

Abstract Submitted
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Ferrimagnetism in Ti and Cr doped α -Fe₂O₃ due to heterostructuring HASAN SADAT NABI, ROSSITZA PENTCHEVA, Department of Earth and Environmental Sciences, Section Crystallography, University of Munich, Germany — Based on DFT calculations including an on-site Coulomb repulsion term (GGA+ U) we perform a comparative study of Ti and Cr substitution in α -Fe₂O₃ by varying the concentration, distribution and magnetic alignment of the cations in the Fe₂O₃ host. In the FeTiO₃-Fe₂O₃ system the charge mismatch at the interface between the room temperature paramagnet ilmenite and the canted antiferromagnet hematite is identified as the driving force towards ferrimagnetism as it leads to the formation of uncompensated spins in a mixed Fe²⁺, Fe³⁺ layer [1-3]. In contrast, in Cr₂O₃-Fe₂O₃ there is no valence discontinuity, but the formation of superlattices opens a path to stabilize a different magnetic order than in the Cr₂O₃ end member leading to a net magnetization in the system. The magnetic properties are discussed based on the magnetic interaction parameters for the interfaces extracted from the DFT calculations. Funding by the DFG (Pe883/4-1) and ESF are gratefully acknowledged.

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