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Supplementary Information for

Ni Doping: A Viable Route to Make Body-Centered-Cubic Fe Stable at Earth's Inner Core

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Text S1 : The P-V third order Birch-Murnaghan's equation of state for bcc-Fe-Ni alloy which is derived from energy versus volume relation obtained using first principles density functional theory . The unit cell contains 128 atoms out of which 6.25% are Ni and the rest are Fe. The configuration adapted for performing this calculation is Model 2 as shown in the inset of Figure 1.

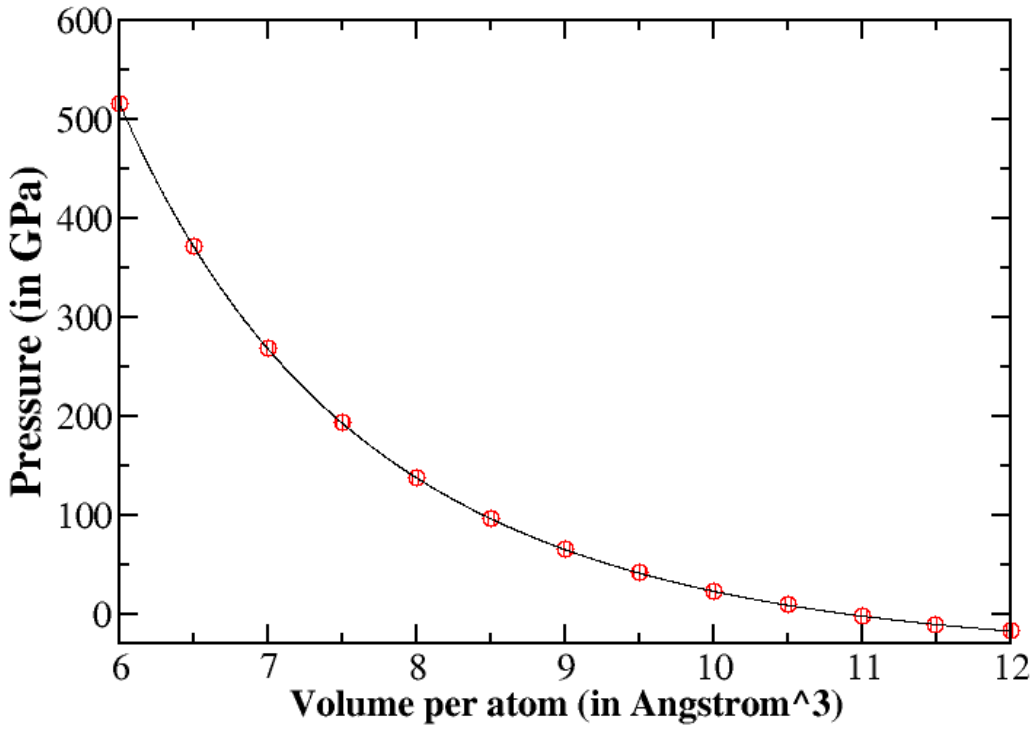

Figure S1.: The P-V third order Birch-Murnaghan equation of state for 6.25% Ni doped bcc-Fe. The black curve shows the curve fitting done using third order Birch-Murnaghan's equation of state on to the theoretically determined dataset as represented by the red circles. The fitting parameters are as follows : V_O (Å^3/atom) = 10.91; K (GPa) = 220.19; K' = 4.49.

Text S2 : Six different models involving 3.125% Ni doped bcc Fe(i.e, there are 4 Ni atoms and 124 Fe atoms per unit cell). The six models scan over different configurations of Ni doping, i.e, uniform, random and clustering of Ni atoms. We find that apart from the cases where Ni is uniformly distributed in the bcc-Fe matrix, the phonon density of states for all the other cases show that the corresponding configurations are dynamically stable.

