Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Ab initio calculation of X-ray absorption spectra for warm dense metals VANINA RECOULES, STÉPHANE MAZEVET, CEA DIF, F-91297 Arpajon — We developed a first principle approach to calculate the x-ray absorption near edge spectra (XANES) of dense plasmas [1] based on density functional electronic structure calculations and quantum molecular dynamics simulations. This approach provides a first principle consistent description of both the electronic structure and the thermodynamics state of the system by using large supercells. We applied the method to the calculation of the XANES spectra near K-edge of aluminium at solid density for temperatures up to 6eV. We show that XANES spectrum loses its room temperature structure, first due to melting and second due to loss of correlation of the liquid. We obtain a good agreement with measurements of XANES spectra performed for an Al foil isochorically heated. We also applied the method to the calculation of the XANES spectra near K-edge of iron at solid density with temperature up to 1eV.

[1] V. Recoules and S. Mazevet, PRB 80, 064110 (2009)

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Date submitted: 25 Nov 2009 Electronic form version 1.4