Abstract Submitted
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Structure and dynamics of bulk liquid iron at pressures up to 58 GPa. A first-principles study[1] DAVID GONZALEZ, MIRIAM MARQUES, LUIS ENRIQUE GONZALEZ, Dpt. Fisica Teorica, Atomica y Optica, Facultad de Ciencias, Universidad de Valladolid, 47011 Valladolid — The static and dynamic properties of bulk liquid Fe at a several high pressure states, have been studied by using first-principles molecular dynamics simulations based on the density functional theory and the projector augmented wave technique. Results are reported for four thermodynamic states at pressures of 27, 42, 50 and 58 GPa for which x-ray scattering data are available. The calculated static structure shows very good agreement with the available experimental data, including an asymmetric second peak which becomes more marked with increasing pressure. The dynamical structure reveals the existence of propagating density fluctuations and the associated dispersion relation has also been determined. The relaxation mechanisms for the density fluctuations have been analyzed in terms of a model with two decay channels (fast and slow, respectively). We found that the thermal relaxation proceeds along the slow decaying channel whereas the fast one is that of the viscoelastic relaxation. Finally, results are also reported for some transport coefficients.

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