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Oral presentation

Computational nanoscience

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Virtually every engineering task in our macroscopic world such as directed motion, pumping, sensing, information storage and processing etc. has already been achieved on a molecular level in nature. There are turbines like the ATP synthase that rotate in a membrane driven by a proton gradient and transforming mechanical into chemical energy, there are molecular vehicles like kinesin carrying vesicles on a tubulin track or repair enzymes moving along DNA strands, recognizing and repairing wrongly paired bases.

Within the last 15 years, based on an increasing knowledge in supramolecular chemistry, a number of artificial molecular machines have been designed and synthesized. The Feringa motor and a large number of rotaxane shuttles could serve as examples. As the dynamic machine-like functions become more sophisticated, computer aided design strategies and the a priori prediction of the properties are needed to guide the chemical (supramolecular) intuition and to minimize the subsequent synthetic efforts.

We currently are pursuing four different "nano-engineering" projects, the synthesis of a supramolecular machine to assemble molecules, a light driven proton pump, a single molecule magnetic switch and an artificial cilia epithelium to induce directed motion on a surface. Geometries, energies, supramolecular interactions and other properties are predicted using density functional theory methods. After "*in silico*" optimization of the properties, we are synthesizing and testing our molecular machines in the lab. Usually, an iterative process switching between calculations and experiments is needed to achieve optimized functions.