# Negative differential conductivity in liquid aluminum from real-time density functional theory

X. Andrade[1], S. Hamel[1], and A. Correa[1]

[1]Quantum Simulations Group, Lawrence Livermore National Laboratory, Livermore CA 94550.

In this talk we will present our approach for the calculation of non-linear electronic conductivy based on time-dependent density functional theory (TDDFT). Based on these simulations, we predict that liquid aluminum exhibits negative-differential conductivity for current densities of the order of $10^{12}$-$10^{13}$ A/cm2. We find that the changes in the conductivity, as the current increases, emerge from a competition between the accumulation of charge around the nuclei, that increases the scattering of the conduction electrons, and a decreasing scattering cross-section at high currents.

Our calculations are based on a new approach that can model, for the first time, non-linear effects in the conductivity of materials from first principles by following in real-time the dynamics of the electrons. In our approach, we induce a current of finite intensity in the system and follow its evolution in time to determine the effective conductivity. The new method is more accurate, computationally efficient, and scalable than the Kubo-Greenwood approach normally used to obtain conducitivities.