

1 Executive Summary

Deliverables D7.3 and D7.4 were specified separately in the Description of Work, but in practice while completing the first one we have also completed the second one and extended the range of applicability of the tools to over 400 atoms. Therefore the content of the reports for the two deliverables are identical, keeping in mind that we are extended even further the range of applicability of the tools we have to be able to address systems with thousand atoms. We expect to have preliminary data confirming this point by the end of 2009, and that those results will clearly go beyond the originally proposed D7.4 and will enhance tremendously the impact of the basic spectroscopic tools offered by the ETSF as part of its ETSF suite of codes.

From the first year and as part of Milestone 7.1 we have added new features to the ETSF codes such as nonlinear optics, spin-orbit and spin-resolved spectroscopy which are now available in the ETSF Yambo, Octopus, DP/EXC and Abinit codes. These are offered on a GPL license to all the scientific community (users). In a test phase (not yet public), we have non-linear spectroscopy of liquids, core-level spectroscopy of molecules, spatially resolved EELS, photo-emission in function of photon energy and polarization and space-and time-resolved density response.

The completion of D7.3 is achieved as we have operative the non-linear optics, a new tool to address femtochemistry at surfaces (relevant for photovoltaics), and circular dichroism in the Octopus code (already available to all users). This work has already give rise to three publications.

The completion of D7.4 is achieved by the testing of the optical properties of a gas of benzene molecules and a large triad system (fullerene plus porphyrine pls carotene) used in hybrid organic/inorganic structures for photovoltaic applications. This work led to two publications.