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Density functional studies of magnetic behavior of layered Ag(II) fluorides SEFA DAG, VINCENT MEUNIER, WILLIAM A. SHELTON, Oak Ridge National Laboratory, DOUGLAS SCALAPINO, University of California at Santa Barbara — We present an extensive study of the structural and magnetic properties of layered Ag(II) fluoride Cs_2AgF_4 by using density functional theory within the local spin density approximation. We find that this material is well described as a two-dimensional ferromagnetism. Our investigations of a number of ground state properties are in good agreement with reported experiments. We also predict Jahn-Teller distortions in the low pressure phase and find that elastic anisotropy and the electric field created by the displacement of F ions does not modify the orbital order and origin of ferromagnetism.

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