

# Chemical Science

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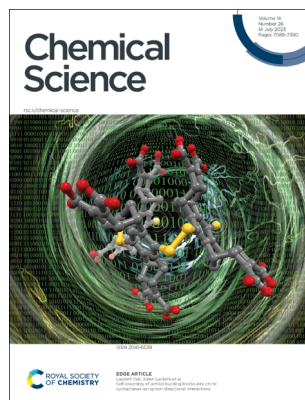
## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 14(26) 7089–7396 (2023)



### Cover

See Wei Han, King Lun Yeung *et al.*, pp. 7114–7125.  
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### Inside cover

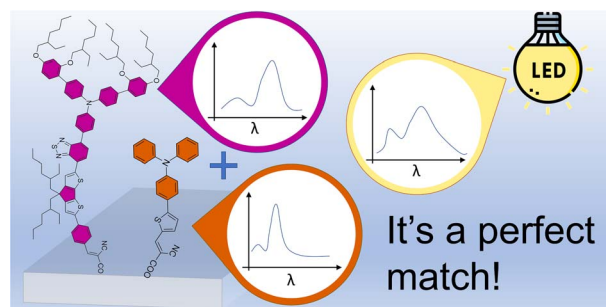
See Laurent Vial, Julien Leclaire *et al.*, pp. 7126–7135.  
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## COMMENTARY

7101

### A focus on sustainable energy management for self-powered IoT devices via indoor photovoltaics

Pablo Docampo\*



## PERSPECTIVE

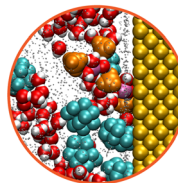
7103

### Fine tuning of electrosynthesis pathways by modulation of the electrolyte solvation structure

Florian Dorchies and Alexis Grimaud\*

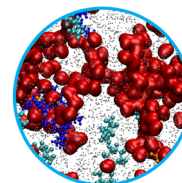
#### Electrochemical Interface

Double layer  
Hydrophilicity/hydrophobicity  
Substrate/product adsorptions



#### Bulk Electrolyte

Substrate/product solvations  
Hydrogen bonding  
Nanostructuring



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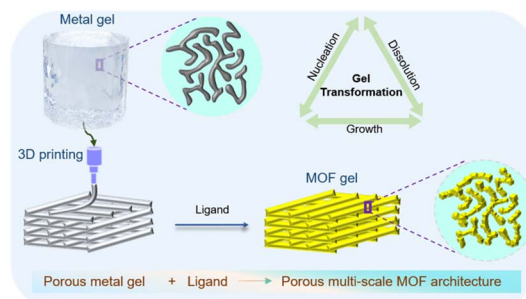
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7114

## Gel transformation as a general strategy for fabrication of highly porous multiscale MOF architectures

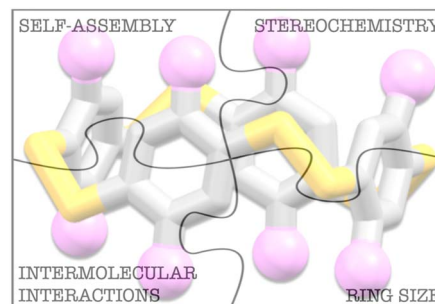
Zhang Liu, Javier Lopez Navas, Wei Han,\*  
Manuel Ricardo Ibarra, Joseph Kai Cho Kwan and  
King Lun Yeung\*



7126

## Self-assembly of achiral building blocks into chiral cyclophanes using non-directional interactions

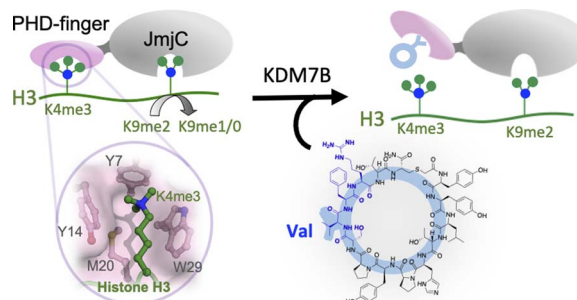
Yuan Zhang, Benjamin Ourri, Pierre-Thomas Skowron,  
Emeric Jeamet, Titouan Chetot, Christian Duchamp,  
Ana M. Belenguer, Nicolas Vanthuyne, Olivier Cala,  
Elise Dumont, Pradeep K. Mandal, Ivan Huc, Florent Perret,  
Laurent Vial\* and Julien Leclaire\*