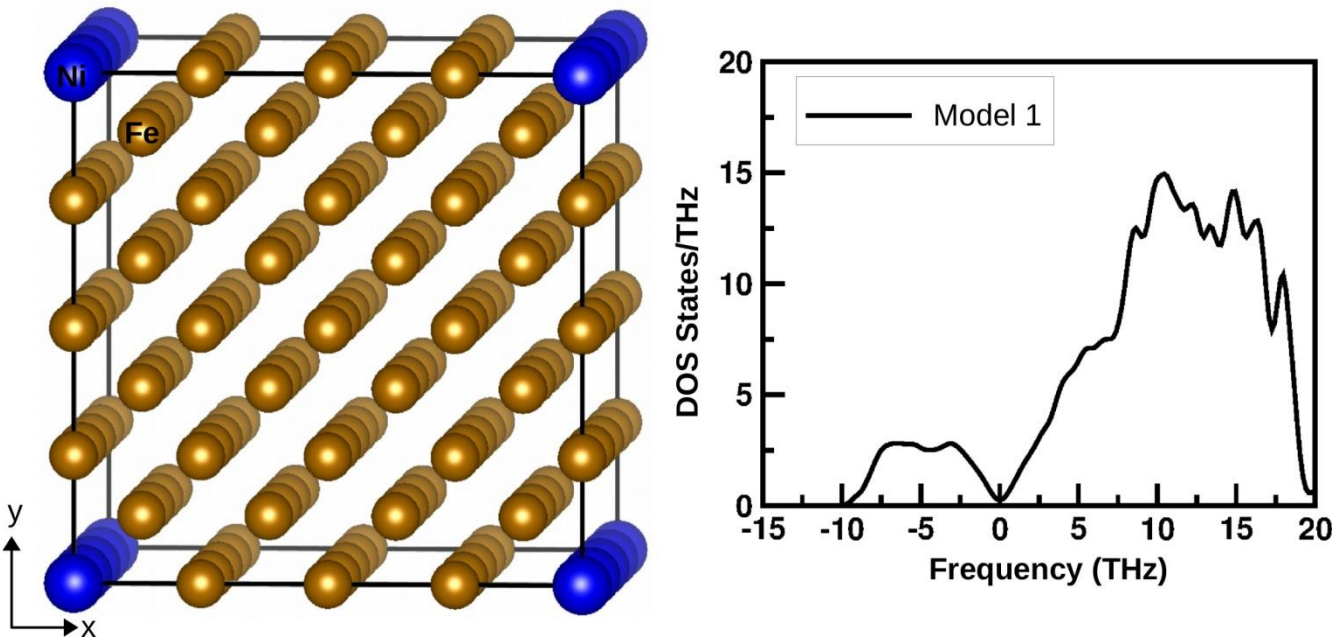

Figure S2.: Here the distribution of Ni is such that they form chains running parallel to c-axis and the distance between each such chain is constant. Therefore the distribution of Ni atoms can be considered as uniform. The crystallographic environment of each Ni atom in the matrix is also found to be similar. The resultant phonon density of states calculated at 364 GPa is found to have imaginary frequencies thereby suggesting that the structure is dynamically unstable at inner core pressures.

