

THEORY OF LATTICE EFFECTS ON MAGNETIC INTERACTIONS IN SOLIDS

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ABSTRACT

This dissertation focuses on studying the effect of lattice distortions on the magnetic properties of nickelates and manganites. These two families of materials have great potential in industrial applications in the fields of magnetic (super-dense hard-drives, fast memory) and charge storage (batteries).

The introduction and methods sections present the main ideas of the dissertation and discuss the various techniques used. Electron-lattice coupling is first examined in chapter three for a two-site model where we estimate the magnitude of the isotope effect on the critical temperature and show that it decreases magnetic exchange. In the next part we study electronic structure and magnetism of NaNiO_2 and show that inter-planar exchange is reduced by lattice coupling. In the fifth chapter we examine the magnetic polaron and discuss the effect of static lattice coupling on its binding energy, and find it to further stabilize the polaron.