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Mineral physics in planetary cores: light elements, seismic properties, electrical and thermal conductivity

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We estimate the necessary amount of several light elements - C, S, P, O, Si - as major alloying components to match the observed seismic properties of the Earth's inner core. For this we compute the elastic constants tensors and determine the seismic properties of Fe_3X compounds, with X = C, S, P, O and Si, using first-principles calculations. Assuming linear relations and similar temperature corrections of velocities, we obtain as most reasonable silicon and oxygen. We perform the same exercise on Fe-Ni alloys and see a minor effect of Ni on the seismic properties of iron.

Then we compute the electrical conductivity of iron and iron alloys at Earth's and superEarths' core conditions from electron-phonon coupling in the ABINIT implementation. We find an excellent agreement with experimental results for pure hcp iron below 1 mbars. We confidently use our results up to core pressure conditions. We show that the conductivity exhibits saturation at high pressures. We estimate the thermal conductivity of the Earth's outer core as well as the cooling rate of superEarths.

We treat in detail the effect of Si on hcp iron and show a marked saturation effect, an increase in anisotropy and a strong dependence with the substitution pattern.