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Systematics of spin crossovers across the RECoO3 family[1]
MEHMET TOPSAKAL, CHRIS LEIGHTON, RENATA WENTZCOVITCH, Univ of Minn - Minneapolis — We have investigated structural and electronic properties of rare-earth cobaltites (RECoO3) using ab initio DFT + U calculations. A structurally consistent and self-consistent Hubbard U treatment is shown to be essential for the proper description of strongly correlated cobalt-d electrons. We successfully capture the experimentally observed structural variations and explain the trend in the spin transition temperature in cobalt across the RE series. We believe that Hubbard U values presented in this study will allow further predictive studies of RE cobaltites.

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