doi:10.2533/chimia.2009.76

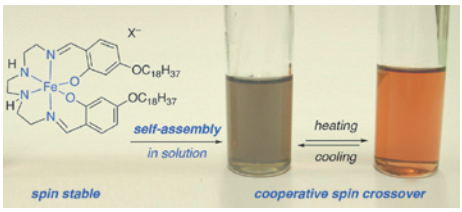
Swiss Science Concentrates

A CHIMIA Column

Short Abstracts of Interesting Recent Publications of Swiss Origin

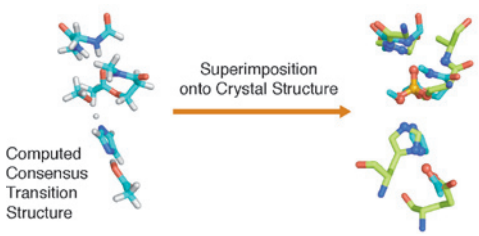
Improved Cooperativity of Spin-labile Iron(III) Centers by Self-assembly in Solution

C. Gandolfi, C. Moitzi, P. Schurtenberger, G. G. Morgan, and M. Albrecht, *J. Am. Chem. Soc.* **2008**, *130*, 14434
University of Fribourg and University College Dublin
In this article, using supramolecular cooperative effects in solution, the spin crossover activity of Fe(sal$_2$tien) iron(III) complexes was improved. By the incorporation of lipophilic side chains onto the polar metallic head, amphiphilic complexes were produced. The authors have further shown that, only in the case of very long side chains, microsized and submicrosized particles are formed which show a markedly increased spin crossover activity. This observation was correlated to an improved cooperativity of the metal centers due to self-assembly, thus connecting supramolecular structural concepts with chemical function.



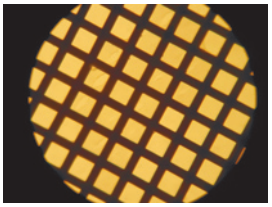
Structural Reorganization and Preorganization in Enzyme Active Sites: Comparisons of Experimental and Theoretically Ideal Active Site Geometries in the Multistep Serine Esterase Reaction Cycle

A. J. T. Smith, R. Müller, M. D. Toscano, P. Kast, H. W. Hellinga, D. Hilvert*, and K. N. Houk*, *J. Am. Chem. Soc.* **2008**, *130*, 15361
ETH Zürich, University of California and Duke University Medical Center
The authors have investigated the compromise between structural reorganization during the catalytic process and preorganization of the active site for a multistep enzyme-catalyzed reaction by generating quantum mechanical geometries which can catalyze each individual step in the mechanism. These geometries are compared to each other by superpositions of catalytic atoms to find 'consensus' geometries that can catalyze all steps with minimal rearrangement. The consensus theoretical geometry of catalytic groups was found to be essentially identical to that obtained from the experimental crystal structures of serine esterases (see below).The results provide a useful guiding principle for *de novo* design of enzymes with multistep mechanisms.



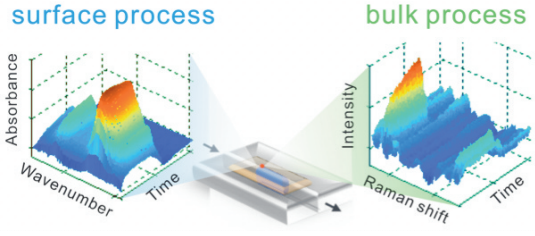
Synthesis of Compounds Presenting Three and Four Anthracene Units as Potential Connectors to Mediate Infinite Lateral Growth at the Air/Water Interface

C. Münzenberg, A. Rossi, K. Feldman, R. Fiolka, A. Stemmer, K. Kita-Tokarczyk, W. Meier, J. Sakamoto, O. Lukin, and A. D. Schlüter*, *Chem. Eur. J.* **2008**, *14*, 10503
ETH Zürich and Universities of Basel and Cagliari
In this article, the authors report the synthesis of molecular sheets based on the photochemically initiated dimerization of monomers with lateral anthracene units. The film thickness and composition were investigated by ellipsometry and X-ray photoelectron spectroscopy (XPS). The mechanical stability of the film was sufficient to span it over 45×45 µm-sized holes. The reported experiments are considered as first steps towards the ultimate goal of the rational synthesis of laterally 'infinite', one-monomer-unit-thick molecular sheets with a long-range positional order and a periodic covalent-bonding pattern.



Space- and Time-Resolved Combined DRIFT and Raman Spectroscopy: Monitoring Dynamic Surface and Bulk Processes during NO_x Storage Reduction

A. Urakawa*, N. Maeda, and A. Baiker *Angew. Chem. Int. Ed.* **2008**, *47*, 9256
ETH Zürich
Various powerful *in-situ* spectroscopic methods and their combinations have been developed to clarify and establish relations between catalytic activity and the atomic-scale environment of catalytic active sites under actual working conditions. In this article, the authors present a combination of both surface-sensitive (diffuse reflectance infrared Fourier transform spectroscopy, DRIFTS) and bulk-sensitive (Raman spectroscopy) space-resolved detection at different catalyst-bed positions as a powerful tool to facilitate deeper understanding of complex dynamic surface and bulk processes and this in the context of the NO_x Storage-Reduction system in particular.



Prepared by M. Austeri, R. Bach, N. Mehanna, A. Sharma, F. Torricelli, W. Zeghida, J. Lacour
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