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Supplementary material: Importance of the many-body effects for structural properties of the novel iron oxide: Fe_2O†

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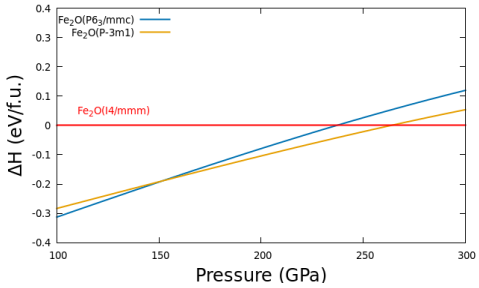

Fig. 1 Plots of relative enthalpy against pressure for Fe_2O as obtained in DFT. The enthalpy of I4/mmm phase is shown as the zero line.

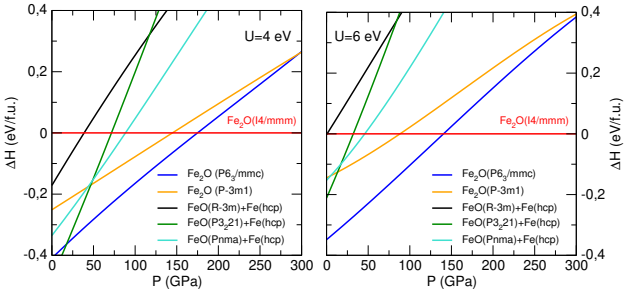

Fig. 2 Plots of relative enthalpy against pressure for Fe_2O and assemblage of FeO and hcp-Fe as obtained in DFT+DMFT at 1000 K calculations for U=4 eV (left panel) and U=6 eV (right panel). The enthalpy of I4/mmm phase is shown as the zero line.

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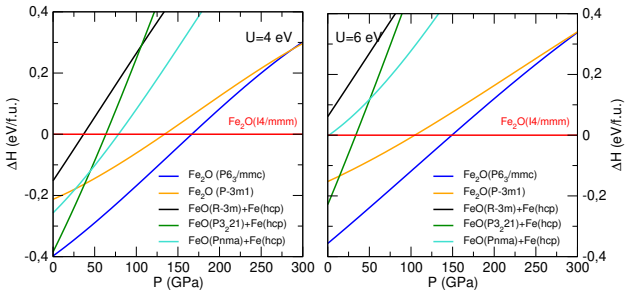

Fig. 3 Plots of relative enthalpy against pressure for Fe_2O and assemblage of FeO and hcp-Fe as obtained in DFT+DMFT at 2000 K calculations for U=4 eV (left panel) and U=6 eV (right panel. The enthalpy of I4/mmm phase is shown as the zero line.

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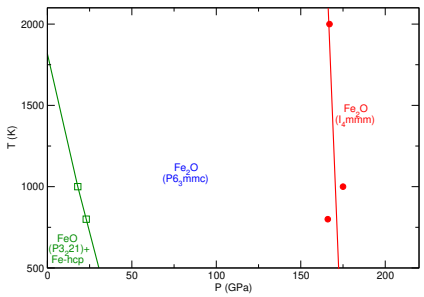

Fig. 4 Phase diagram obtained in DFT+DMFT for U= 4 eV. Circles shows the crossing points of $P6_3/mmc$ and I4/mmm enthalpies at different temperatures. Dashed line is shown as a guide for eyes.

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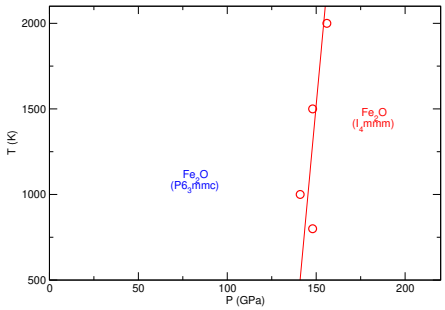

Fig. 5 Phase diagram obtained in DFT+DMFT for U= 6 eV. Circles shows the crossing points of $P6_3/mmc$ and I4/mmm enthalpies at different temperatures. Dashed line is shown as a guide for eyes.