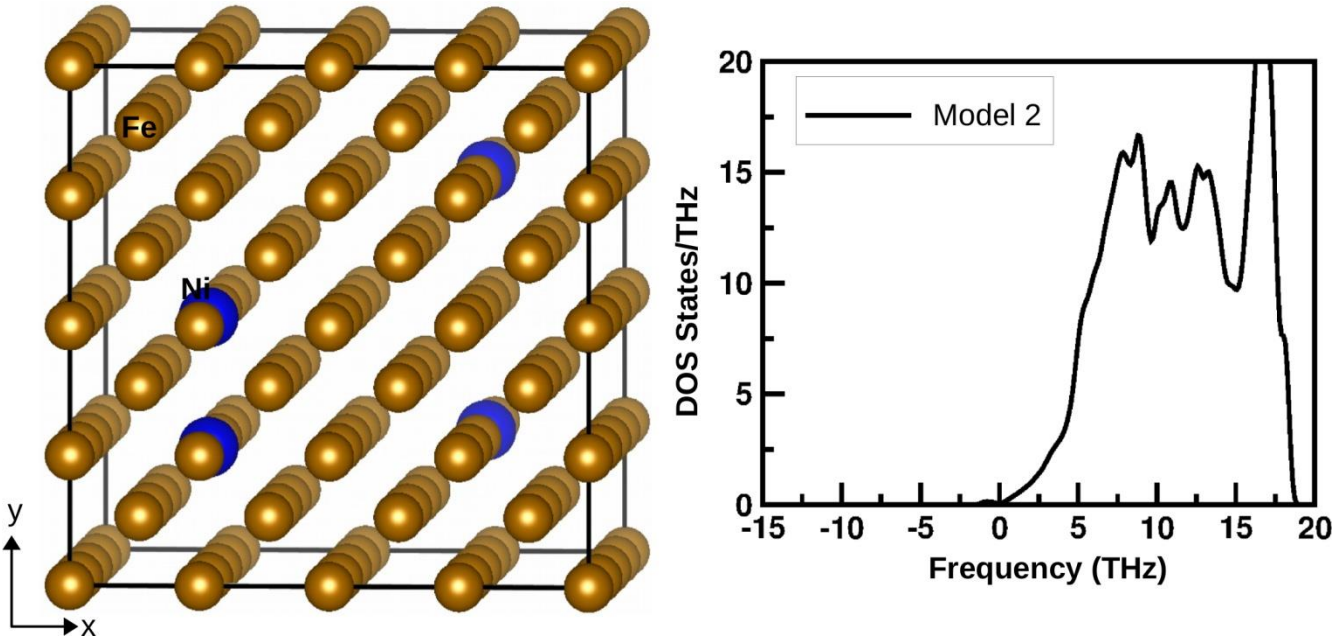

Figure S3.: Here out of 4 Ni atoms, two Ni atoms are made to cluster whereas the other two are located farther apart. The distribution of Ni is, therefore far from being uniform. The calculated phonon density of states at inner core pressures finds the structure to be dynamically stable.

