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Ab initio calculations on the frustrated magnet $ZnCr_2O_4$ KEVIN T. CHAN, JAY D. SAU, MARVIN L. COHEN, UC Berkeley and Lawrence Berkeley National Laboratory, PEIHONG ZHANG, University at Buffalo — The complex oxide $ZnCr_2O_4$ is a good realization of the Heisenberg antiferromagnet on a pyrochlore lattice and is a strongly frustrated magnetic system. Recent experiments have shown that $ZnCr_2O_4$ undergoes a lattice distortion and a transition from paramagnetic to antiferromagnetic order at $T_c = 12.5\ K$. Infrared spectroscopy has shown a large splitting of a phonon mode involving magnetic ions. We perform ab initio total energy calculations of the exchange coupling constant and phonon modes using the plane-wave pseudopotential formalism with the LSDA+U method, and we compare the results to experiment. This work was supported by National Science Foundation Grant No. DMR04-39768 and by the Director, Office of Science, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, U.S. Department of Energy under Contract No. DE-AC03-76SF00098. Computational resources have been provided by NPACI and NERSC.

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