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Many body effects on the formal charge state of 3d - Transition Metal Doped $BaTiO_3$ SUBHASISH MANDAL, Department of Applied Physics, Yale University, New Haven, Connecticut & Geophysical Laboratory, Carnegie Institution of Washington, Washington D. C, R.E. COHEN, Geophysical Laboratory, Carnegie Institution of Washington, Washington D.C. USA & Dept of Earth Sciences, University College London, London, U.K, K. HAULE, Department of Physics, Rutgers University, Piscataway, New Jersey, USA — Using density functional theory in combination with dynamical mean field theory in Mn doped $BaTiO_3$, we find a different charge state and 3d - orbital occupations than obtained from either DFT or DFT+U. We find that the explicit treatment of many-body effects induced by the Hund's rule coupling in Mn shows a donor charge state of Mn^{2+}, instead of usual acceptor charge state of Mn^{4+} as is found in both DFT and DFT+U. The differences in electron density reveal that charge transfer due to strong Hubbard interactions is not sufficient to describe the electron correlations in transition metal doped ferroelectrics.

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