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LETTER

Density functional calculation of the infrared spectrum of surface hydroxyl groups on goethite (α-FeOOH)

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ABSTRACT

We present density functional calculations of vibrational frequencies of OH groups on an idealized goethite (110) surface, represented by a large embedded cluster model. The calculations show that isolated surface groups bound to one, two, and three metal ions can have nearly identical OH stretching frequencies. This finding provides a strong constraint on interpretations of infrared spectra of oxide surfaces, and resolves a long-standing problem in OH vibrational assignments on goethite surfaces, where, in general, too few peaks have been observed relative to the expected heterogeneity of surface functional groups.

Keywords: IR spectroscopy, quantum mechanical calculations, surface studies, goethite, iron oxide