Abstract

It has recently become possible to calculate the free energy and other thermodynamic functions of solids and liquids using density functional theory to treat the quantum mechanics of the electrons[a,b,c]. We present the main ideas that have made this possible, emphasising the key role of thermodynamic integration and the importance of well adapted reference systems in the computation of the free energy. We show how *ab initio* methods have been used to calculate the melting properties of Iron under Earth's core conditions, and we present our results for the melting curve of Iron in the range of pressures spanning from that at the

in the range of pressures spanning from that at the boundary between the Earth's mantle and the outer liquid core, to the pressure at the boundary between the outer liquid core and the inner solid Earth's core.

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[a] Sugino, O.; Car, R. Phys Rev Lett 1995, 74, 1823.

[b] de Wijs, G. A.; Kresse, G.; Gillan, M. J. Phys Rev B 1998, 57, 8223.

[c] Smargiassi, E.; Car, R. Phys Rev B 1996, 53, 9760.