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Origin of magnetism in the Fe_2O_3-$FeTiO_3$ system from correlated band theory[1] ROSSITZA PENTCHEVA, HASAN SADAT NABI, University of Munich — The high remanent magnetization measured in exsolutions of the canted antiferromagnet hematite (Fe_2O_3) and room-temperature paramagnet ilmenite ($FeTiO_3$) has recently received considerable attention not only in the geoscience community [1] but also for possible spintronics applications. To resolve the microscopic origin of magnetism in this system, we have performed density functional theory calculations, varying systematically the concentration, distribution, and charge state of Ti (Fe) in a hematite (ilmenite) host. We find that including electronic correlation within the LDA+U approach is decisive to obtain the correct ground state of the end members, α-$Fe^{3+}{}_2O_3$ and $Fe^{2+}Ti^{4+}O_3$. In a single Ti layer in the hematite host, Ti is not inert as commonly assumed but plays an active role in compensating the charge mismatch at the interface and the emergence of magnetism and the preferred charge state is Ti^{3+}, Fe^{3+}. As soon as a thicker ilmenite-like block forms, the most favorable compensation mechanism is through Ti^{4+} and a disproportionation in the Fe contact layer in Fe^{2+}, Fe^{3+} giving theoretical evidence for the *lamellar magnetism hypothesis* [1]. The substitution of Ti (or Fe) in Fe_2O_3 ($FeTiO_3$) leads to impurity levels in the band gap and in some cases to half-metallic behavior.

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