

Molecular modeling of the cytochrome c on a gold surface

Magdalena Siwko

INFM National Research Center on nanoStructures and bioSystems at Surfaces (S3) and University of Modena and Reggio-Emilia via Campi 213/A, I-41100, Modena Italy.

Redox metalloproteins are of great interest in the design of biosensors and/or electronic nano-devices due to the capability to the transfer of electrons (ET) between molecular partners. In the cytochrome c electron is transferred from its cofactor, i.e. heme group to the other proteins through the surface cysteine residue. Experiments show that the ET rate from heme to the cysteine anchored to the gold cathode can be reversibly modulated by changing pH and temperature of the solution, or by introducing mutations. At low pH both axial ligands are detached from the heme iron. These rearrangements allow binding the molecular oxygen to the heme what is not possible at physiological pH. The property of the pH-induced conformational transitions could be used as a molecular switch for bioelectronic devices. By changing the position of the surface cysteine the rate of ET can be increased. In this project we investigated the interaction of the cytochrome c with a gold substrate using molecular dynamics (MD) techniques. The MD simulations performed provide information about the structural changes within the protein and favorable orientation of the protein with respect to the gold surface. The rate of ET has been also estimated for both native and mutated cytochrome c.