Atto-second out-of-equilibrium dynamics in germanium

L. J. D'Onofrio,[1] A. Eskandari-asl,[1] and A. Avella[1,2,3]

[1] *Dipartimento di Fisica "E.R. Caianiello", Università degli Studi di Salerno, I-84084 Fisciano (SA), Italy*

[2] *CNR-SPIN, UOS di Salerno, I-84084 Fisciano (SA), Italy*

[3] *Unità CNISM di Salerno, Università degli Studi di Salerno, I-84084 Fisciano (SA), Italy*

Implementing XUV-ray spectroscopy is one of the challenging topics in solid-state physics [1-5]: indeed, it can be a crucial step to unveil the early time dynamics of fundamental processes in systems such as semiconductors, metals, superconductors and topological materials. Therefore, it is essential to build theoretical tools in order to understand the experimental results and what actually happens in solid-state systems on a new and finer time-scale: the atto-second scale. Studying and simulating electron dynamics on the atto-second scale is a new element useful for revealing the fundamental forces driving electron dynamics and leading to the physics related to topological phase transitions. With this in mind, we have developed a theoretical-numerical tool in order to control the time evolution of the electronic band populations in germanium on the atto-second scale when perturbed by a near-IR pump probe. First of all, we have had to deduce the unperturbed germanium band structure by Elk. After that, we have resorted to Wannier90 to compute Maximally-Localized Wannier Functions (MLWFs) from a specific number of Bloch wave functions and obtain the hopping terms. Subsequently, we studied the perturbed case by the Peierls substitution method. We have inferred a system of coupled first-order differential equations describing the out-of-equilibrium time evolution of band populations. The results obtained describe electronic transitions from the valence to the conduction band on the atto-second scale. The overall tool can be extended to other systems like superconductors and topological materials.

References:

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