Scientific Report "Short Visit Grant"
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Aim of the visit

The purpose of my visit was to learn a recent implemented theoretical/computational approach combining ab-initio DFT and many-body simulations applied to the study of the electronic and optical properties of materials, beyond the "state of the art" clamped nuclei approximation. Dr. Elena Cannuccia, I visited in Grenoble, and Dr. Andrea Marini are indeed the main developers of a recent theoretical and computational tool based on the dynamical extension of the Allen and Cardona approach to the study of the electron-phonon interaction, presently implemented in the code yambo (www.yambo-code.org).

A preliminary study of the theory background at the base of this formulation has been necessary to carry on the computational steps on which this methodology is built up.

Our aim is to investigate the effect of the electron-phonon (el-ph) interaction on the electronic properties of several bulk oxides and hopefully then to the corresponding nano-structured phases of these materials. The first materials under study were MgO and TiO2. On MgO several publications on the electronic gap renormalization, due to the el-ph interaction, appeared in the last years. We aim to compare our results with the available literature. Regarding the anatase phase of TiO2, whose ab-initio description at the T=0 many-body level (GW,BSE) has been recently published (see Phys. Rev. B 82, 045207) and a very recent publication (Phys. Rev. Lett. **110**, 196403), reported several measurements by ARPES techniques of the spectral functions at different level of doping and several temperatures.

We want to verify if the actual stage of the developed theoretical framework is able to reproduce the available experimental data or if, other diagrams of the e-ph self-energy, or a different description will be necessary for a complete and correct description of the electronic and optical spectra beyond the clamped nuclei approximation.

Description of the work carried out during the visit:

We had first to install a dedicate version of Quantum Espresso (to calculate the self-consistent potential and the e-p matrix elements within the DFPT) and yambo codes (to calculate the Fan and Debye-Waller contribution to the el-ph interaction) on a parallel Supercomputer. In particular we were able to install these codes on EURORA and PLX of Cineca Supercomputer center (www.cineca.it). Here some CPU time from past projects will be used in the next months to carry on the present project.

As first step, we relaxed the MgO and anatase TiO2 bulk structures, using norm-conserving pseudo-potentials and finding the relaxed equilibrium constants, in good agreement with the experimental ones. Then we calculated the phonon-dispersion bands of MgO and we found a perfect agreement with available experimental and theoretical data. An analogous calculation for anatase phase of TiO2 is under way. In particular during my visit, I learned the computational procedure to calculate the electronic gap renormalization due to the el-ph interaction: calculation of the self-consistent potential within DFPT, the el-ph matrix elements, followed by the renormalization of the bare electronic energies due to the el-ph interaction.

Description of main results obtained:

At the moment convergence calculations on the main ingredients of the el-ph self-energy terms (q-points grid, number of bands) are under way. Finally we will obtain convergence on the band-gap renormalization value and on the spectral functions.

Future collaboration with the host institution: Dr. Elena Cannuccia will probably come in Rome after the summer to continue this collaboration.

Projected publications : although the described research activity is still at the initial stage, our aim is to publish at least one or two dedicated publications on the oxides under study hopefully within 2014.