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## Cyclic peptides target the aromatic cage of a PHD-finger reader domain to modulate epigenetic protein function

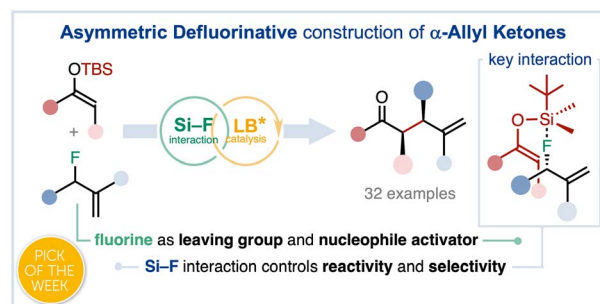
Oliver D. Coleman, Jessica Macdonald, Ben Thomson,  
Jennifer A. Ward, Christopher J. Stubbs, Tom E. McAllister,  
Shane Clark, Siddique Amin, Yimang Cao,  
Martine I. Abboud, Yijia Zhang, Hitesh Sanganeer,  
Kilian V. M. Huber, Tim D. W. Claridge\*  
and Akane Kawamura\*



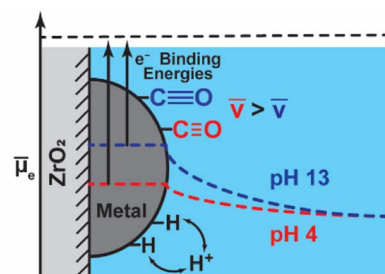
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## Catalytic asymmetric defluorinative allylation of silyl enol ethers

Jordi Duran, Javier Mateos, Albert Moyano  
and Xavier Companyó\*



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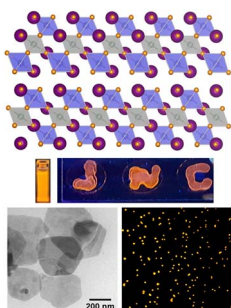


IR &amp; AP-XPS Reveal Spontaneous Polarization

### Metal nanoparticles supported on a nonconductive oxide undergo pH-dependent spontaneous polarization

Thejas S. Wesley, Max J. Hülsey, Karl S. Westendorff, Noah B. Lewis, Ethan J. Crumlin,\* Yuriy Román-Leshkov\* and Yogesh Surendranath\*

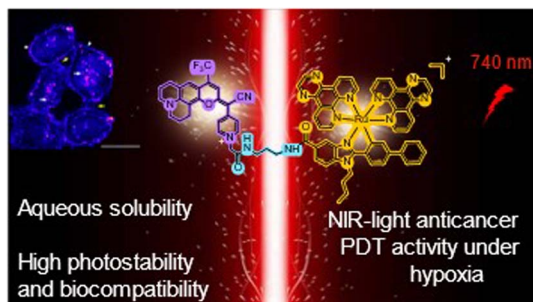
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### 2D nanosheets of layered double perovskites: synthesis, photostable bright orange emission and photoluminescence blinking

Aditya Bhardwaj, Kaushik Kundu, Ranjan Sasmal, Paribesh Acharyya, Jayita Pradhan, Simanta Kalita, Sarit S. Agasti\* and Kanishka Biswas\*

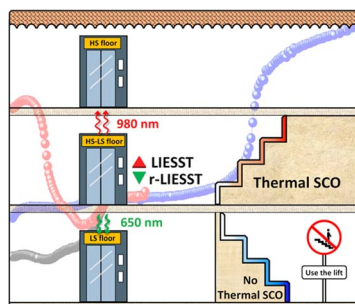
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### A near-infrared light-activatable Ru(II)-coumarin photosensitizer active under hypoxic conditions

