universität innsbruck

Department of
Theoretical Physics

Theory Colloquium

Prof. Pietro Faccioli, University of Trento

"Investigating protein dynamics with theoretical physics methods"

Abstract

Biomolecules and in particular proteins are extremely complex many body systems. Not only they are made by many thousands of atoms interacting through up to 4-body forces, but also they are prototypical examples of open systems since their dynamics is shaped by dissipation and thermal fluctuations provided by the environment (mostly water). The combination of strong correlation and large fluctuations gives rise to nonperturbative phenomena such as frustration, meta-stability and cooperativity.

Large-scale computer simulations of their classical structural dynamics and their quantum electronic structure can in principle provide a powerful and theoretically sound framework for theoretical investigations. Unfortunately, they are intrinsically limited by the co-existence of multiple widely separated time scales. As a result, a gap of many orders of magnitude exists between the time scales which can be simulated and those which are biologically relevant.

In this seminar, I will show that many of these computational difficulties can be overcome using theoretical physics techniques originally developed in the context of subnuclear physics, such as path integrals, quantum field theory and renormalization group. In particular, I will discuss an approach developed in almost 10 years of research which has recently opened the way simulate biologically relevant conformational transitions (such as protein folding) or study the relaxation, transport and decoherence of optically excited electronic excitations.

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Seminar room 2S17 | ICT building