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Ab-initio calculations of the X-ray absorption spectra of shocked compressed aluminum STEPHANE MAZEVET, VANINA RECOULES, GILLES ZERAH, CEA-DIF F91297 Arpajon France — Molecular dynamics (MD) simulations, using density functional (DF) electronic structure techniques, provide a powerful, predictive tool for examining materials from solids to plasmas over a wide range of densities and temperatures. Using the Kubo-Greenwood formulation, we can access to the frequency-dependent electrical conductivity as well as additional optical properties consistent with the Equation of State. Due to the use of pseudopotentials, the calculations of these properties have, so far, been limited to low photon frequencies, i.e. below 100eV, where only the valence electrons contribute. We recently extended those calculations into the X-ray domain within the PAW formalism. This allows us to describe for the first time, X-ray absorption spectra of shocked compressed aluminum from an ab-initio standpoint.

Stephane Mazevet
CEA-DAM

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