Core-hole Calculations of Hematite

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In this work we present the results of ab-initio calculations realized for Fe_2O_3. The aim of this work is to study the (total and partial) density of states of Fe_2O_3 with a core hole. This system is a strongly correlated material and exhibits antiferromagnetism [1-3]. For strongly correlated systems spin-polarized plus LDA+U calculations are required to accurately reproduce observations [4]. The methodology followed in this work is, first, to carry out spin-polarized plus LDA+U calculations without core hole. This will serve as a basis for core-hole calculations. Later we do the core-hole calculations for cores from the 1s, 2p and 3s levels and compare with results without core hole. The calculations were performed using the full-potential Linearized Augmented Plane Wave (FP-LAPW) method as implemented in Wien2k code [5].

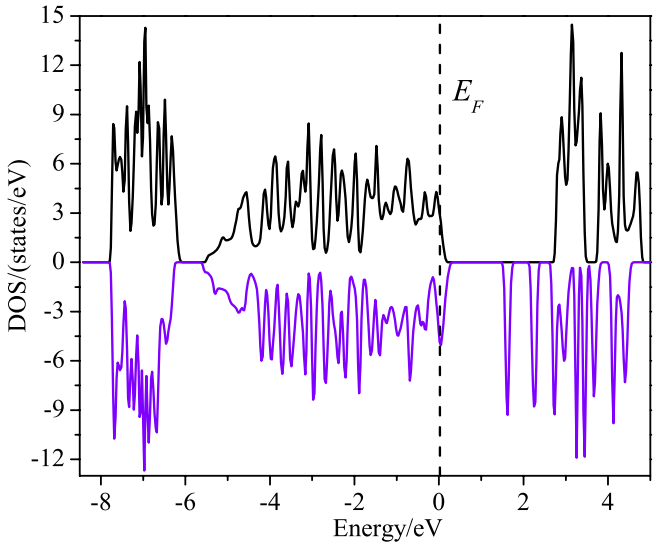

Figure 1 – Projected density of states for LDA+U calculations of Fe2O3

Key Words: Core hole, LDA+U, Density of states, ab-initio calculations.

References

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