Modeling of Reactions in Confined Spaces

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Abstract:
In this talk, I will describe our recent effort in using quantum chemistry to model binding and reactions inside self-assembled capsules.[1-4] Description of these systems requires: 1) structural and energetic characterization of the capsules, 2) accurate determination of the binding free energies of all possible guests, including reactants, solvent and solvent impurities, and 3) calculation of the reaction pathways inside and outside the capsule.
We show that the modern density functional theory (DFT) methodology provides a reasonable approach for this purpose. Detailed energy decomposition analysis is applied to identify the factors causing the rate enhancement and the selectivity introduced by the capsule. However, host-guest binding free energies in aqueous solution require special treatment. A new approach is presented which gives very promising results.

References:

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Biography:

Fahmi Himo did his undergraduate studies in physics at Stockholm University (1992-1995), where he also received his Ph.D. degree in 2000 (with Leif Eriksson and Per Siegbahn). He then received a special postdoctoral gran from the Wenner-Gren Foundations, where he spent two years at the Scripps Research Institute (with Louis Noodleman) and three years back in Sweden at the Royal Institute of Technology (KTH). 2005-2009 he was assistant professor at KTH before he moved to his current position as professor in quantum chemistry at Stockholm University.
His work is concerned with quantum chemical modeling of both homogeneous and enzymatic catalysis.

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