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Composition and temperature of the Earth's core constrained by combining ab initio calculations and seismic data

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Ab initio calculations using density functional theory are used to constrain the temperature and composition of the Earth's core. The constraints stem from continuity of the chemical potentials of iron and dissolved impurities across the inner−core/outer−core boundary (ICB). Chemical potential calculations of sulfur, oxygen and silicon impurities indicate that the known solid and liquid densities at the ICB require ~ 8 mol % of oxygen and a similar amount of sulfur and/or silicon in the outer core. The calculated depression of melting point indicates an ICB temperature ~ 800 K below the melting point of iron.
