

Tue May 29, 2012 @ 14.00 a.m.

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SISSA - first floor - room 132

Abstract:

Many important physico-chemical processes "live" in a high-dimensional free energy landscape, which makes difficult their study by computer simulations. I will present some recently-developed methodologies which tackle this challenge: 1) Social PeRmutation INvariantT (SPRINT) topological coordinates, which in combination with ab-initio metadynamics allowed to discover the mechanism of the experimentally-observed transformation of a graphene flake into fullerene, and 2) conformational cluster models of protein dynamics built from all-atom bias-exchange simulations, applied to the early unfolding events of protein SH3 (compared with conventional replica exchange and with experiments) and to the full folding pathway of the WW domain.