

# 1 Executive Summary

The suite of codes and knowledge made available to all users of the ETSF at the beginning of the project offered scope for expansion in both the techniques being provided and the concepts being implemented. The scope of this deliverable, as with the others related to Work Package 7, concerns either the development of a new technique or the implementation of new physical, chemical and biological concepts into the existing ETSF tools. The present deliverable is the natural continuation of deliverable D7.3 in which we made 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) and add the following new spectroscopy tools to the whole scientific community: non-linear spectroscopy of liquids, charge transport in organic crystals, core-level spectroscopy of molecules, and chiroptical responses of solids and molecules.

All these new features have been implemented in the ETSF codes<sup>1</sup> such Yambo, Octopus, DP/EXC and Abinit, which are offered on a GPL license to the scientific community (users), and some of the features have also been implemented in VASP (not GPL). Presently in a test phase (not yet public) are spatially resolved EELS, photo-emission in function of photon energy and polarization and space-and time-resolved density response, *GW* many-body based scheme without sum over empty states, non-adiabatic dynamics and time-dependent transport in TDDFT and Baym-Kadanof formalisms.

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<sup>1</sup> <http://www.etsf.eu/resources/software>