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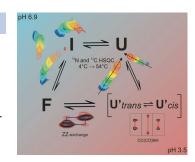


#### Protein Folding

P. Rovó, P. Stráner, A. Láng, I. Bartha, K. Huszár, L. Nyitray, A. Perczel\*

Structural Insights into the Trp-Cage Folding Intermediate Formation

Observing the invisible: Trp-cage miniprotein folds in a multistate process into its native structure. Heteronuclear NMR spectroscopy studies combined with molecular dynamics simulations provide direct evidence for the  $3_{10}$ - to  $\alpha$ -helix rearrangement as an initial step during the unfolding. The  $G^{11}-P^{12}$  peptide bond isomerization slows down the folding under acidic conditions (see figure; F = folded, I = intermediate, and U = unfolded structures).



Chem. Eur. J.

DOI: 10.1002/chem.201203764

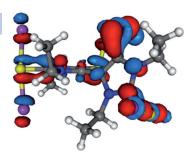


# Charge Transfer

A. Mancini, M. C. Aragoni, N. Bricklebank, C. Castellano, F. Demartin, F. Isaia, V. Lippolis, A. Pintus, M. Arca\*

Formation of T-Shaped versus Charge-Transfer Molecular Adducts in the Reactions Between Bis(thiocarbonyl) Donors and  $Br_2$  and  $I_2$ 

**T for two**: The reactions of 4,5,6,7-tetrathiocino-[1,2-b:3,4-b']-1,3,8,10-tetrasubstituted-diimidazolyl-2,9-dithiones ( $R_2$ , $R'_2$ -todit; **1**: R=R'=Et; **2**: R=R'=Ph; **3**: R=Et, R'=Ph) with  $Br_2$  exclusively afforded "T-shaped" compounds, whereas the reactions of compounds **1–3** with  $I_2$  provided CT adducts. The nature of all of the reaction products was elucidated based on XRD analysis, FT-Raman spectroscopy, and DFT calculations.



Chem. Asian I.

DOI: 10.1002/asia.201201043

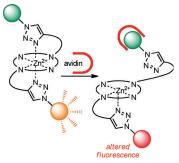


#### Fluorescence

M. Yu, Q. Yu, P. J. Rutledge,\* M. H. Todd\*

A Fluorescent "Allosteric Scorpionand" Complex Visualizes a Biological Recognition Event

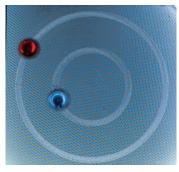
A new class of fluorescent metal complex with "ballerina"-like geometry is described. When functionalized with biotin (green) and a dye (orange/red), the zinc(II) complex can be used to visualize interactions with avidin. Metal complexes that can exhibit selective fluorescence changes in response to a macromolecular binding event have great potential for imaging applications.



ChemBioChem

DOI: 10.1002/cbic.201200637





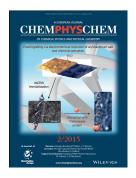
ChemPhysChem
DOI: 10.1002/cphc.201200929

### Microfluidics

I. You, N. Yun, H. Lee\*

Surface-Tension-Confined Microfluidics and Their Applications

**Showing the way**: Emerging microfluidic systems called surface-tension-confined microfluidic (STCM) devices are reviewed. STCM devices utilize surface energy that can control the movement of fluid droplets. Unlike conventional microfluidics, which confine the movement of fluids by three-dimensional microchannels, STCM systems provide two-dimensional platforms for microfluidics.





## **Antitubercular Agents**

L. Ballell,\* R. H. Bates, R. J. Young, D. Alvarez-Gomez, E. Alvarez-Ruiz, V. Barroso, D. Blanco, B. Crespo, J. Escribano, R. González, S. Lozano, S. Huss, A. Santos-Villarejo, J. J. Martín-Plaza, A. Mendoza, M. J. Rebollo-Lopez, M. Remuiñan-Blanco, J. L. Lavandera, E. Pérez-Herran, F. J. Gamo-Benito, J. F. García-Bustos, D. Barros, J. P. Castro, N. Cammack

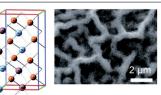
Fueling Open-Source Drug Discovery: 177 Small-Molecule Leads against Tuberculosis

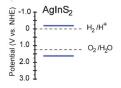
Needles from the haystack: As part of GlaxoSmithKline's commitment to open innovation research against neglected diseases such as TB, herein we report the results of a high-throughput phenotypic screen of two million compounds. A set of 177 potent, non-cytotoxic hits against *Mycobacterium tuberculosis* H37Rv are described. Samples of these compounds will be made available in an effort to promote further research against this critical disease.



ChemMedChem

DOI: 10.1002/cmdc.201200428





ChemSusChem

DOI: 10.1002/cssc.201200588

# Photoelectrochemistry

Q. Cheng, X. Peng, C. K. Chan\*

Structural and Photoelectrochemical Evaluation of Nanotextured Sn-Doped AgInS<sub>2</sub> Films Prepared by Spray Pyrolysis

**Tin best or tin pest?** The role of Sn extrinsic dopants in chalcopyrite  $AgInS_2$  is investigated to understand their effects on the optical, electronic, and photoelectrochemical properties of this promising photoanode material. We found that at low amounts, Sn increased the  $AgInS_2$  carrier concentration and photocurrent, but was detrimental at higher dopant concentrations.



