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Thermodynamic Stability of Cobalt Oxide's Low-index Surfaces from Density Functional Theory Calculations

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Abstract

Low-index surfaces and morphologies of cobalt spinel (Co_3O_4) are studied using density functional theory calculations. For each of the surfaces (100), (110), and (111), a set of terminations with different surface compositions and atomic structures are assessed to study their thermodynamic stability under different environmental conditions. Surface energies are calculated as functions of oxygen's chemical potential, which in turn is a function of temperature and partial pressure. We select seven typical shapes of cobalt oxide nanoparticles and compute their free energies of formation using the surface energies of all the surrounding facets. The results show that the shapes of octahedron and cuboctahedron have the lowest Gibbs free energies among the seven shapes for all the environmental conditions being explored.

Keywords: cobalt oxide; thermodynamic morphology; surface energy; density functional theory calculation