Strong effect of defects on the electronic and dynamical properties of FeO

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Electronic structure and vibrational dynamics of FeO crystal containing cation vacancies are theoretically studied within density functional theory incorporating strong local Coulomb interactions at iron atoms. Our investigations show a strong effect of Fe vacancies on the structural, electronic, and vibrational properties of wustite [1]. They also uncover qualitative difference between stoichiometric and defected FeO containing either 3% or 6% of cation vacancies. The insulating gap of iron oxide is reduced by about 50% due to unoccupied electronic bands introduced by trivalent Fe ions stabilized by cation vacancies. Significant changes in the electronic structure along with atomic displacements induced by cation vacancies affect strongly phonon dispersions via modified force constants, including those at atoms beyond nearest neighbors of defects. It is shown for the first time that theoretical phonon dispersions and their densities of states reproduce the results of inelastic neutron and nuclear resonant inelastic x-ray scattering experiments [2,3] only when Fe vacancies and Coulomb interaction are both included explicitly in ab initio simulations.

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