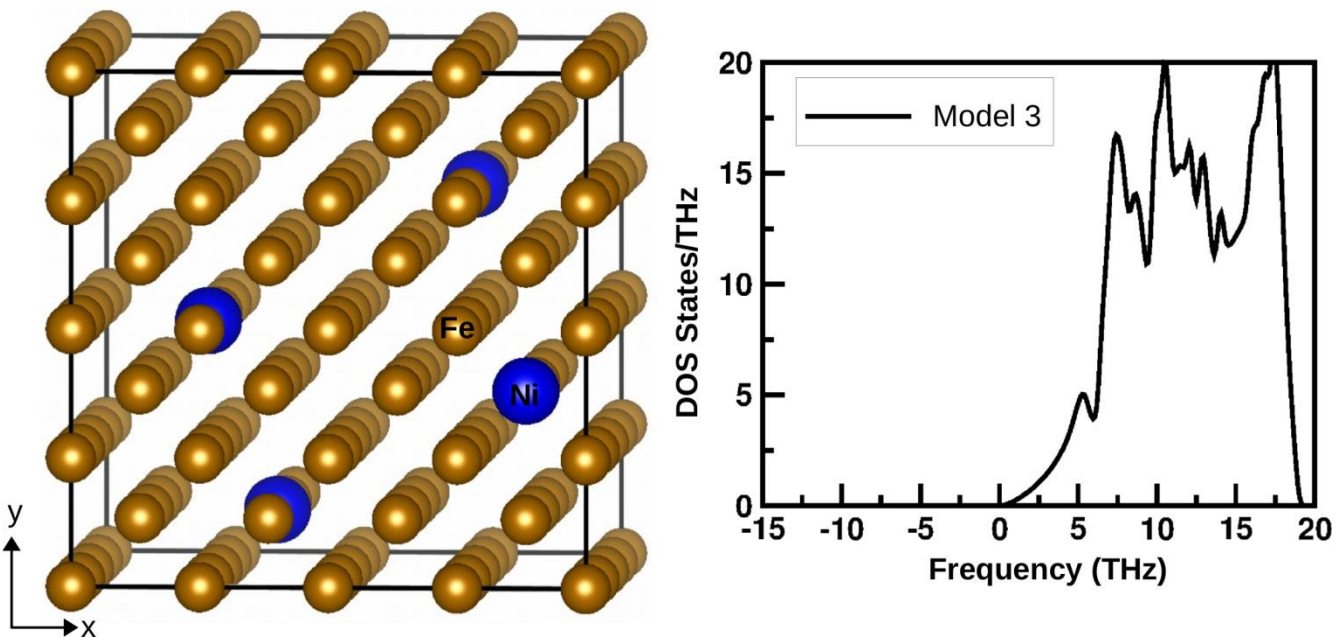

Figure S4.: In this figure all the Ni atoms are separated from each other. However the distribution is still random and the crystallographic environment of the four Ni atoms is also very different. The calulated phonon DOS at 364 GPa finds the structure to be dynamically stable.

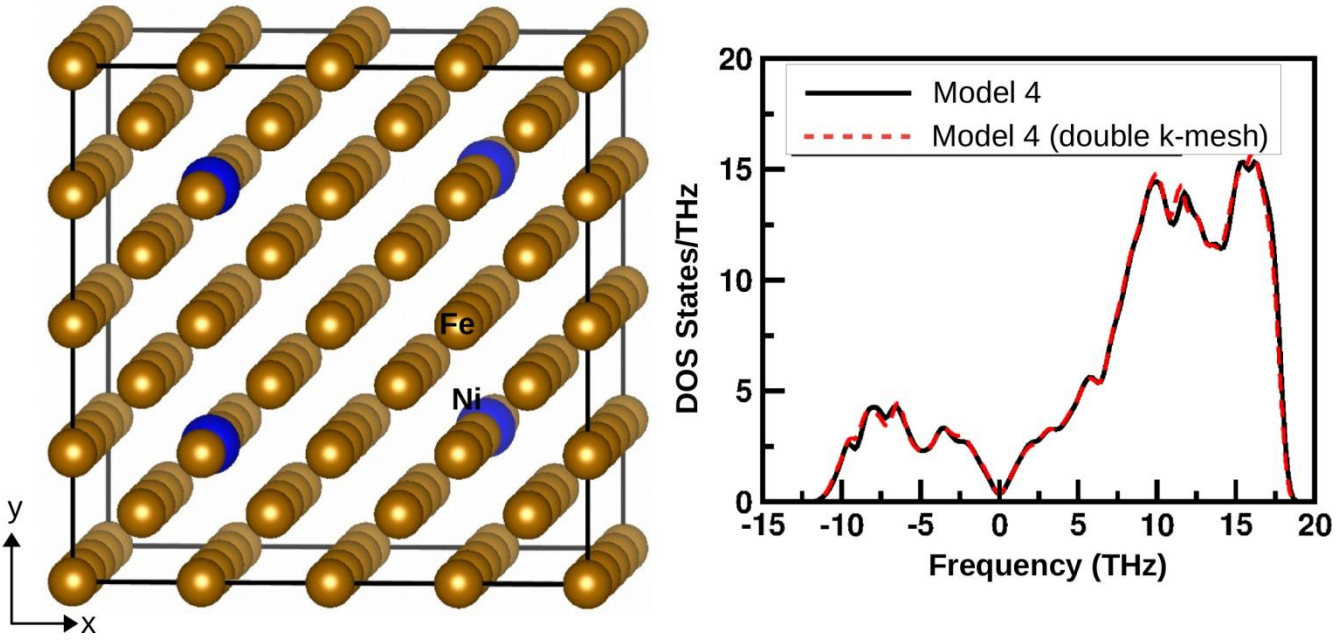

Figure S5.: Here the four Ni atoms are distributed such that the crystallographic environment of all the four Ni atoms is same. Therefore the structure has a uniform distribution of Ni atoms. The calculated phonon DOS shows it to be unstable at inner core pressures. In order to verify our calculations and check upon its accuracy, we have re-calculated the phonon DOS using doubled k-mesh, which however is found to give similar results.

