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 communications [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 understanding of hot carrier dynamics in graphene and other 2D materials, as well as reveal strategies for the control of such dynamics, with an eye toward future applications in photodetection, optical communications, and energy conversion.

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References

[1] M Romagnoli et al, *Nat Rev Mater* **3**, 392 (2018)
[2] M Massicotte, G Soavi, A Principi, K-J Tielrooij, *Nanoscale* **13**, 8376 (2021)

Figures

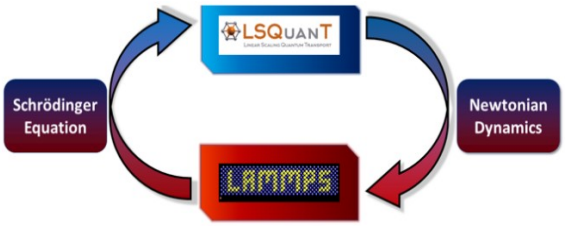

Figure 1. Schematic of the self-consistency cycle for the atomistic simulation of coupled charge and ion dynamics.

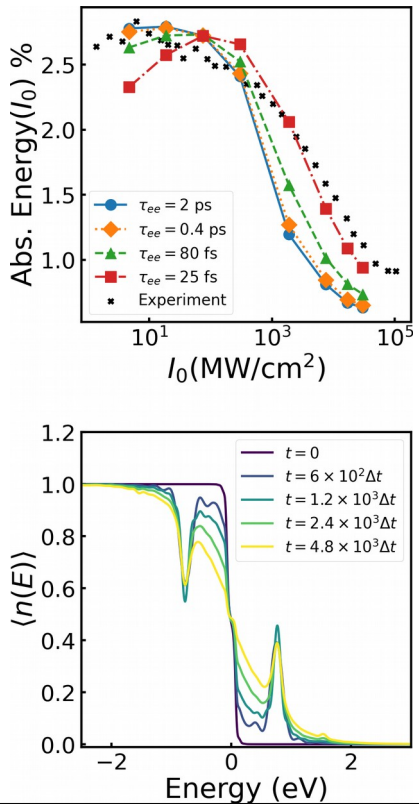

Figure 2. *Top*: absorption efficiency of a finite optical pulse in graphene, as a function of optical power. Colored curves are simulation results and black symbols are from experiments. *Bottom*: time evolution of the electronic carrier distribution under the optical pulse, with competing vertical absorption and thermalization effects.