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Adopting the ab-initio method to unravel the antiferromagnetic hematite bulk and surface properties

This study employed ab-initio density functional theory (DFT) with Grimme's D3 dispersion correction to investigate the bulk and surface properties of hematite. The Hubbard U parameters 5.0 eV was adopted which gave a band gap of 2.55 eV and lattice parameters of a = b = 5.045 Å and c = 13.774 Å, which were in good agreement with experimental values (band gap: 1.9–2.6 eV; lattice parameters: a = b = 5.035 Å, c = 13.75 Å). The computed electronic properties confirmed the antiferromagnetic nature of bulk hematite, arising from alternating spin-states (spin-up and spin-down) on the Fe atom layers. Various surface orientations including (012), (104), (110), and (116) were modelled to assess surface geometry, relaxation, and energetics to unravel the most stable surface. Among these surfaces, the (104) and (110) surfaces were found to be the most stable based on their relaxations which exhibited the surface energies of 5.61 J/m2 and 5.22 J/m2, respectively. These were in agreement with the computed X-ray diffraction (XRD). These findings revealed the effectiveness of DFT+D3 methods in predicting the bulk and surface of hematite mineral. Furthermore, these form a base for adsorption of collectors to unravel the recovery separation of hematite from other minerals.

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