

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. Being able to predict spectroscopic properties of materials at finite temperature is essential and will be required by many users of the facility. This work implies development of new algorithms to make tractable the computation of spectra at finite temperature.

At the starting of the I3-e- ETSF project we already had the case for describing ground-state (dynamics) of complex systems as a function of temperature but this was not the case for optical and other spectroscopic tools. During the first year and before we have developed a large amount of human and computational resources to put this in shape, and now it is being offered in at least two codes of the ETSF (octopus and Yambo). The successful development of this study has lead to one publication in 2008¹ with more to come in 2009, plus an internal report. Both the published paper and an invited Editorial are attached to this deliverable report.

1 <http://nano-bio.ehu.es/files/articles/article-405.pdf>