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Ab-initio study of the excited state properties of liquid water

LUCIA REINING, Ecole Polytechnique, Paris, France

In the last decades, we have witnessed an increasing interest on water and many studies on the geometry and ground state properties have appeared in the literature. Nevertheless, its excited state properties, which are essential to study the chemical and physical behavior of many biological and industrial processes, have not been investigated yet. We present here ab-initio calculations, in the framework of many body Green's function formalism, of liquid water. We use snapshots taken from classical molecular dynamics as input geometries for the study of the electronic and optical spectra. The excitation spectra are first obtained within the Density Functional Theory (DFT) and then corrected within the "GW" approximation. The optical absorption spectra are calculated by solving the Bethe-Salpeter equation; they result modified, with respect to the DFT spectra, suggesting the presence of important excitonic effects at low energies.