

Ab Initio Calculations and the Composition of the Earth's Core

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The Earth's liquid core consists mainly of iron, but its density is too low to be pure iron, so it must contain some light impurity, like S, Si or O. To a lesser extent, this is true for the solid core too. We propose a novel approach to the problem of the composition of the Earth's core. The technique is based on the ab-initio calculations of the chemical potentials of light elements in solid and liquid iron. To demonstrate the technique, we first assume that the core is the binary mixture Fe/S. At the solid-liquid boundary the chemical potentials of S in solid and liquid iron must be equal. This provides a constraint on the partitioning of S, which in turn fixes the densities of the solid

and the liquid. A comparison with seismological data leads to the conclusion that the binary Fe/S mixture is almost certainly untenable as model for core composition (Alfè et al 2000 and Price 2000). In this presentation, we report new results for Fe/Si and Fe/O, and we show that also these two hypothetical compositions are incompatible with the density of the core. Finally, we discuss the possibility of the ternary mixtures Fe/S/O and Fe/Si/O.

Alfè D, Gillan MJ, Price GD, *Nature*, **405**, 172-175, (2000).