1 Executive Summary

The rapid advances in theory and software development, together with the availability of increasingly powerful computer hardware, means that more and more complex problems in materials science can be tackled by modern ab initio methods. In particular, this is also true for theoretical spectroscopy, which can now be applied to increasingly complex systems. As a consequence, research fields that were so far dominated by purely experimental work or phenomenological theories can now benefit from predictive quantitative simulations to solve problems of practical technological interest. The ETSF intends to reach out to these communities and thus make contact with new prospective users. For this purpose, the ETSF advertises its services at scientific conferences, in bulletins of the targeted research communities and in the general media.

The object of the present deliverable is a review about theoretical spectroscopy, which also aims at promoting the expertise of the ETSF and reaching out to new user communities. Therefore, the target audience are experimental and industrial researchers from different scientific fields. To best meet the information needs of this readership, we decided not to write a monograph with an extensive coverage of theory background, but rather a collection of shorter essays, each of which focuses on an example from a particular research field and illustrates how theoretical spectroscopy with modern ab initio methods can help to solve problems of practical relevance. Altogether, the collection comprises nine essays and covers such diverse topics as biomolecules, organic semiconductors, phase-change materials, silicon nanostructures and various experimental spectroscopies.

The essay collection was edited by Lucia Reining from Palaiseau, who also contributed a foreword and overview, and published as a special issue of Comptes Rendus Physique (Volume 10, Issue 6, Pages 465-586) in July-August 2009[1]. The formal publication in a peer-reviewed journal not only lends further authority to this display of ETSF capabilities, but the publisher, Elsevier, also guarantees additional promotion, wide outreach and long-term electronic archiving. The essay collection is furthermore highlighted on the ETSF homepage[2]. It is hoped that the essays attract the interest of researchers from different fields and make them aware of the benefits that ETSF services can bring to their projects.

1 http://dx.doi.org/10.1016/j.crhy.2009.08.002
2 http://www.etsf.eu/about_etsf/theoretical_spectroscopy