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Comparison of A12O3 and Fe2O3 surfaces using First Principle method

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ABSTRACT
Al2O3 and Fe2O3 are oxide materials that are widely used in a variety of applications, including catalysis, ceramic-based semiconductors, corrosion protection, and thermal barrier coatings. However, most of the material strength applications depend on its surface properties. The purpose of the study was to investigate the structural. In this study First Principle calculations based on density functional theory were performed with Cambridge Serial Total Energy to investigate the surface stability between Al2O3 and Fe2O3 surfaces. The results show that the surface energy of Al2O3 is lower than that of Fe2O3 in all three planes. Therefore, the surface energy values of Al2O3 increase in this order 100< 111<110 Al2O3 and for Fe2O3 it increases in this order 111<110<100, which explains that the 100 plane has the lowest surface energy for Al2O3 and 111 has the lowest surface energy for Fe2O3 The results suggest that Al2O3 is more stable and energetically favorable, since it exhibits a low surface energy on all planes than Fe2O3surfaces. In addition, partial density of states and work function were computed and analyzed.

Keyword: Oxide materials, First principle, Millar index, Aluminum oxide, Iron oxide

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