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Ab initio studies on lattice dynamics and Verwey transition in magnetite

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Magnetite is the first discovered magnetic material. At T=125˜K, the Verwey phase transition is observed, in which the electric conductivity decreases by two orders of magnitude [1]. At room temperature, magnetite crystallizes in an inverse spinel structure, in which tetrahedrally coordinated A-sites are occupied by Fe^{3+} ions, while octahedrally coordinated B-sites are occupied by randomly distributed Fe^{3+} and Fe^{2+} ions. At the Verwey temperature, magnetite exhibits the structural phase transition from the cubic to monoclinic phase with the charge-orbital order [2].

Using the density functional theory, we studied the lattice dynamical properties of magnetite in the cubic symmetry [3]. We found a strong electron-phonon coupling, which plays the important role in the Verwey transition. The anomalous phonon broadening resulting from this interaction was observed by the inelastic X-ray scattering studies [4]. The discrepancy between the calculated and measured phonon density of states (DOS) indicates the existence of short-range order with local deformations in the cubic phase. In contrast, the phonon DOS obtained for the monoclinic structure shows a very good agreement with the nuclear inelastic scattering [5]. The interplay between the structural and dynamical properties of magnetite was demonstrated by the recent pump-probe experiments [6], which revealed new features of the collective modes.

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