1 Executive Summary

The scope of this deliverable, as with the others of Work Package 7, is concerned with either the development of a new technique or the implementation of new physical/chemical/biological concepts into the existing ETSF tools. It is clear from this statement that being able to predict spectroscopic properties of materials in solution is a must that continues the line of development started with the previous D7.1 deliverable where modelling of temperature effects was made available to ETSF users. Clearly, many chemical and biological processes happen in solution; therefore to have tools in place able to tackle spectroscopic properties of molecules and nanostructures in solution will be required by many users of the facility. This work implies not only code implementation but also the development of new algorithms to handle the complexity of solvated molecular systems.

The successful development of this study has led to two publications, one submitted in 2008 and published in 2009[1] and another that has been selected as the front page of the corresponding journal ChemPhysChem Vol.8 in 2009[2].

1 Conte *et al.*, Journal of Chemical Theory and Computation 2009: appended as Annex I to this report.

2 Kirketerp *et al.*, ChemPhysChem, August 2009: appended as Annex II to this report.