Enrique Ortega-Forte, Anna Rovira, Marta López-Corrales, Alba Hernández-García, Francisco José Ballester, Eduardo Izquierdo-García, Mireia Jordà-Redondo, Manel Bosch, Santi Nonell, María Dolores Santana, José Ruiz,\* Vicente Marchán\* and Gilles Gasser\*

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### Bidirectional photoswitchability in an iron(III) spin crossover complex: symmetry-breaking and solvent effects

Raúl Díaz-Torres, Guillaume Chastanet, Eric Collet, Elzbieta Trzop, Phimpaka Harding\* and David J. Harding\*

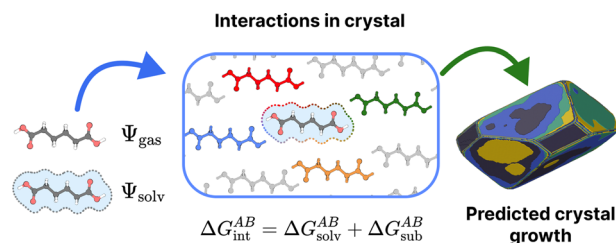




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### CrystalClear: an open, modular protocol for predicting molecular crystal growth from solution

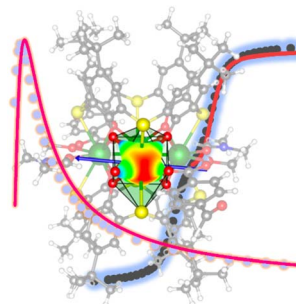
Peter R. Spackman,\* Alvin J. Walisinghe,  
Michael W. Anderson and Julian D. Gale



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### Toroidal moment and dynamical control in luminescent 1D and 3D terbium calixarene compounds

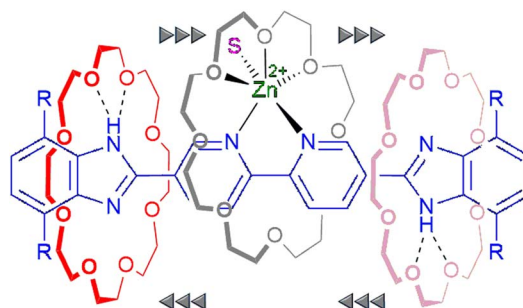
Hao Wang, Zhenhua Zhu, Léo La Droitte, Wuping Liao,\*  
Olivier Cador, Boris Le Guennic\* and Jinkui Tang\*



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### A translationally active ligand based on a [2]rotaxane molecular shuttle with a 2,2'-bipyridyl core

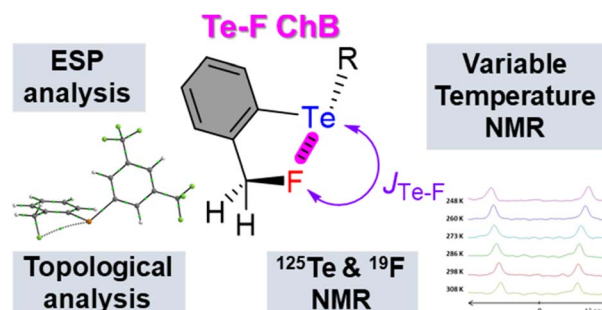
Ayan Dhara, Anton Dmitrienko, Rahaf N. Hussein,  
Ariel Sotomayor, Benjamin H. Wilson and  
Stephen J. Loeb\*



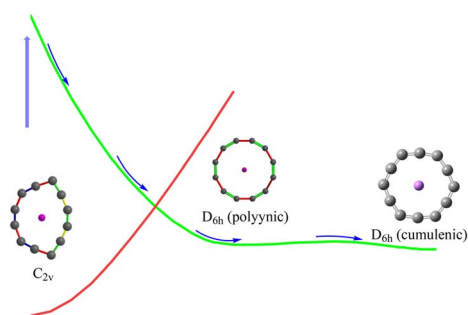
7221

### Evidence for and evaluation of fluorine–tellurium chalcogen bonding

Robin Weiss, Emmanuel Aubert, Loic Gros Lambert,  
Patrick Pale\* and Victor Mamane\*



