



SCHOOL OF NATURAL SCIENCES PHYSICS COLLOQUIUM 293

Negative Differential Conductivity in Liquid Aluminum from Real-time Time-dependent Density Functional Theory

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ABSTRACT

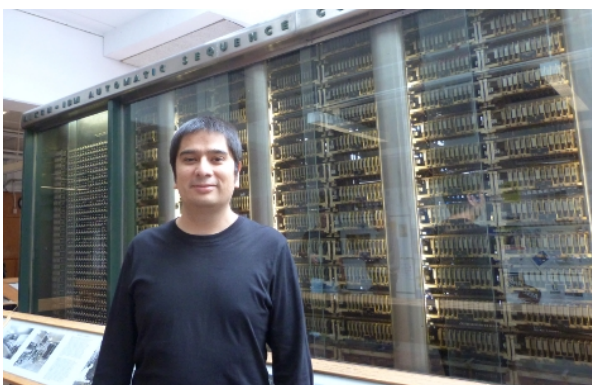
In this presentation, I explore the application of real-time electron dynamics, the explicit simulation of the quantum dynamics of electrons in time, to study the conduction of electricity in metals. These simulations give us access to many current related properties, in particular, the calculation of electrical conductivities in different regimes.

We have implemented this approach using time-dependent density functional theory (TDDFT) in its real-time formalism. This implementation allows us to induce, measure and visualize the current density as a function of time in realistic systems. The computational efficiency of the method allows us to perform simulations with hundreds and even thousands of atoms.

We have found that real-time TDDFT can describe how currents naturally decay in metals, and 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. Since our method deals with finite-intensity electric fields, we gain access to properties beyond the linear regime for intense electric fields and current densities.

We illustrate our approach by simulating the linear and non-linear conductivity of aluminum at high temperature. Our calculations predict that the conductivity of liquid aluminum changes for very-high currents and that it even exhibits negative differential conductivity.

BIO:



Xavier Andrade is a research scientist in the Quantum Simulations Group at Lawrence Livermore National Laboratory. His research focuses on the development of new methods and tools for the simulation of the dynamics of electrons in materials, in particular approaches based on time-dependent density functional theory. He is also interested in the application of new high-performance computing paradigms to large scale scientific codes.

Xavier holds a B. Sc. and a M. Sc. in physics from the University of Chile, and a Ph. D. from the University of the Basque Country, Spain. Before joining Lawrence Livermore, he was a postdoc in the Department of Chemistry and Chemical Biology at Harvard University. Xavier has contributed to several scientific computing codes, and he is one of the main developers of Octopus, a real-space density functional code, used by many researchers around the world.