

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Effective model parameters for the spin-Peierls system TiOCl from first principles YUZHONG ZHANG, ROSER VALENTI, HARALD JESCHKE, Johann Wolfgang Goethe-Universität, Institut für Theoretische Physik — The inorganic spin-Peierls system TiOCl is studied in the frame of Density Functional Theory (DFT) by the projector augmented wave (PAW) and linearized augmented plane wave (LAPW) methods. A two-dimensional frustrated spin Peierls model is proposed to describe the system. The model parameters, such as spin exchange couplings in a, b, and c directions, are estimated by the LAPW method. With the help of the eigenvectors of the dynamical matrix, the spin-phonon couplings and the elastic constant are determined by the PAW method. The reliability of these model parameters is demonstrated by an exact diagonalization and a mean-field calculation as well as by comparison to available experiments.

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Date submitted: 26 Nov 2007

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