Crystalline Fe under TPa pressures: simple or complex?

***Stefaan Cottenier (1); Matt Probert (2); Veronique Vanspeybroeck (1); Michel Waroquier (1)**
1. Ghent University (Center for Molecular Modeling) , Belgium; 2. University of York (Department of Physics) , United Kingdom

Corresponding Author: Stefaan Cottenier (stefaan.cottenier@ugent.be)

The pressure-temperature phase diagram for pure Fe plays an important role in Earth and planetary science. Pure Fe is the simplest approximation for the Fe-rich alloy that is believed to be the material forming the solid inner core of terrestrial planets. In the planet Earth, the inner core material is subject to a pressure of about 350 GPa and a temperature of about 6000 K. In more massive terrestrial planets that might exist in other solar systems (exoplanets or super-Earths), the relevant pressures and temperatures might be considerably larger.

Searching for the most stable crystal structure of a given element (or number of elements) under a given pressure and temperature is a "structure prediction" type of problem. Unbiased, systematic structure prediction goes beyond regular DFT applications – in the latter, the crystal symmetry is usually considered to be input knowledge. Recently, various methods for ab initio structure prediction have been proposed[1,2,3].

At 0 K, pure Fe transforms from its bcc ground state structure to a hcp structure already at moderate pressure (14 GPa). No unambiguous (experimental) evidence for other phase transitions at higher pressures relevant for the Earth's inner core is available. A recent computational study[4] that applied the 'random search' ab initio structure prediction method, identified a window at much higher pressures (8-20 TPa) where the fcc phase is more stable than the hcp phase. At even higher pressures (>30 TPa), the same study found a dramatic take-over by the bcc phase. No other phases were found with enthalpies that are competitive with these simple phases (bcc, hcp, fcc).

In the present contribution, we present ab initio calculated enthalpies as a function of pressure up to 100 TPa, for a family of crystal structures that do compete with the simple bcc, fcc and hcp phases in the TPa region.

References: [1] A.R. Oganov et al., J. Chem. Phys. 124 (2006) 244704 [2] N. L. Abraham et al., Physical Review B 73 (2006) 224104 [3] C.J. Pickard et al., Phys. Rev. Lett. 97 (2006) 045504 [4] C.J. Pickard et al., J. Phys.: Condens. Matter 21 (2009) 452205