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First-principles calculation of the infrared spectrum of hematite

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Abstract

The theoretical infrared spectrum of hematite (α-Fe_2O_3) was computed using ab initio quantum mechanical calculations. Frequencies of the normal vibrational modes and Born effective charges were computed using the density functional theory (DFT) with and without the addition of a Hubbard *U* correction. The infrared reflection spectra of a single crystal of hematite were calculated as well as the infrared powder absorption spectrum using an electrostatic model that takes into account the shape of hematite particles. The theoretical behavior of the absorption bands is in agreement with experimental observations and provides a firm basis for the interpretation of the bands in term of vibrational modes. Overall, results suggest that the use of DFT + *U*, which is necessary to describe correctly the electronic and magnetic properties of hematite, does not improve noticeably the prediction of vibrational properties.

Keywords: Iron oxide, density functional theory, infrared spectroscopy