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A New look into the spin transition in Fe_2O_3 DIPTA BHANU GHOSH, STEFANO DE GIRONCOLI, SISSA and DEMOCRITOS — The wide range of intriguing characteristics exhibited by Fe_2O_3 with pressure and temperature has renewed the attention of the scientific community in the last decade. Experimental and theoretical efforts are on to address and unravel the complexity of the system. The ambient pressure phase, hematite (α-Fe_2O_3) transforms to a new structural phase (HP1). That the HP1 phase is orthorhombic perovskite (Pbnm) or Rh_2O_3-II type (Pbcn) is still a debate and yet to be explored theoretically. On top of this ambiguous assignment of HP1, there has been a long-standing issue of an isostructural high spin (HS) to low spin (LS) transition. Experimental data till date are divided into two horizons–one assigning the spin transition in the hematite phase and the other in the HP1 phase. In this work, motivated by these exotic unresolved controversies of the system, we have tried to gain an insight of the system from first principles density functional calculations. Our results favor the Rh_2O_3-II type as the HP1 phase, in agreement with recent experiments. Also a (new) mechanism governing the HS to LS transition is proposed. This mechanism, we believe, might help in removing the boundary between the two horizons as mentioned above.

Stefano de Gironcoli
SISSA and DEMOCRITOS

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