Abstract Submitted
for the DPP07 Meeting of
The American Physical Society

ab initio **Molecular Dynamics simulations of dense boron plasmas up to the semiclassical Thomas Fermi regime** CLEROUIN JEAN, MAZEVET STEPHANE, LAMBERT FLAVIEN, BOTTIN FRANCOIS, ZERAH GILLES, CEA/DIF Bruyeres Le Chatel France — We have performed *ab initio* simulations of dense boron along the 1 and 4 eV isotherms [1], starting from the regime where quantum mechanical effects are important to the regime where semiclassical simulations based on the Thomas Fermi approach are, by default, the only simulation method currently available. To overcome the limitations of *ab initio* simulations at high density, we have build an "all electron" norm conserving pseudopotential for boron which allows simulations up to 50 times the normal density, ρ_0. We show that, at high pressure, all electrons *ab initio* simulations are necessary to get a correct pressure, which is in close agreement with the one given by the, much faster, Thomas-Fermi molecular dynamics method [2].We further compare the Kubo-Greenwood and the Ziman formulations for the electrical conductivity.

[1] S. Mazevet et al. PRE **75**, 056404 (2007).
[2] F. Lambert et al. PRE **73**, 016403 (2006).

Clerouin Jean
CEA/DIF

Date submitted: 17 Jul 2007 Electronic form version 1.4