**Computational Studies of Biological Systems Related to Human Diseases**

Alessandra Magistrato

CNR-IOM and International School for Advanced Studies, Trieste. Italy

Computational biology is playing an ever-increasing important role in understanding at atomistic level of detail the complex mechanisms of biological processes, complementing experimental data and predicting novel aspects of those processes, which are inaccessible to experiments. In this talk multi-scale simulations ranging from force field based molecular dynamics to hybrid quantum-classical (QM/MM) simulations, in combination with state of the art advanced sampling techniques, will be used to understand the molecular mechanisms of biological processes related to human diseases. In particular, I will focus on enzymes metabolizing hormones, on repair enzymes and on inorganic molecules that selectively recognize the presence of damaged bases in DNA sequences, and finally, on membrane proteins, which transport nutrients across the cellular membranes.