Report on the outcomes of a Short-Term Scientific Mission[1]

Action number:

Grantee name:

Details of the STSM

Title: **Attosecond transient Absorption spectroscopy in topological materials via Wannier orbitals**

Start and end date: 01/12/2021 to 15/12/2021

Description of the work carried out during the STSM

Description of the activities carried out during the STSM. Any deviations from the initial working plan shall also be described in this section.

The main goal of this short stay was to understand the main properties of topological materials, the classification that is used in literature to distinguish them and, as a final step, choose one or more that seems promising for its geometrical and topological properties, in order to find track of the non trivial topology directly from the ATA spectrum.

During the STSM, I interacted with people from EPFL that have expertise in the field of topological materials, and it has been easier for me to understand all the features of this subject.

I collected some of the main papers and reviews about topological materials, from Weyl semimetals to Chern insulators. As it seems that most of the materials that are nowadays known are Weyl semimetals, I decided to focus on them. Weyl semimetals have some symmetry broken because of the spin-orbit coupling, and this produce two nodes in the Brillouin zone with non trivial topology. The fact that there are two nodes is caused by the properties of the spin-orbit coupling, that splits one node into two, and breaks the symmetry of the crystal. The Berry curvature is not zero, and this makes these materials interesting for a future study from their ATA spectra.

[1] This report is submitted by the grantee to the Action MC for approval and for claiming payment of the awarded grant. The Grant Awarding Coordinator coordinates the evaluation of this report on behalf of the Action MC and instructs the GH for payment of the Grant.

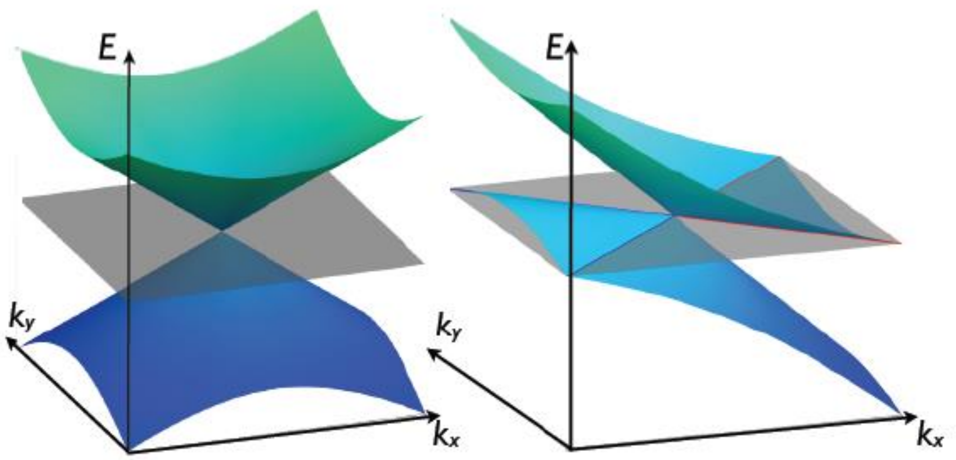

Fig. Schematic representation of type I (left) and type II (right) Weyl semimetals, from Solyuanov et al. Nature **527**, 495 (2015)

As it is shown in figure, there are two types of Weyl semimetals, and since the type II have many bands crossing the Fermi level that can produce "noise" for the properties that I want to study, I focused on the first ones.

Among them, I chosed TaAs and TaP as possible materials to study. Their band structure show two Weyl nodes, that I want to study with tools provided by DFT codes.

Even if I still don't have the Wannier functions of the materials, everything is already settled to do the DFT calculations and I learnt during my experience how to study the properties (as the Berry curvature) of the Weyl nodes via post-DFT tools (as WannierBerry).

Description of the STSM main achievements and planned follow-up activities

Description and assessment of whether the STSM achieved its planned goals and expected outcomes, including specific contribution to Action objective and deliverables, or publications resulting from the STSM. Agreed plans for future follow-up collaborations shall also be described in this section.

(max. 500 words)

During my short stay, I managed to have a good knowledge of the properties of topological materials, and I spent my time to understand which are the materials that are nowadays studied and with non trivial topology in their properties. Among them, I decided to focus on type I Weyl semimetals, which have a band dispersion similar to the one of graphene, but the cone exists in 3D and this makes the material more appealing for its properties. I have also learnt to use the Aiida framework, with which it will be easier to perform the time-independent part of my calculations (DFT and Wannierization).

I am planning to obtain an ATA spectrum of two materials in particular, TaAs and TaP, in order to understand if their non trivial topology leaves a trace in their optical properties. It will be very nice for the community of ultrafast spectroscopy to achieve this goal, and to show that also the field of topological *materials, that is nowadays appealing for the scientific community, can have a good contribution from attochemistry.*

The collaboration with the group at EPFL is continuing, and besides what I explained, I am also trying with their collaboration to fix a known bug inside the wannier90 code, related to the position operator in the basis of wannier functions.