

Abstract Submitted
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Electrical conductivity of metals from real-time time-dependent density functional theory XAVIER ANDRADE, ALFREDO CORREA, Lawrence Livermore National Laboratory — In this presentation, I will discuss how to apply real-time electron dynamics to study electronic currents in crystalline systems and, in particular, how to use this method to predict electrical conductivities in different regimes. This approach presents many interesting theoretical challenges associated to the representation of bulk systems as infinitely periodic. For example, in order to induce electronic currents in the system, we use a gauge transformation that allows us to include finite electric fields in the simulation. We have implemented this approach using time-dependent density functional theory (TDDFT). This implementation allows us to induce, measure and visualize the current density as a function of time, in simulations with thousands of electrons (hundreds and even thousands of atoms). We have found that real-time TDDFT can describe how currents naturally decay in metals. From this dissipation process we can directly calculate the frequency-dependent conductivity, including the direct current (DC) conductivity that is not accessible from linear-response approaches like Kubo-Greenwood.

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