SHORT TERM SCIENTIFIC MISSION (STSM)
SCIENTIFIC REPORT

This report is submitted for approval by the STSM applicant to the STSM coordinator

Action number: CA18222-Attosecond chemistry
STSM title: Attosecond transient absorption spectroscopy via Wannier orbitals
STSM start and end date: 15/09/2021 to 15/10/2021
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PURPOSE OF THE STSM:

When dealing with Bloch functions, it is common to have an interaction potential that diverges at some points of the reciprocal space. This is because the manifold in which the electrons wavepacket move presents discontinuities. As a consequence, it is very difficult to reach convergence for the electron dynamics simulations.
Wannier90 is a post-processing *DFT tool* that *allows* the *interpolation of band structures and wave functions of an extended system. It has been developed by the host institution and provides a good solution to avoid discontinuities since the wavefunctions are interpolated with wannier* functions, that *are well localized in space; thus, their representation in reciprocal space does not present any discontinuity.*
The program that I developed during the last years propagates the electronic density matrix of an extended system under the presence of an external field. It needs as a starting point the bands and the position operator in the basis of Bloch functions, all observables that can be extracted after a wannierization. Building an interface of my program with wannier90 can lead to the possibility to perform realistic calculations to compare with experiments.

DESCRIPTION OF WORK CARRIED OUT DURING THE STSMS

As a first step, I managed to do a *DFT calculation of the systems that I wanted to simulate. Since I* had already *some* tight-binding *calculations for those systems to compare with, the choice was to perform calculations for the band structures of a 2D semimetal, graphene, and its corresponding 3D semimetal, graphite.*
The wavefunctions of both materials have discontinuities in reciprocal space, corresponding to the points K and K' of the Brillouin zone. As the final goal was to have a good position operator, which depends on the gradient of the wavefunctions, these discontinuities must be canceled*.*
I learned *to wannierize the DFT calculations performed with quantum espresso. In particular, by using wannier90, the wavefunctions are "mixed". At the end of the calculation, one can extract the Hamiltonian matrix and the position operator matrix in terms of wannier functions (thus in real space). A "Fourier transform" allows to go to reciprocal space form of the wavefunction, where the semiconductor Bloch equations are derived.*
With all this implemented and working, it has been possible to propagate in time the electronic density matrix of those systems. This allows to describe realistic pump-probe experiments, in which an IR laser pulse drives the electron dynamics while an attosecond X-ray pulse probes the induced dynamics by resonantly exciting the core bands with the valence/conduction bands. I calculated the ATA spectrum, i.e. the absorption of the attosecond X-ray pulse going through *the medium under the presence of the strong IR laser pulse. There are similarities and differences between my previous* tight-binding *calculations and the one that I performed here. This comparison is a first step to understand the limits of the* tight-binding *models.*

DESCRIPTION OF THE MAIN RESULTS OBTAINED

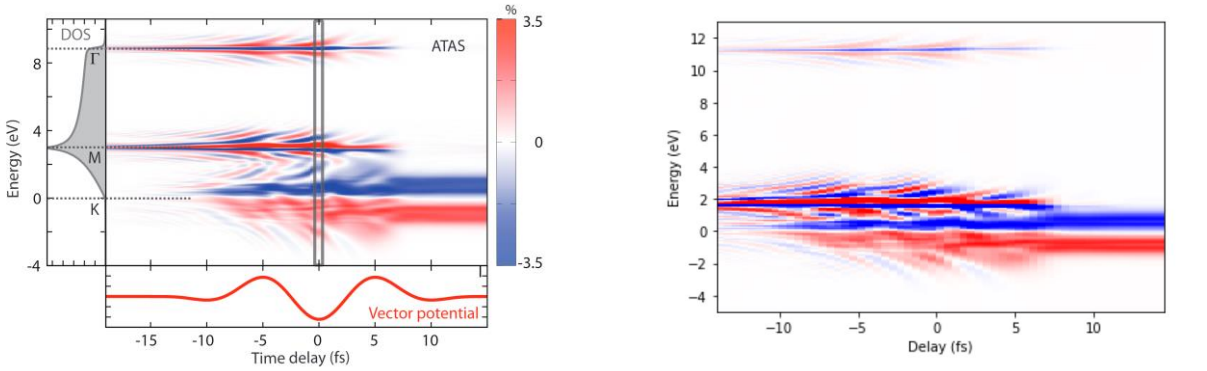

Fig: ATA spectra for TB graphene (left) and graphene from wannier90 (right)

The results regarding this collaboration *are mainly related to the observable of my calculations, the ATA spectra, as well as some output I produce from my calculation, for example*, *the density of electrons in direct and reciprocal space. The ATA spectra can be compared with the one that I already have, which I already published. We can notice that there are differences in the spectra, related mostly to the change in the energy dispersion of the system, and some similarities. The behavior of the Van Hove singularity is similar, with some difference related to a different slope of the energy dispersion.*
The movement of the electron in reciprocal space results mostly the same. In the resolution given by the images, it is not possible to notice any significant difference.

FUTURE COLLABORATIONS (if applicable)

I am currently planning to apply for a new STSM at EPFL, since the group that I worked with has a lot of knowledge in many other fields of condensed matter that sound interesting for my research. In particular, I would like to learn more about topological material and understand which ones are the best candidates to *perform a pump-probe experiment. I would like to develop a method to understand the topology of the material in which the electric field creates excitations. We already tried to do it with* tight-binding *models, and applying it to real material can be the key to* compare *the results with experimental results.*