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Magnetic properties of $CuZrTiO_5$ H.M. ALYAHYAEI, Department of Physics and Astronomy, University of California, Riverside, Riverside, California 92521, USA, R.A. JISHI, D.M. GUZMAN, Department of Physics, California State University, Los Angeles, California 90032, USA, O. TA, A.A. SHARIF, Department of Mechanical Engineering, California State University, Los Angeles, California 90032, USA — $CuZrTiO_5$ is a newly synthesized crystal that contains copper oxide planes [1]. We have carried out first-principles calculations using density functional theory in order to determine the ground state of this crystal. We considered various nonmagnetic and magnetic phases and calculated the corresponding total energies. We found that in the ground state, the magnetic moments on the copper ions adopt an antiferromagnetic arrangement. The effects of doping on the electronic properties of this crystal are investigated.

[1] U. Troitzsch et al., Journal of Solid State Chemistry 183, 668(2010).

H. M. Alyahyaei
Dept of Physics and Astronomy, University of California, Riverside,
Riverside, California 92521, USA

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