FeS polymorphs: stability and thermodynamics from *ab initio* modelling

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Iron sulfide polymorphs with formula FeS are thought to compose the cores of Earth and Mars, which is suggested by the presence of troilite, the most stable FeS phase at ambient conditions, in many meteorites [1]. This possibility has sparked interest in investigating the FeS phases forming at extreme thermodynamic conditions that are relevant to planetary science [2, 3].

In this work, we have applied the quasi-harmonic approximation within a density functional theory approach to provide fundamental insights into the stability and the thermodynamic properties of the FeS phases at high pressure and temperature. We show that, although significant differences arise in the values of the transition pressures, the sequence of polymorphs forming under pressure at room temperature is in line with the results in the literature. In addition, our *ab initio* p-T diagram confirms the experimental observations from X-ray diffraction studies. Finally, we reliably predict the thermodynamic properties of the FeS phases at conditions difficult to reproduce experimentally. For troilite, the calculated data are in excellent agreement with those available from measurements.

[1] Fei, Y. *et al. Science* 1995, **268**, 1892. [2] Vočadlo, L. *et al. J. Phys. Earth Planet. Inter.* 2000, **120**, 145-152. [3] Urakawa, S. *et al. Phys. Earth Planet. Inter.* 2004, **143**, 469-479.