

Abstract Submitted
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Ab-initio calculations of the sound velocities of iron at high pressure and temperature. JOHANN BOUCHET, FRANCOIS BOTTIN, FRANCOISE REMUS, CEA DAM DIF, DANIELE ANTONANGELI, GUILLAUME MORARD, IMPMC Universit Pierre et Marie Curie, Paris — By means of *ab initio* molecular dynamics calculations and the temperature dependent effective potential method (TDEP) we have calculated the vibrational properties of hcp iron as a function of density and temperature. From the interatomic force constants we derived the elastic constants and the compressional and shear velocities. We compare our results with the experimental data in the range of densities and temperatures where they are available and to previous theoretical work. We show that our data respect the Birch's law with a linear dependence in density at any fixed temperature and we give a fit of our values covering a large scale of densities and temperatures (10-14g/cc, 0-7000K). We also compare our results with the Preliminary Reference Earth Model (PREM) and we discuss the effect of light elements on the sound velocities of iron.

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