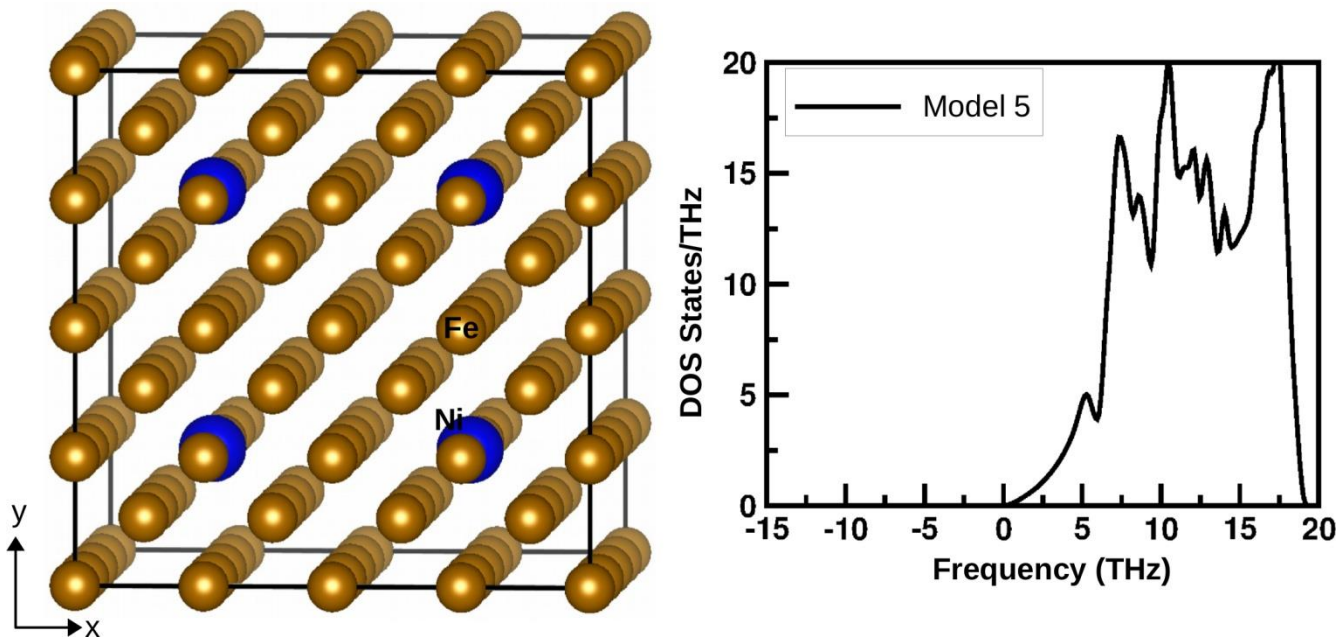

Figure S6.: The structure can be viewed as sheets of Fe-Ni alloy sandwiched between five sheet of pure Fe, all stacked along the z-direction. However, since the Ni-Ni distance along the z-direction is significantly large, the distortion in the lattice created by one the Ni containing sheets cannot be effectively counter-balanced by next Ni-containing sheet which lies at a distance which is five times the lattice parameter. Therefore, although the structure is apparently uniform, the calculated phonon DOS at 364 GPa finds it to be dynamically stable at inner core pressures.

