Abstract Submitted
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Structure and dynamics of bulk liquid iron near melting. A first principles study[1] DAVID J. GONZALEZ, MIRIAM MARQUES, LUIS E. GONZALEZ, Dept. Fisica Teorica, Atomica y Optica, Facultad de Ciencias, Universidad de Valladolid, 47011 Valladolid — First principles molecular dynamics simulations, based on the density functional theory and the projector augmented wave technique, have been performed in order to study several static and dynamic properties of bulk liquid Fe at a thermodynamic state near melting. As for the static properties, the obtained results for the pair distribution function and the static structure factor show a good agreement with the available X-ray and neutron diffraction data. The calculated dynamical structure reveals collective density excitations with an associated dispersion relation which closely follows recent experimental data; moreover, its slope at the long-wavelength limit provides an estimate for the velocity of sound. The dynamical structure factors have been calculated and they are compared with their experimental counterparts, which have recently been measured by inelastic X-ray diffraction experiments. Finally, results are also reported for some transport coefficients.

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