hao Chen<sup>\*</sup> and Zijian Guo<sup>\*</sup>

Here, an application of a biomolecular probe based on a peptide–oligonucleotide conjugate is presented as a novel method for investigating the recognition of cisplatin–DNA lesions by HMGB1 *in vivo*.





2079

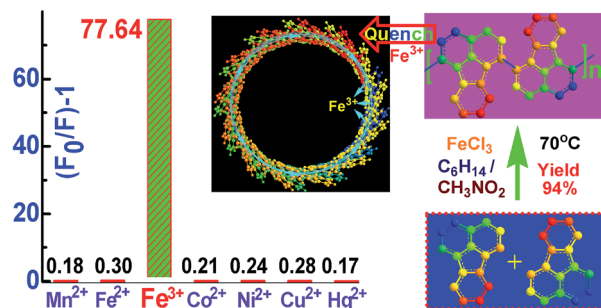


### Adaptive binding and selection of compressed 1,ω-diammonium-alkanes *via* molecular encapsulation in water

Dan Dumitrescu, Yves-Marie Legrand, Eddy Petit, Arie van der Lee and Mihail Barboiu\*

Alkane chains may be encapsulated inside rigid crystalline capsules, adopting specific conformations of different levels of compression that are sufficiently kinetically stable under the confined conditions, to allow a conventional structure determination by X-ray diffraction.

2087

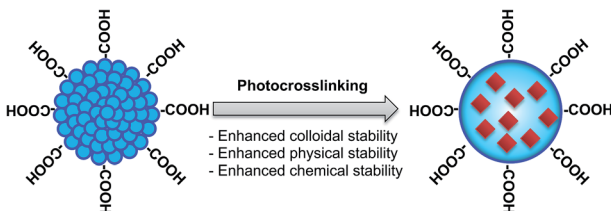


### Interfacial chemical oxidative synthesis of multifunctional polyfluoranthene

Xin-Gui Li,\* Yaozu Liao, Mei-Rong Huang\* and Richard B. Kaner\*

Polyfluoranthene, synthesized by an interfacial cationic oxidative polymerization of fluoranthene, emits visible fluorescence that shows highly selective sensitivity to Fe<sup>3+</sup>.

2102

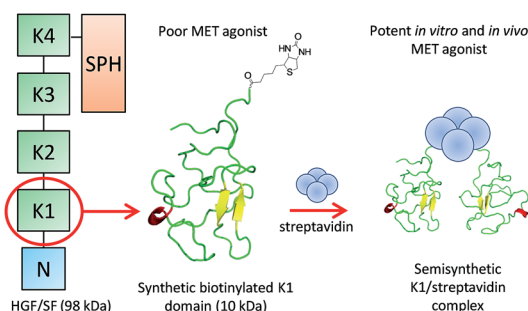


### Light-induced crosslinkable semiconducting polymer dots

Yue Zhang, Fangmao Ye, Wei Sun, Jiangbo Yu, I-Che Wu, Yu Rong, Yong Zhang and Daniel T. Chiu\*

This paper describes photocrosslinkable Pdots with enhanced colloidal, physical, and chemical stability, and excellent encapsulating ability of functional small molecules.

2110



### Semi-synthesis of a HGF/SF kringle one (K1) domain scaffold generates a potent *in vivo* MET receptor agonist

Claire Simonneau, Bérénice Leclercq, Alexandra Mougel, Eric Adriaenssens, Charlotte Paquet, Laurent Raibaut, Nathalie Ollivier, Hervé Drobecq, Julien Marcoux, Sarah Cianférani, David Tulasne, Hugo de Jonge, Oleg Melnyk\* and Jérôme Vicogne\*

Clustering of synthetic biotinylated K1 domain from HGF/SF by streptavidin is sufficient to generate a potent MET agonist.





## CORRECTION

2122

**Correction: Utilizing the bioorthogonal base-pairing system of L-DNA to design ideal DNA nanocarriers for enhanced delivery of nucleic acid cargos**

Kyoung-Ran Kim, Taemin Lee, Byeong-Su Kim and Dae-Ro Ahn\*

