**Non adiabatic vibrational spectra from first principles**

**Final Report**

PIIFR-GA-2011-911070

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**1. Executive Summary**

The main goals of the PIIFR-GA-2011-911070, Non adiabatic phonon project were the following:

1. To perform an interface with a self-consistent phonon implementation to extract the ionic forces from a diversity of electronic structure codes such as Vasp, Abinit, Siesta, Quantum Expresso, ELK and Castep and use them to calculate the temperature dependence of the phonon spectra by using the Self Consistent Ab initio Lattice Dynamics (SCAILD).
2. To use the created interface in item (1) to study specific thermoelectric materials, where the influence of the anharmonicities is very important to understand the material behavior. In particular, PbTe has been chosen for being one of the most studied materials in this field, where there is still some unanswered questions about its large termoelectric response.
3. To establish the basic components to perform Non adiabatic phonon dispersion calculations, in particular to identify the effect of the complex character of the phonon self-energy that contains the lifetime of the phonon, a measure of the anharmonic thermal effects within the material.
4. To set up long-range collaborations with groups within the Max Planck Institute in Halle and other groups in Europe, that can make use of the expertise of the responsible members of this proposal and in particular to establish proposals that will impact the research of both groups.

After a year of intense research and development activities, the majority of the goals proposed in the original project were reached and a plan to finish the pending research has been established in a long-term collaboration. In particular, target (1) was completely finished and a Perl script that interfaces between the self-consistent ab initio lattice dynamics method (SCAILD) and different first principle codes was put in production. For such purpose, we set up a collaboration with the group of Prof. Matthieu Verstraete at Liege University, where this script has been used and with Dr. Olle Hellman, Linköping University in Sweden, who has done a different implementation based on *ab initio* molecular dynamics. This takes us to target (2), where all calculations for the case of PbTe has been performed but in order to insure the physical observations based on our implementation, we have decided to coordinate our efforts with Dr Hellman, which is performing a similar calculation but now using his approach. We expect to be able to compare directly those two approaches and to learn about the different approximations and the relevance of the observed physics. Goal (3) was more complicated and we were unable to complete this task. The fact that the physical observables depend quite strongly on the K-point density used to describe the wavefunction in reciprocal space took us into a different path, where we did have to perform an implementation of the Maximally Localized Wannier functions within the software ELK, that will allow us to extrapolate energies and wave functions into a much larger grid based on a coarse grid. At this point, the Wannier functions interface has been partially finished with the software Wannier90 ([www.wannier.org](http://www.wannier.org)). Right now, we are able to project the Kohn-Sham states into a random set of states but we need to go further and perform the projection on a pre-chosen set of atomic orbitals, this is lacking at this moment but within this effort we will perform this implementation in the next few months. Last goal (4) was more than successful. Besides establishing a strong collaboration with the developers of ELK and interfacing with them a lot for the Wannier implementation, some other additional projects were initialized with scientists within the MPI in Halle and at the MPI in Dusseldorf. The description of such collaborations is discussed below.

The development of this project was not only focused on the technical aspects of the problem of non-adiabatic phonons but also to establish a collaboration network with different institutions in Europe that were visited during the course of the project. This goal was achieved by participating in conferences but in particular with direct visits to institutions and deliver specific talks related somewhat to this proposal. These visits allowed us to have direct contact with groups outside the project and create an awareness of our efforts as well as to be able to build new collaborations with other groups that will remain in the long run.

In the first part of this report, we describe the most technical aspects of the research performed during the year of the project. Technical issues as well as the encountered problems will be discussed. In the second part of the report, we focused more on the dissemination, productivity and planned activities derived from this project.