

Abstract Submitted
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Optical signature of the OCP crystallization in a boron plasma

FLAVIEN LAMBERT, STÉPHANE MAZEVET, JEAN CLÉROUIN, CEA, DAM, DIF — We have calculated the DC conductivity of a boron plasma along the 1 eV isotherm up to 25 times the normal density. We use both the quantum and orbital free molecular dynamics coupled with, respectively, the Kubo-Greenwood formulation and the semi-classical Ziman theory. We find that the DC conductivity obtained using a full quantum mechanical treatment exhibits a significant jump at the one component plasma phase transition – specifically the OCP crystallization – jump that is not reproduced using the semi-classical Ziman description. This difference – reaching up to a factor of four – remains well beyond the phase transition and up to the highest density explored. This shows that a full quantum mechanical treatment of the optical and electrical quantities is required in this regime even if semi-classical theories are reliable to obtain both the thermodynamical, and, ionic dynamical and structural properties.

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