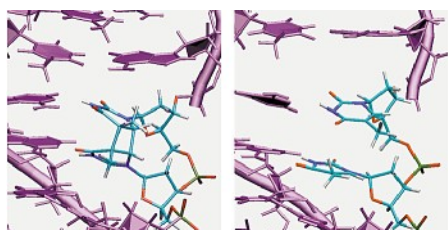


Science Concentrates

Computational Study of Thymine Dimer Radical Anion Splitting in the Self-Repair Process of Duplex DNA

F. Masson,* T. Laino, I. Tavernelli, U. Röthlisberger, and J. Hutter, *J. Am. Chem. Soc.* **2008**, *130*, 3443
Universität Zürich & EPFL

UV-induced cyclobutane thymine dimerisation is one of the most important types of DNA damage that results in several biological pathologies, notably skin cancer. A self-repair mechanism was recently discovered using an autocatalytic activity of the DNA itself. This paper provides the first molecular dynamics study of the splitting of thymine dimer radical anions, using a quantum mechanical/molecular mechanics (QM/MM) approach based on density functional theory (DFT) to describe the quantum region. The results characterize the dimer splitting process as an asynchronous concerted reaction with no or little energy barriers (2.5 kcal/mol max.). All these data tag the whole process as an ultra-fast reaction.



Protein Structure Determination from ¹³C Spin-Diffusion Solid-State NMR Spectroscopy

T. Manolikas, T. Herrmann, and B. H. Meier*, *J. Am. Chem. Soc.* **2008**, *130*, 3959
ETH Zurich

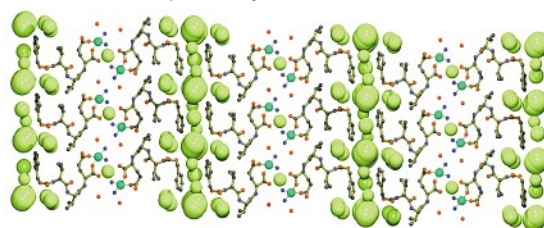
While first atomic structures from (microcrystalline) proteins have been obtained, an established protocol for structure determination by solid-state NMR is not yet available and any progress towards this goal is important. In this paper, it is demonstrated that proton-driven ¹³C spin diffusion (PDS), a simple and robust two-dimensional NMR experiment, can be used and leads to spectra with a high signal-to-noise ratio in which cross-peaks contain information about internuclear distances. It is shown that the total information content is sufficient to determine the atomic-resolution structure of a small protein from a single, uniformly ¹³C-, ¹⁵N-labeled microcrystalline sample – and ubiquitin in particular.



Metal–Peptide Frameworks (MPFs): ‘Bioinspired’ Metal Organic Frameworks

A. Manton,* L. Massüger, P. Rabu, C. Palivan, L. B. McCusker, and A. Taubert*, *J. Am. Chem. Soc.* **2008**, *130*, 2517
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Chiral metal–organic frameworks attract a growing interest for their potential use in energy technologies, asymmetric catalysis, and chiral separation. In this paper, the authors report the first metal peptide framework (MPF) constructed from an oligovaline peptide family. Using simple oligopeptide Z-(L-Val)₂-L-Glu(OH)-OH, porous copper and calcium MPFs are grown thanks to the self assembling properties of the peptide and specific metal–peptide and metal–ammonia interactions. These MPFs are stable up to ~250 °C and possess some internal porosity.



Linear Polynuclear Helicates as a Link between Discrete Supramolecular Complexes and Programmed Infinite Polymetallic Chains

N. Dalla-Favera, J. Hamacek, M. Borkovec, D. Jeannerat, F. Gummy, J.-C. G. Bünzli, G. Ercolani, and C. Piguet*, *Chem. Eur. J.* **2008**, *14*, 2994.

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The contribution of the solvation energies to the assembly of polynuclear helicates reduces the free energy of intermetallic repulsion in condensed phase so much that stable *D*₃-symmetrical tetranuclear lanthanide-containing triple-stranded helicates [Ln₄(L)₃]¹²⁺ are quantitatively produced at millimolar concentrations, despite the 12+ charge. Modelling of the formation constants using statistical factors provides a set of five microscopic parameters, which can be used for rationalizing the stepwise generation of the linear analogues. Photophysical studies of [Eu₄(L)₃]¹²⁺ confirm the existence of two different binding sites producing differentiated metal-centred emission at 10 K, which transforms into single site luminescence at 295 K.

