Electronic energy losses in collision cascade simulations

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Electrons couple to atoms through two distinct processes, i.e. electronic stopping in the high energy limit and electron-phonon coupling in the low energy limit. In collision cascades, atoms transition smoothly from one regime to the other, and a clear physically motivated threshold between these two regimes cannot be determined. This gives rise to significant challenges for incorporating electronic effects in large scale atomistic simulations. In this talk, I present the latest developments towards this goal.

By extensive quantum mechanical calculations, we can determine the electronic energy losses in specific local environments, in particular, as a function of the local electronic density seen by the projectile or atom. Using a model that approximates the energy losses as a function of the electronic density modelled in the atomic system, we are able to simulate energetic collision cascades in multi-million atom systems with both electronic stopping and electron-phonon coupling, without imposing cut-off parameters. We find that two energy loss regimes during cascade evolution emerge from this model, with a transition in the rate of energy losses occurring between the early ballistic phase and later relaxation phase of the cascade. The two stages of energy losses clearly capture the two different coupling regimes, with energy losses corresponding to electronic stopping in the early phase of a cascade and electron-phonon coupling in the later phase.