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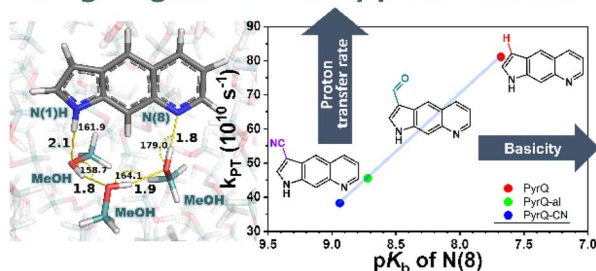


### Can anions possess bound doubly-excited electronic states?

Shi-Jie Hou, Yi-Fan Yang,\* Zhong-hua Cui\* and Lorenz S. Cederbaum\*

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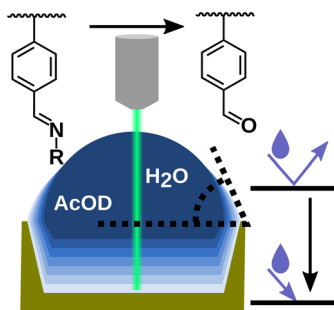
### Long range solvent relay proton transfer



### Long-range hydrogen-bond relay catalyses the excited-state proton transfer reaction

Kai-Hsin Chang, Yu-Chiang Peng, Kuan-Hsuan Su, Yi-Hsien Lin, Jiun-Chi Liu, Ying-Hsuan Liu, Chao-Hsien Hsu, Hsiao-Ching Yang\* and Pi-Tai Chou\*

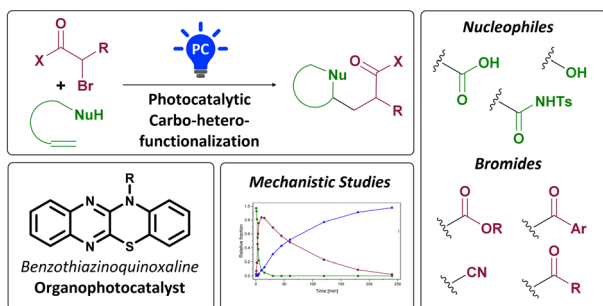
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### Molecular *in situ* monitoring of the pH-triggered response in adaptive polymers by two-dimensional Raman micro-correlation-spectroscopy

Julian Hniopek, Josefine Meurer, Stefan Zechel, Michael Schmitt, Martin D. Hager\* and Jürgen Popp\*

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### Organophotocatalytic carbo-heterofunctionalization of unactivated olefins with pendant nucleophiles

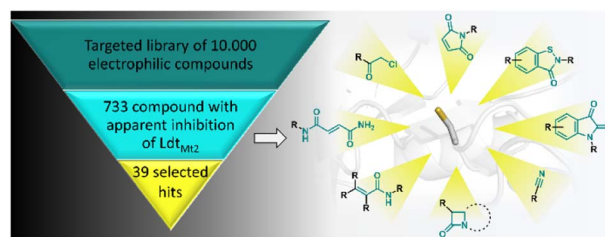
David M. Fischer, Manuel Freis, Willi M. Amberg, Henry Lindner and Erick M. Carreira\*



7262

### High-throughput screen with the $L,D$ -transpeptidase $Ldt_{Mt2}$ of *Mycobacterium tuberculosis* reveals novel classes of covalently reacting inhibitors

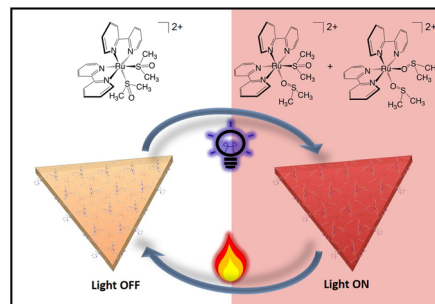
Mariska de Munnik, Pauline A. Lang, Francisco De Dios Anton, Mónica Cacho, Robert H. Bates, Jürgen Brem, Beatriz Rodríguez Miquel\* and Christopher J. Schofield\*



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### Photocrystallography of $[Ru(bpy)_2(dmsO)_2]^{2+}$ reveals an O-bonded metastable state

