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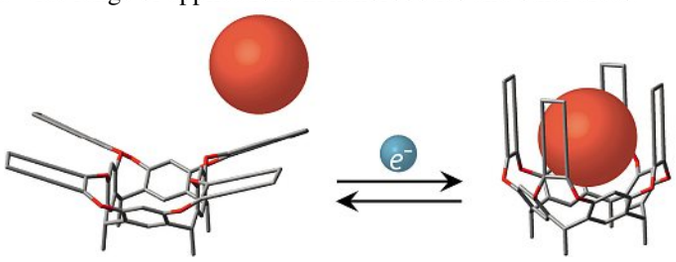
Swiss Science Concentrates

A CHIMIA Column

Short Abstracts of Interesting Recent Publications of Swiss Origin

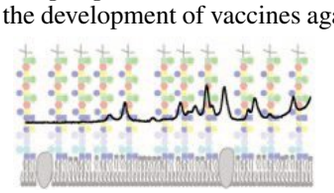
Redox-Switchable Resorcin[4]arene Cavitands: Molecular Grippers

I. Pochorovski, M.-O. Ebert, J.-P. Gisselbrecht, C. Boudon, W. B. Schweizer, and F. Diederich*, *J. Am. Chem. Soc.* **2012**, *134*, 14702.
ETH Zürich and Université de Strasbourg (F)
Devising molecular machines is a fascinating and fast-growing field in organic and supramolecular chemistry. In this paper Diederich and co-workers describe the preparation and behavior of novel resorcin[4]arene cavitands that act as molecular grippers, opening and closing upon a change in redox state of their quinone walls. A change in the oxidation state allows formation of intramolecular H–bonds that are responsible for the conformational switching process from a kite to a vase shape. Interestingly, these molecular grippers are able to grab and release guest molecules, demonstrating fascinating potential for a wide range of applications in nanorobotics and other areas.



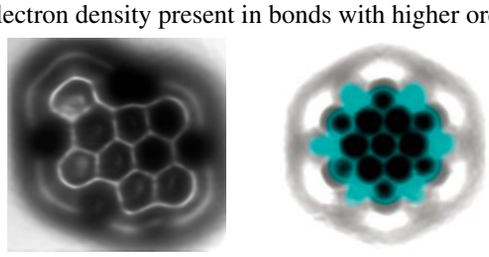
On-cell MAS NMR: Physiological Clues from Living Cells

G. Zandomeneghi, K. Ilg, M. Aebi*, and B. H. Meier*, *J. Am. Chem. Soc.* **2012**, *134*, 17513.
ETH Zürich
Magic-angle sample spinning (MAS) enables recording of high-resolution spectra of rigid bacterial cell components by NMR. In Gram-negative bacteria, lipopolysaccharides are the main constituent of the outer membrane and include the O-antigen, a polysaccharide chain of up to 100 repeats of an oligosaccharide. In the investigated *Salmonella Typhimurium* cells, one of the sugars in the repeating unit, abequose, is O-acetylated at C(2). The *in vivo* NMR study showed that the O-acetylation level is substantially altered during the stationary growth phase and is correlated to a pH-change in the growth medium. The change in the O-acetylation state can be also induced by artificially modifying the pH of the medium and, remarkably, it is much more pronounced in living cells. The investigation introduces a new method for the study of physiological processes and can thereby lead to new perspectives on bacteria. This may have a direct impact on the development of vaccines against pathogenic bacteria.



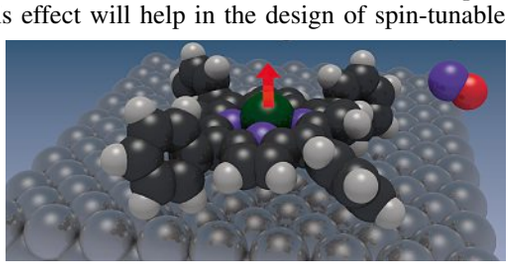
Bond-Order Discrimination by Atomic Force Microscopy

L. Gross*, F. Mohn, N. Moll, B. Schuler, A. Criado, E. Guitián, D. Peña, A. Gourdon, and G. Meyer, *Science* **2012**, *337*, 1326.
IBM Research – Zurich, Univ. Santiago de Compostela (ES), CEMES-CNRS, Toulouse (F)
Whereas diffraction methods allow the determination of averaged bond lengths over large ensembles, scanning probe microscopy offers the opportunity to scrutinize geometric properties of single molecules. Herein, the authors rely on non-contact atomic force microscopy to detect differences of individual C–C bond lengths with remarkable precision (down to 0.03 Å). For this purpose, a CO-functionalized AFM tip is used to reveal differences in contrast caused by the Pauli repulsion between the tip and the higher electron density present in bonds with higher order.



On-surface Coordination Chemistry of Planar Molecular Spin Systems: Novel Magnetochemical Effects Induced by Axial Ligands

C. Wäckerlin, K. Tarafder, D. Siewert, J. Girovsky, T. Hählen, C. Iacovita, A. Kleibert, F. Nolting, T. A. Jung*, P. M. Oppeneer*, and N. Ballav*, *Chem. Sci.* **2012**, *3*, 3154.
Paul Scherrer Institut, Uppsala University (SE), University of Basel, SLS at PSI, IISER (IND)
Paramagnetic metal-organic complexes assembled on surfaces have great potential for organic spintronics. However, the subtle interaction between the spin of a metal ion center, axial ligand, and ferromagnetic surface is poorly understood. To address this, the authors combined X-ray magnetic circular dichroism and quantum-chemical simulations. The interplay between external axial ligands like NH_3 or NO and Ni and Co ferromagnetic surfaces affecting the spin of Co(II), Fe(II) and Mn(II) tetraphenylporphyrins and Mn(II) phthalocyanine was highlighted. The structural *trans*-effect on the surface determines the molecular spin state, as well as the sign and strength of the exchange interaction with the substrate. The authors coin this observation as the surface spin-*trans* effect. This effect will help in the design of spin-tunable interfaces with applications in quantum computing building blocks.



Prepared by Nico Bruns, Valentin Köhler, Mark R. Ringenberg, Paolo Tosatti and Thomas R. Ward
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