Mercoledì 13 settembre 2017 alle ore 15:00 presso l’aula L2

il Dr. Stefano Caprasecca

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terrà il seminario dal titolo:

Plasmons meet coherences in light-harvesting systems

The photophysical properties of chromophoric systems can be greatly affected by the proximity of plasmonic devices. In particular, light-harvesting systems, typically containing many chromophores, can show a marked enhancement of their fluorescence and absorption properties when they are placed in proximity of metal nanoparticles (NPs) [1].

An accurate description of such effects is challenging, since the processes under study require performing electronic structure calculations; at the same time, the system is extremely large and inhomogeneous. We therefore employ a quantum/classical multiscale approach, fully polarisable, where the chromophores of the light-harvesting system are treated at quantum-mechanical level, within an excitonic description, while the protein environment is represented classically, using a discrete polarisable characterisation in terms of atomic charges and induced dipoles [2]. At the same time, the metal nanoparticle is described using a modified version of the polarisable continuum model (PCM) [3]. This multiscale model allows to account for the effect of the protein and the nanoparticle both on the properties of the individual chromophores and on the electronic couplings between them. We study the LH2 light-harvesting complex, whose electronic states are strongly excitonic. We show how its photophysical properties can be modified by the presence, orientation and geometry of the NP, inducing enhancements of absorption and fluorescence [4]. We also analyse the effect of the NP on the excitonic character of the states. Our study proves valuable not only to dissect the metal-induced effects on light-harvesting systems, but also to correctly interpret and analyse the experimental results available.


La presenza della S. V. sarà molto gradita

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Stefano Corni

Il Direttore del Dipartimento
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