

Modeling (bio-)molecular aggregation to understand their interaction with light

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Resumen

Aggregation, the formation of molecular assemblies or condensates, is a critical element in many processes of relevance in material science, soft matter and biophysics. Molecular aggregates are a challenging case to model from scratch, as experimental information about their structure(s) are scarce. Details involved in the intermolecular interactions are crucial to determine their properties, such as the response to light: optical properties, photophysics or photochemistry. To attempt the modeling of these systems, hybrid (multiscale) modeling is employed as a general strategy. First, molecular dynamics (MD) is employed to model a reliable (set of) structure(s) for the aggregate. Next, electronic-structure methods (such as Density-Functional Theory, DFT) and/or model hamiltonian are employed to describe the properties of interest. I will present few examples, such as: i) modelling (chiro)-optical properties of molecular chiral aggregates combining MD and coarse-grain model hamiltonian to build a valuable interpretation of the experimental results; ii) how biological assemblies based on different building blocks, can be structurally modeled and their optical properties simulated employing time-dependent DFT.