

Final Report on the short visit grant entitled: Non-equilibrium dynamics from first principles

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Purpose of the visit

The purpose of the visit in the group *Theory and Numerical Simulation of Electronic Properties* at the NEEL laboratory (neel.cnrs.fr), was to develop theoretical approaches, algorithms and numerical codes to simulate the physical properties of realistic systems out-of-the-equilibrium.

In addition to the tight collaboration with the theoretical group of Prof. BLASE the visit was supposed to promote discussions with local members of the institute that are currently involved in the study of models and theoretical approaches to the study of transport in nano-scale materials.

Description of the work carried out during the visit

Much to my satisfaction, during my visit, I had the opportunity to have deep and exhaustive discussions with two members of the NEEL laboratory: Dr. Simone FRATINI and Dr. Didier MAYOU on the theoretical approaches to the study of non-equilibrium transport they have derived. I also had the opportunity to discuss with Dr. Yann-Michel NIQUET, of the local Atomistic simulation laboratory, about the numerical and theoretical tools he uses to describe intrinsic transport properties in nano-scale materials.

At the same time I continued my fruitful collaboration with Dr. Claudio ATTACCALITE of the NEEL institute on the device of a controllable approach to the non-equilibrium dynamics in realistic materials. With Dr. ATTACCALITE I discussed further projects to be carried on in the following months and we had also very constructive discussions on various theoretical aspects of the non-equilibrium dynamics.

Description of the main results obtained

The discussions with the members of the local scientific community gave me an extended overview of the state-of-the-art approaches to the non-equilibrium dynamics, as far as transport properties are concerned. I received several references to review papers and works carried on in the NEEL institute. These will represent a basis for my future work and for future collaborations.

With Dr. ATTACCALITE I discussed the steps necessary to embody the electron-phonon scattering in the non-equilibrium dynamics. We derived a coherent approach to describe the temperature evolution as due to the relaxation of the electronic degrees of freedom following the excitation by means of an ultra-strong laser pulse.

We also discussed further applications of the approach we proposed¹ recently such as: second and third harmonic generation in carbon nano-tubes and the description of the dynamical Franz-Keldysh effect from first principles.

Future collaboration with host institution

The collaboration with Dr. ATTACCALITE will continue in the forthcoming months. We are already collaborating and, thanks to this visit, new projects have been planned for the future. I will also start a project on conductivity and mobility in molecular crystals. This will permit me to start collaborations with other members of the NEEL institute.

¹ *Real-time approach to the optical properties of solids and nanostructures: Time-dependent Bethe-Salpeter equation*, by C. Attaccalite, M. Gruning and A. Marini, Phys. Rev. B, in press.

Projected publications/articles resulting or to result from your grant

There are several publications that will result from the present grant. The study of second and third harmonics generation in carbon nano-tubes, the modeling of electron-phonon scattering (with Dr. ATTACCALITE) and my separate project on conductivity and mobility in molecular crystals. These projects are expected to be concluded by the summer of 2012.