Ab Initio Description of the Photoionization of Graphene Under Laser Pulses

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Graphene (Gr) is the archetype of a 2D material. With a zero-gap and excellent mechanical properties, Gr seems to be an endless source of research topics, with a huge range of potential applications. However, most of the theoretical works on Gr are based in models (e.g. tight binding) or in regular Density Functional Theory (DFT) calculations. With such approaches, the time evolution of the electrons in the material is rarely considered. Thus, several ultrafast processes, in the range from attoseconds up to a few femtoseconds, cannot be studied with standard calculations.

However, using our methodology [1], based on the Wave Packet Propagation (WPP) technique, we are able to describe the electron dynamics taking into account the full atomistic structure, thanks to the inputs of high-level ab initio DFT calculations.
This methodology, which has been used to follow the dynamics of electrons attached to molecules adsorbed on metal surfaces [2] and on metal surfaces decoupled with ultrathin insulator layers [3], allows the inclusion of time-dependent potentials, such as ultra-short and/or ultra-intense laser pulses.

Here, we present a WPP study of the photo-excitation and photo-ionization of Gr under the action of infrared (IR) laser fields. Our results show a strong relation of the coordinate of the Brillouin zone of the initial state and the probability of the photoionization.
Also, we observe the transition from the multiphoton to the strong field regime when intense IR laser sources are applied to the material.

References

[1] F. Aguilar-Galindo et al. Journal of Chemical Theory and Computation, 17 (2021), 639
[2] F. Aguilar-Galindo et al. Applied Surface Science, 554 (2021), 149311
[3] F. Aguilar-Galindo et al., ACS Photonics, Accepted (2021)

Figures

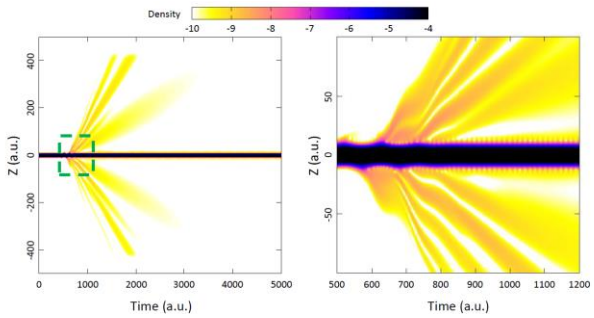

Figure 1: Density of the emitted electrons as function of time under the action of the laser pulse. Graphene is located at z=0.