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The Application of ab Initio Quantum Mechanical Methods to the Study of the Earth's Core

G David Price (d.price@ucl.ac.uk)[1], **Lidunka Vocadlo** (l.vocadlo@ucl.ac.uk), **Dario Alfe** (d.alfe@ucl.ac.uk) & **Michael J Gillan** (m.gillan@ucl.ac.uk)[2]

[1] Dept Geol. Sci., UCL, Gower St, London., UK
[2] Dept Physics&Astronomy, UCL, Gower St, London, UK

The experimental investigation of the properties of the materials that form the Earth's deep interior is difficult because of the very high pressures and temperatures involved. As a result computational and theoretical approaches have been adopted to supplement experimental studies. In the past decade, the technique of choice for these studies has been quantum mechanical simulation, involving the use of density functional theory. Contributions have been made by a number of groups, using either all electron methods or pseudo-potentials. More recently, it has become possible to use quantum mechanical molecular dynamics to model the effect of high T and to simulate the properties of liquids. In this talk, we will focus upon the work performed on Fe and its alloys, aimed at attempting to constrain the temperature, composition and physical properties of the inner and outer core. Specifically, we will review work aimed at determining the structure of Fe at core conditions, the melting temperature of Fe as a function of P, the viscosity of liquid Fe in the outer core, the equation of state and rheological properties of Fe under core conditions, the densities and properties of liquid Fe-O, Fe-S and other alloy systems under outer core condition, and the possible composition of the outer core.