



## DoNuTS Technical Meeting

**Time:** 1600 Wednesday, 4 June 2008

**Place:** NE Conference Room, 4101 Etcheverry

**Speaker:** Julius Su, California Institute of Technology

**Subject:** Simulation of large-scale excited electron dynamics

We introduce eFF, a molecular dynamics model with electrons included in a way that accounts for the effects of Heisenberg uncertainty and Pauli exclusion. It can simulate highly excited systems where the Born-Oppenheimer approximation may break down over long times, and where excitations may be distributed in a spatially heterogeneous nonequilibrium fashion over tens of thousands of electrons. Using eFF, we explore the thermodynamics of warm dense hydrogen, and find excellent agreement with path integral methods and diamond anvil and shock compression experiments over a temperature range of 0 to 100,000 °K and densities up to  $1 \text{ g cm}^{-3}$ . We also simulate the Auger process in a diamond nanoparticle ( $\text{C}_{196}\text{H}_{112}$ ), and discover direct and indirect pathways for the desorption of atomic fragments from the surface, in agreement with recent experiments.