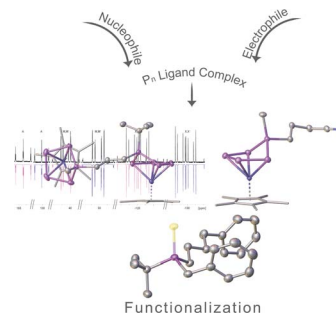
Zoe Y. Marr, Rajani Thapa Magar, Bertrand Fournier, Jason B. Benedict\* and Jeffrey J. Rack\*



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### Controlled introduction of functional groups at one P atom in $[Cp^*Fe(\eta^5-P_5)]$ and release of functionalised phosphines

Stephan Reichl, Felix Riedlberger, Martin Piesch, Gábor Balázs, Michael Seidl and Manfred Scheer\*



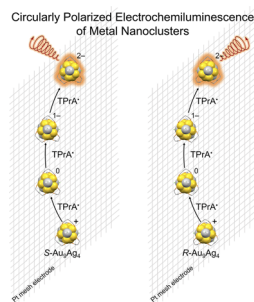
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### Cobalt-catalyzed enantioselective C–H/N–H annulation of aryl sulfonamides with allenes or alkynes: facile access to C–N axially chiral sultams

Xiao-Ju Si, Xiaofang Zhao, Jianli Wang, Xinhai Wang, Yuanshuo Zhang, Dandan Yang,\* Mao-Ping Song and Jun-Long Niu\*



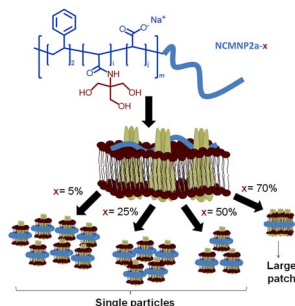
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### Bright near-infrared circularly polarized electrochemiluminescence from Au<sub>9</sub>Ag<sub>4</sub> nanoclusters

Lirong Jiang, Mengmeng Jing, Bing Yin, Wenjun Du, Xiaojian Wang, Ying Liu, Shuang Chen\* and Manzhou Zhu\*

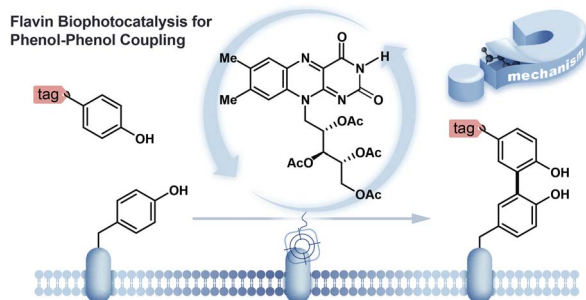
7310



### pH-tunable membrane-active polymers, NCMNP2a-x, and their potential membrane protein applications

Thi Kim Hoang Trinh, Andres Jorge Cabezas, Soumil Joshi, Claudio Catalano, Abu Bakkar Siddique, Weihua Qiu, Sanket Deshmukh, Amedee des Georges and Youzhong Guo\*

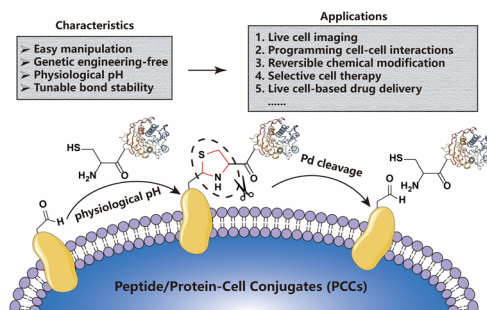
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### Targeted proximity-labelling of protein tyrosines via flavin-dependent photoredox catalysis with mechanistic evidence for a radical-radical recombination pathway

Taylor O. Hope, Tamara Reyes-Robles, Keun Ah Ryu, Steven Mauries, Nicole Removski, Jacinthe Maisonneuve, Rob C. Oslund,\* Olugbeminiyi O. Fadeyi\* and Mathieu Frenette\*

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### Catalyst-free thiazolidine formation chemistry enables the facile construction of peptide/protein-cell conjugates (PCCs) at physiological pH

