

In silico approaches to model spectroscopic properties and chemical reactions in complex systems

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In this talk, I would like to present some recent results on the theoretical-computational modelling of the UV absorption spectrum of water in alkaline conditions and the spontaneous deamidation of Asparagine occurring in a simple model peptide.

Both these works are based on the possibility to estimate the electronic properties of interest by a QM/MM approach where the dynamical effect of the environment on the Quantum Center - treated at quantum-mechanical level of details - is taken into account.

Our results, in close agreement with experimental data, point out that an accurate modeling requires a high-level treatment of the electronic properties of the region of interest coupled to a proper sampling of the environment as provided by extended Molecular Dynamics simulations.