Mean Field study of induced magnetic moment in a 2d-multiband Hubbard model

A possible approach to some main group binary compounds

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Mean Field study of induced magnetic moment in a 2d-multiband Hubbard model.
A possible approach to some main group binary compounds.

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We set a possible 2-d Hubbard Hamiltonian including an itinerant p-band hybridized with localized orbitals. Inspired in recent studies of magnetism in compounds with no transition metal, we look at the magnetic moment induced by external field. Our model is solved in the Mean field approximation and several thermodynamic quantities are computed. We obtain a variety of behaviors strongly dependent on the fine tuning of the accounted interactions.

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[2] M. Imada et al, *Rev. Mod. Phys.* **1998**, *70*, 1039.
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Novel phthalocyanine-based stopcock for zeolite L

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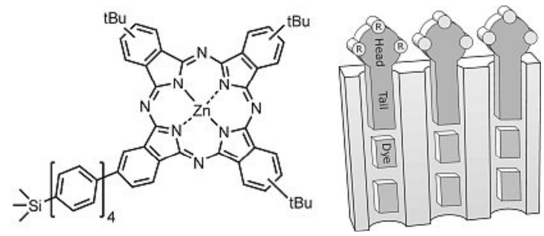
The one-dimensional channel system of zeolite L offers possibilities to obtain defined arrangements of monomeric dyes, resulting in efficient energy transfer materials. Communication with external objects is established by functionalization of the channel entrances of the zeolite crystals with fluorescent stopcock molecules. We report the first phthalocyanine-based stopcock for selective adsorption to the channel entrances of zeolite L and the realisation of a new electronic dipole moment coupling situation between dyes in the zeolite channels and stopcock molecules [1]. Photonic antenna systems based on this concept are of particular interest in the design of sensitised organic solar cells [2].



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Insight into fuel cell membrane degradation by pulse radiolysis experiments

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Membrane durability has become a central issue for the progress of polymer electrolyte fuel cells, PEFCs. Accordingly, understanding the mechanism of membrane degradation is crucial to improve suitable membrane materials. Free radical species, such as the $^{\bullet}OH$ and $^{\bullet}OOH$, directly produced on the platinum catalyst at the fuel cell electrodes, are assumed to considerably contribute to the ageing process of the polymer. In order to obtain insight into possible polymer-chain-degradation mechanisms relevant for fuel cell applications, this work focuses on the kinetics of the $^{\bullet}OH$ towards low-molecular-weight soluble polymers of poly(styrene sulfonic acid) as model systems.

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Repair of Protein Radicals by Ascorbate

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Proteins are significant biological targets for partially reduced oxygen species *in vivo*. The subsequently random formed radicals on the surface of proteins yield often tryptophan and tyrosyl radicals through intramolecular electron transfer. We generated these radicals specifically by azide radicals in insulin, β-lactoglobulin, pepsin, chymotrypsin, and bovine serum albumin. The rate constants measured varied between 10^8 to 10^9 $M^{-1}s^{-1}$, depending on the protein. The formation and disappearance of tyrosyl and tryptophanyl radicals was followed at 405 and 510 nm, respectively. The free tyrosyl and tryptophanyl radical are known to react with monohydroascorbate with rate constants close to 10^8 $M^{-1}s^{-1}$. The rate constants for reactions of protein-bound tryptophanyl radicals with monohydroascorbate in chymotrypsin and pepsin are quite similar, while that of β-lactoglobulin is smaller by a factor of 5. The corresponding rate constant values for protein-bound tyrosyl radicals are ca. 30 – 40 % of that of the free tyrosyl radical, with the exception of that of β-lactoglobulin, which is smaller by a factor of 400. These results are similar to those obtained with lysozyme by others. Previously, we found that glutathione reduces the tryptophanyl radical in lysozyme with a rate constant of 10^5 $M^{-1}s^{-1}$ [1]. Although monohydroascorbate is present in cells in 10-fold smaller concentrations than glutathione, it appears to be more important for the repair of protein radicals. The results suggest that the loss of ascorbate in living organisms subjected to oxidative stress may result from repair of protein radicals.

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