Research Networking Programmes

Short Visit Grant ☒ or Exchange Visit Grant ☐

(please tick the relevant box)

Scientific Report

The scientific report (WORD or PDF file – maximum of eight A4 pages) should be submitted online within one month of the event. It will be published on the ESF website.

***Proposal Title**:* First-principles study of second-order Resonance Raman scattering

Application Reference N°: 6689

1) Purpose of the visit

The ongoing collaboration between theoretical and development work done in Louvain-la-Neuve (group of Xavier Gonze), Berlin (group of Claudia Draxl) and with experimental work done in Luxembourg (group of Jens Kreisel) aims at advancing the ab-initio simulation of Raman intensities in general, by assessing different approximations and different levels of theories.

In the proposed collaborative visit, we wanted to investigate the evolution of the second-order Raman scattering process with the laser frequency. The second-order intensity can be computed from the generalization of the approach used for first-order intensity [Y. Gillet et al, Phys. Rev. B 88, 094305 (2013) and C. Ambrosch-Draxl et al, Phys. Rev. B 65, 064501 (2002)], combining multiple finite difference calculations with supercells for different points in the Brillouin Zone. This requires some code development in the framework of both Abinit and exciting codes.

2) Description of the work carried out during the visit

During this visit, we have first settled the methodology to be applied to compute these second-order Raman intensities. Since the "brute force" approach requires a huge amount of different calculations, we have focussed on reducing the total amount of calculations by using symmetries.

After this step, we have developed scripts for the automatic generation of input files and automatic post-processing of the results within the Abipy python framework for Abinit.

Finally, calculations have been performed on silicon thanks to these automated tools using the CISM/CECI infrastructure in Belgium and the Dune cluster in Berlin.

3) Description of the main results obtained

From the results of the calculations, we have shown that the relative intensities of the peaks associated to different points in the Brillouin Zone change drastically when the laser frequency increases. These changes appear as soon as (even indirect) transitions are reached. The results obtained so far show a very good agreement between theoretical results and measurements [Renucci et al, Phys. Rev. B 11, 3885 (1975)].

4) Future collaboration with host institution (if applicable)

In the future, we want to develop a similar methodology in the exciting code, by generalizing what is already coded for first-order and based on what we have done during this visit. Then applications on systems of interest (i.e. BiFe03 or carbon-based structures) will be performed with Abinit and exciting.

These future perspectives will require future collaboration and visits between our two groups in Berlin and Louvain-la-Neuve.

5) Projected publications / articles resulting or to result from the grant *(ESF must be acknowledged in publications resulting from the grantee's work in relation with the grant)*

We have already started writing a publication during this visit, based on the results we have obtained for the second-order Raman spectrum of silicon. It should be submitted in the next coming months to an international peer reviewed journal.

We envision a second more detailed common publication on the methodology.

6) Other comments (if any)

We thank the ESF/Psi-k 2 programme for the support of Short Visit Grants.