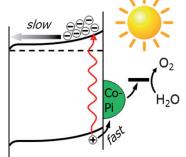
#### Catalyst Doping



Efficient BiVO<sub>4</sub> Thin Film Photoanodes Modified with Cobalt Phosphate Catalyst and W-doping

**Strengthening the weakest link**: A chain is no stronger than its weakest link. In this study, we show two important performance limiting factors in BiVO<sub>4</sub> photoanodes; water oxidation kinetics and electron transport. Based on this knowledge, the photoanode is modified by surface catalysis and doping, resulting in approximately 3-fold photocurrent improvement.



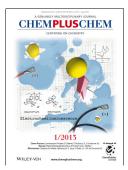


ChemCatChem

DOI: 10.1002/cctc.201200472





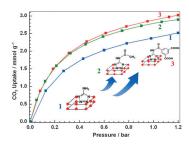


## Metal-Organic Framework

Q. Yan, Y. Lin, P. Wu, L. Zhao, L. Cao, L. Peng, C. Kong,\* L. Chen\*

Designed Synthesis of Functionalized Two-Dimensional Metal-Organic Frameworks with Preferential CO<sub>2</sub> Capture

What a catch! A series of three functionalized metal-organic frameworks have been fabricated by the combination of direct synthesis (template-free) and covalent modification. The resulting frameworks display fairly good thermal stability and moisture resistance. Regardless of the moderate surface area, the grafted carbonyl functionalities enhance the selective CO<sub>2</sub> adsorption capacity (see figure).



ChemPlusChem

DOI: 10.1002/cplu.201200270

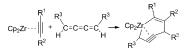


## Metallacycloalkynes

N. Suzuki,\* T. Tsuchiya, N. Aihara, M. Iwasaki, M. Saburi, T. Chihara, Y. Masuyama

Synthesis and Structure of Seven-Membered Metallacycloalkynes

Seven-membered metallacycloalkyne compounds were synthesized and structurally characterized. Zirconocene—alkyne complexes, such as those of 1-(trimethylsilyl)prop-1-yne and diphenylacetylene reacted with [3]cumulene to give 1-zirconacyclohept-2-en-5-yne in good yields. Coupling of benzyne and [3]cumulenes on the metal also gave the corresponding metallacycles.



Eur. J. Inorg. Chem.

DOI: 10.1002/ejic.201201245

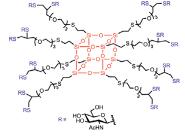


## **Photoinduced Reactions**

A. Marra, S. Staderini, N. Berthet, P. Dumy, O. Renaudet, A. Dondoni\*

Thiyl Glycosylation of Propargylated Octasilsesquioxane: Synthesis and Lectin-Binding Properties of Densely Glycosylated Clusters on a Cubic Platform

Typical hexadecavalent glyco-POSS prepared by thiol-yne coupling. A measured IC<sub>50</sub> of 2 nM was found by ELLA with tetrameric wheat germ agglutinin (WGA).



Eur. J. Org. Chem.

DOI: 10.1002/ejoc.201201453

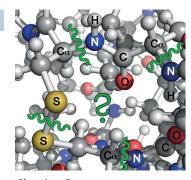


# Mass Spectrometry

B. Ganisl, K. Breuker\*

Does Electron Capture Dissociation Cleave Protein Disulfide Bonds?

**Runner-up!** Disulfide bond cleavage comes second in gas phase radical ion chemistry. Cleavage of N–C $\alpha$  backbone bonds is preferred over disulfide bond cleavage in electron capture dissociation (ECD) of peptides and proteins, but disulfide bonds can be cleaved by vibrational excitation or secondary radical reactions.



ChemistryOpen

DOI: 10.1002/open.201200038





Asian J. Org. Chem. DOI: 10.1002/ajoc.201200114

# Fullerooxazole Synthesis

Y. Takeda, S. Enokijima, T. Nagamachi, K. Nakayama, S. Minakata\*

Straightforward and Versatile Synthesis of Fullerooxazoles from  $C_{60}$  and Carboxamides through Radical Reactions under Mild Conditions

**Sixty plus**: A direct synthetic method for producing oxazoline-fused fullerenes, that is, fullerooxazoles, from [60] fullerene and readily available carboxamides by radical pathways has been developed. The method presented allows efficient access to a variety of fullerooxazoles with a high tolerance of functional groups under mild reaction conditions







Sunggyu Lee on the Future of Energy Technology

Solutions to the pressing problem of energy demand will vary depending upon regional strengths, technoeconomic factors, and resource utilization and availability according to Professor Sunggyu Lee, Director of the Sustainable Energy and Advanced Materials Laboratory at Ohio University, USA. He talks about where energy technology is heading, the role of governments in its development, and his latest research.



ChemViews magazine DOI: 10.1002/chemv.201200150