Plasmon-Controlled Light-Harvesting: Design Rules for Biohybrid Devices via Multiscale Modeling

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Photosynthesis is triggered by the absorption of light by light-harvesting (LH) pigment−protein complexes followed by excitation energy transfer to the reaction center(s). A promising strategy to achieve control on and to improve light harvesting is to complement the LH complexes with plasmonic particles.

An extension of the Polarizable Continuum Model (PCM) is used to couple the complex dielectric response of plasmonic nanoparticles to the electronic properties of organic chromophores [1-2], thus allowing the characterization of plasmon-enhanced optical properties of atomistic systems, treated with full details. By combining such a continuum approach with a polarizable QM/MM method, the resulting multiscale model can be used to investigate the LH process of the peridinin-chlorophyll-protein (PCP) complex on a silver island film [3].

The simulations not only reproduce and interpret the experiments [4] but they also suggest general rules to design novel biohybrid devices; hot-spot configurations in which the LH complex is sandwiched between couples of metal aggregates are found to produce the largest amplifications. Indications about the best distances and orientations are also reported together with illumination and emission geometries of the PCP−NP system necessary to achieve the maximum enhancement.

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[3] O. Andreussi, A. Biancardi, S. Corni and B. Mennucci, *Nano Lett.* 13 (2013) 4475.

[4] S. Mackowski et al. *Nano Lett.* 8 (2008) 558.