



Melting of iron at Earth's core conditions from quantum Monte Carlo free energy calculations

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The Earth's core is formed by an inner part of almost pure solid iron, surrounded by a shell liquid iron which extends roughly half way towards the surface of the planet. The temperature at the centre of the Earth is a crucial parameter in building models for its thermal structure, yet it is impossible to measure. Indirect information can be gathered by exploiting the presence of a solid/liquid boundary (the ICB), which implies that the temperature at this boundary must be the melting temperature. Experiments on the melting of iron under these conditions (pressure of 330 GPa and temperatures in excess of 6000 K) are extremely challenging, and it is not surprising that a large variability of data is found in the literature.

Numerous attempts have been made to calculate the melting temperature of iron using various flavours of approximations to quantum mechanics, the most notable ones employing density functional theory.

In this talk I will summarise some of these past endeavors first, then present new data obtained with quantum Monte Carlo simulations, a technique generally expected to be one order of magnitude more accurate than density functional theory.