Ab initio study of Iron-Nickel alloys in Super-Earths cores

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Iron-nickel alloys are considered the main components of Earth and Super-Earth cores, which make them crucial systems in order to comprehend the properties of these planets. While the relative nickel content is anticipated to be around 10% in the Earth, this value could differ slightly in other planets because of different host star metallicity and formation history. It is thus important to understand the properties of iron-nickel systems with various compositions in the multi-megabar regime.

While pure iron is anticipated to have hexagonal close packing at high pressure, nickel is expected to have face-centered cubic packing. This means there is a structural change as the composition is modified, which can also mean a limited stability of the solid solutions of iron-nickel.

We will discuss the properties of iron-nickel alloys in the megabar regime as predicted by *ab initio* simulations. We will examine the relative stability of different iron-nickel solid solution compositions and the interplay of the spin states. After characterizing the properties of these alloys at pressure-temperature conditions relevant for Super-Earth, we will discuss possible consequences their cores.

Keywords: Super-Earth, iron core, Ab initio simulations

