Hot electron dynamics in graphene –a linear-scaling atomistic approach

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Graphene holds significant promise for a variety of applications. in particular, graphene photodetectors have been shown to be very fast, highly sensitive, and consume minimal power, making them extremely promising for next-generation optical communication technologies[1].

Hot electrons – electrons whose temperature is higher than the surrounding lattice – play a fundamental role in such graphene photodetectors. A variety of theories and measurements have been developed and conducted to understand the main factors controlling the dynamics and relaxation of hot carriers in graphene, but fundamental questions remain to be examined [2].

Here, we present our development of a numerical simulation tool that can capture the dynamics of hot carriers in graphene with arbitrary lattice vibrations, defects, and disorder. Our methods are linear-scaling, meaning we can simulate systems with millions of atoms – this permits an atomic description of the system while allowing for system sizes that approach the experimental scale. Such a tool will allow for a deeper fundamental understanding of hot carrier dynamics in graphene, as well as reveal strategies for the control of such dynamics, with an eye toward future applications in photodetection, optical communications, and energy conversion.

References

[1] M. Romagnoli, V. Sorianello, M. Midrio, et al. Nat. Rev. Mater., 3, 392 (2018).

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Figures

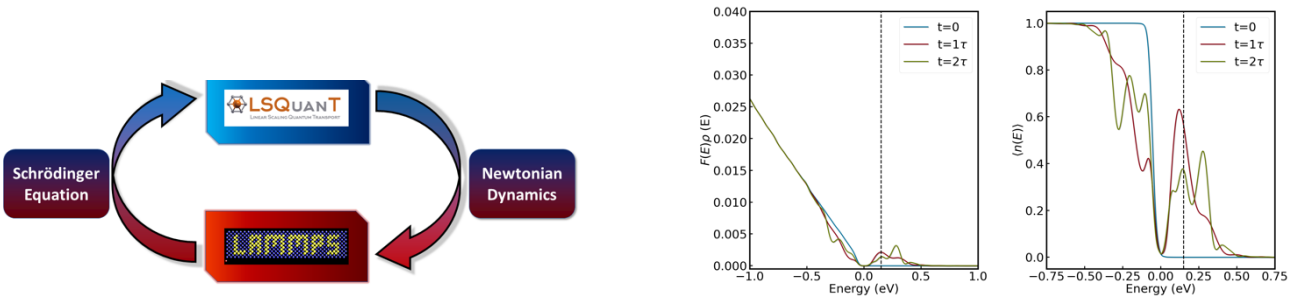

Figure 1 ***Left***: Schematic representation of the self-consistency cycle for the atomistic simulation of coupled charge and ion dynamics. ***Right***: Time and energy resolved phonon absorption in monolayer graphene.