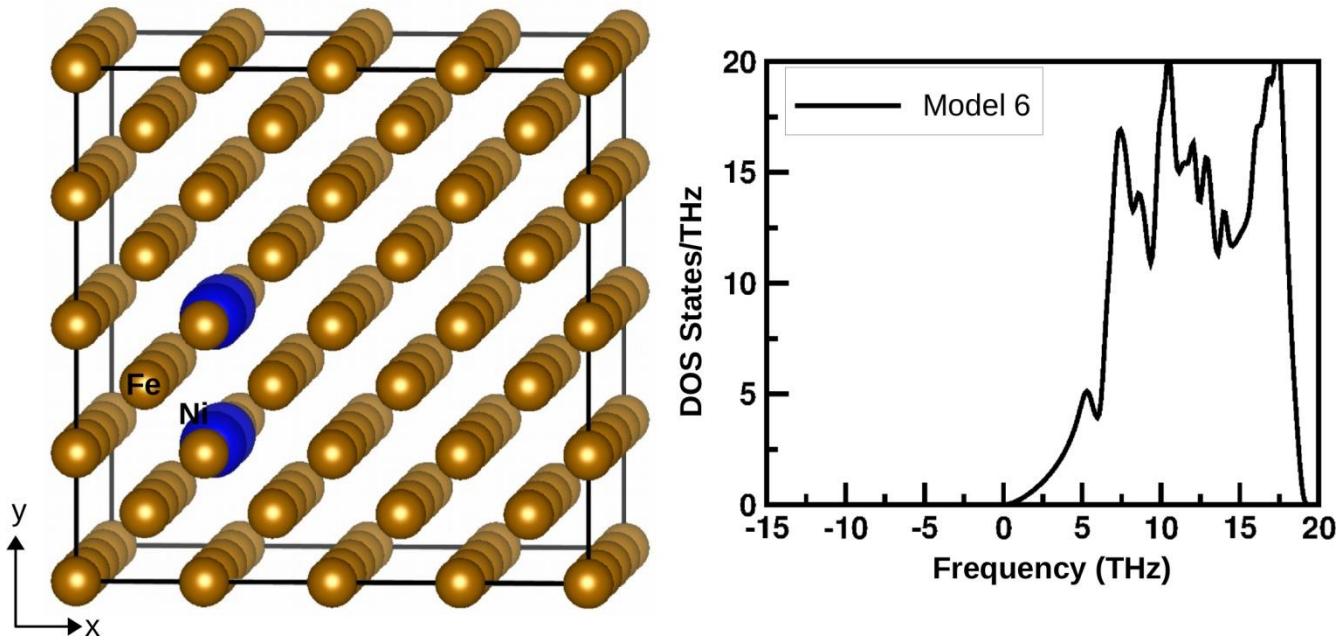

Figure S7.: Here all the four Ni atoms are made to cluster. The calculated phonon DOS at 364 GPa indicates that the structure is dynamically stable at inner core pressures.

Text S3: The third order Birch-Murnaghan's equation of state(3B-M) fitting parameters for the different compositions considered in this study presented in comparison with previous first principles based studies.

System	Reference	Method	EOS	V_o (Å^3/atom)	K(GPa)	K'
Bcc-Fe	This study	PBE, VASP	3B-M	11.36	188.15	5.14
Bcc-Fe	Vočadlo 2006	GGA, VASP	3B-M	11.36	201.50	4.29
Bcc-Fe	Stixrude 1994	GGA, LAPW	3B-M	11.45	189	4.9
Bcc-Fe with 6.25% Ni	This study	PBE, VASP	3B-M	10.91	220.19	4.49
Bcc-Fe with 3.5% Ni	Vočadlo 2006	GGA, VASP	3B-M	11.49	184.74	4.53
Hcp-Fe	This study	PBE, VASP	3B-M	10.17	288.56	4.68
Hcp-Fe	Vočadlo 2006	GGA, VASP	3B-M	10.19	293.05	4.36
Hcp-Fe	Neumann 1999	GGA, LAPW	3B-M	10.28	292	4.4
Hcp-Fe	Stixrude 1994	GGA, LAPW	3B-M	10.26	291	4.4
Hcp-Fe with 6.25% Ni	This study	PBE, VASP	3B-M	10.25	290.6	4.29
Hcp-Fe with 7% Ni	Vočadlo 2006	GGA, LAPW	3B-M	10.22	298.88	4.24
Fcc Fe	This study	VASP, PBE	3B-M	10.34	272.6	4.4
Fcc-Fe	Vočadlo 2006	VASP, GGA	3B-M	10.37	278.50	4.5
Fcc-Fe with 6.25% Ni	This study	VASP, PBE	3B-M	10.31	275.93	4.45
Fcc-Fe with 7% Ni	Vočadlo 2006	VASP, GGA	3B-M	10.34	283.65	4.42

