We introduce an electron force field (eFF) that makes simulation of large scale excited electron dynamics possible and practical. The forces acting on thousands of electrons and nuclei can be computed in less than a second on a single modern processor.

Just as conventional force fields parameterize the ground state potential between nuclei, with electrons implicitly included, electron force fields parameterize the potential between nuclei and simplified electrons, with more detailed degrees of freedom implicitly included. The electrons in an electron force field are Gaussian wave packets whose only parameters are its position and its size.

With this eFF, we compute the dissociation and ionization behavior of dense hydrogen, and obtain equations of state and shock Hugoniot curves that are in agreement with results obtained from vastly more expensive path integral Monte Carlo methods. We also compute the Auger dissociation of hydrocarbons, and observe core hole decays, valence electron ionizations, and nuclear fragmentation patterns consistent with experiment.