Abstract Submitted for the DPP11 Meeting of The American Physical Society

Properties of metals during the heating by intense laser irradiation using *ab initio* simulations BASTIAN HOLST¹, VANINA RECOULES, MARC TORRENT, CEA, DAM, DIF, 91297 Arpajon, France, STEPHANE MAZEVET, LUTh, Observatoire de Paris, 92195 Meudon, France — Ultrashort laser pulses irradiating a target heat the electrons to very high temperatures. In contrast, the ionic lattice is unaffected on the time scale of the laser pulse since the heat capacity of electrons is much smaller than that of the lattice. This nonequilibrium system can be described as a composition of two subsystems: one consisting of hot electrons and the other of an ionic lattice at low temperature. We studied the effect of this intense electronic excitations on the optical properties of gold using *ab initio* simulations. We additionally use *ab initio* linear response to compute the phonon spectrum and the electron-phonon coupling constant within Density Functional Theory for several electronic temperatures of few eV.

¹LULI, Ecole Polytechnique, CNRS, CEA, UPMC, 91128 Palaiseau, France

Bastian Holst CEA, DAM, DIF, 91297 Arpajon, France

Date submitted: 13 Jul 2011

Electronic form version 1.4