Xiangquan Liu, Youyu Wang, Bangce Ye\* and Xiaobao Bi\*

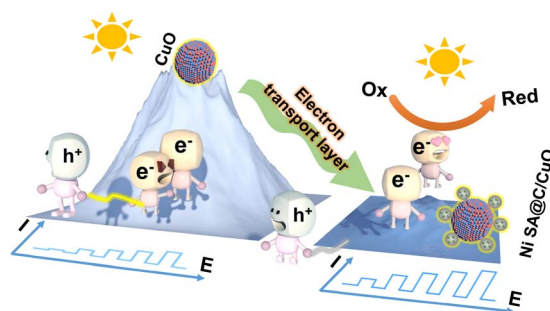




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### Engineering the microenvironment of electron transport layers with nickel single-atom sites for boosting photoelectrochemical performance

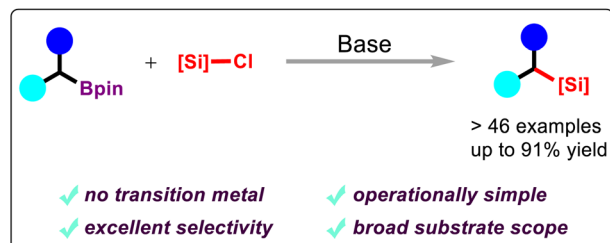
Ying Qin, Rong Tan, Jing Wen, Qikang Huang, Hengjia Wang, Mingwang Liu, Jinli Li, Canglong Wang, Yan Shen, Liuyong Hu,\* Wenling Gu\* and Chengzhou Zhu\*



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### Facile preparation of organosilanes from benzylboronates and *gem*-diborylalkanes mediated by KO<sup>t</sup>Bu

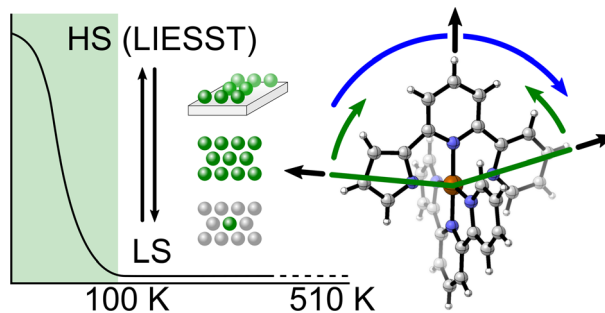
Man Tang, Wenyan Zhu, Huaxing Sun, Jing Wang, Su Jing,\* Minyan Wang,\* Zhuangzhi Shi and Jiefeng Hu\*



7361

### Defying the inverse energy gap law: a vacuum-evaporable Fe(II) low-spin complex with a long-lived LIESST state

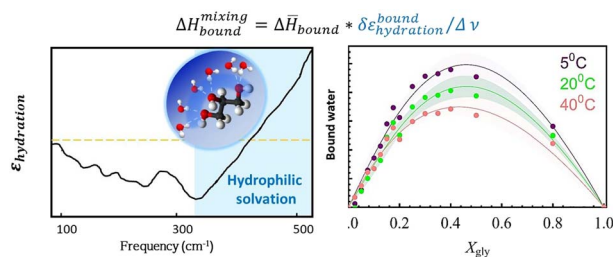
Jan Grunwald, Jorge Torres, Axel Buchholz, Christian Näther, Lea Kämmerer, Manuel Gruber, Sebastian Rohlf, Sangeeta Thakur, Heiko Wende, Winfried Plass, Wolfgang Kuch\* and Felix Tuczek\*



7381

### Local solvation structures govern the mixing thermodynamics of glycerol–water solutions

Debasish Das Mahanta, Dennis Robinson Brown, Simone Pezzotti, Songi Han, Gerhard Schwaab, M. Scott Shell\* and Martina Havenith\*



## CORRECTION

7393

**Correction: The influence of chirality on the behavior of oligonucleotides inside cells: revealing the potent cytotoxicity of G-rich L-RNA**

Chen-Hsu Yu and Jonathan T. Szczepanski\*

