Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

First principles investigation of the dielectric function of gold under ultrafast laser excitation[1] TADASHI OGITSU, LLNL, DAVID PRENDERGAST, LLBL, ERIC SCHWEGLER, YUAN PING, ANDREW NG, LLNL — Recently, a quasi-steady state in ultrathin, ∼30 nm gold foils exposed to an ultrafast laser pulse has been observed, which includes an enhanced interband transition peak at 2.6 eV in the imaginary part of the dielectric function [1]. Simulations of this system assuming a two-temperature model for the electronic and ionic degrees of freedom do not provide this enhancement in optical absorption, possibly indicating that both of these degrees of freedom are not in equilibrium. Our approach is to treat this as an inverse problem: to reproduce experiment by sampling various states of electrons and ions. We employ an efficient first principles technique to quickly estimate the dielectric function of this fcc metal for various finite temperature and non-equilibrium model distributions. Converged Brillouin zone sampling is achieved using a compact k-dependent Hamiltonian derived from first principles calculations [2]. [1] Y. Ping et al., Phys Rev Lett **96**, 25503 (2006). [2] E. L. Shirley, Phys Rev B **54**, 16464 (1996).

[1]Work at the Molecular Foundry was supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Prepared by LLNL under Contract DE-AC52-07NA27344.

David Prendergast
Molecular Foundry, LBNL

Date submitted: 06 Dec 2007 Electronic form version 1.4