Dottorato di Ricerca in Fisica dell'Università degli Studi di Messina

25 Marzo 2010, ore 15.00, Aula E. Majorana, Dip.to di Fisica,
Ctr. Papardo Sperone, 31, S. Agata, Messina

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Collective dynamics of membrane proteins: A molecular dynamics simulation study

Function of membranes and membrane proteins depend on their dynamics and relaxation behavior. Proteins have close-packed structures, and changes in their conformation require the collective motion of a large fraction of the protein atoms. These collective modes may be in principle probed using-neutron and x-ray-scattering techniques, yet, coherent inelastic data probing low frequency modes of globular and membrane proteins are very scarce and difficult to interpret. In the past we have shown that, combined with experiments, Molecular Dynamics (MD) simulations are able of providing exquisite details about the dynamics of membranes, that of globular proteins and of their associated hydration-water. After an introduction of MD techniques and a brief summary of previous results, we show here how to generate *in silico* neutron and x-ray scattering measurements in order to probe collective modes of bacterorhodopsin trimers in their purple membrane environment. We discuss the appropriate experimental conditions allowing one to extract the maximum information from scattering techniques. A principal components analysis is performed in order to shed light onto the essential collective modes of the protein occurring on the nanosecond time regime.

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