Text S4: The calculated enthalpy of hcp-Fe and fcc-Fe with respect to bcc-Fe in eV/atom in the range 0 GPa to 100 GPa. The bcc phase is found to be stable with respect to the hcp phase upto 12 GPa, whereas it is found to be stable upto 42 GPa with respect to fcc. The phase relations and the corresponding transition pressures are in good agreement with those reports by Stixrude and Cohen (1995).

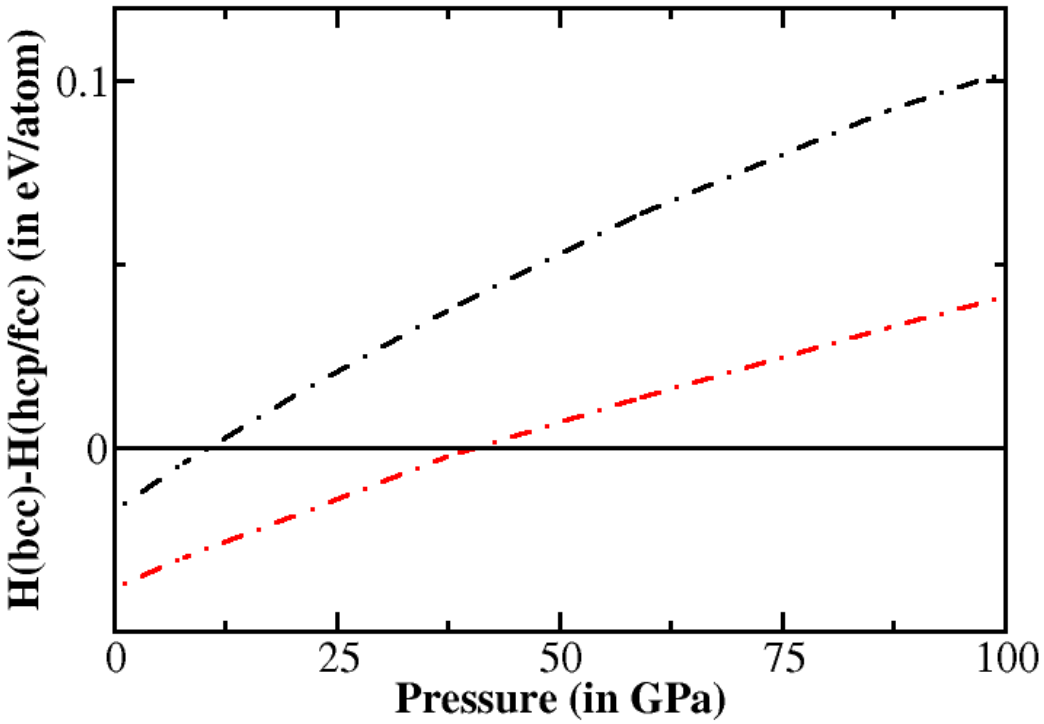

Figure S8.: Difference in enthalpy between (i) bcc-Fe [H(bcc)] and hcp-Fe [H(hcp)] plotted as a function of pressure (black dashed line); (ii) bcc-Fe [H(bcc)] and fcc-Fe[H(fcc)] as a function of pressure (red dashed line).

References:

Steile-Neumann, G., Stixrude, L., Cohen, R.E.(1999) First-principles elastic constants for the hcp transition metals Fe, Co and Re at high pressure, Phys. Rev. B, 60, 2, 791-799.

Stixrude, L., Cohen, R. E., Singh, D.J.(1994) Iron at high pressure : Linearized augmented plane wave computations in the generalized gradient approximation, Phys. Rev. B, 50, 9, 6442-6445.

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