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Ab initio investigation of ground state magnetic and ferroelectric properties of monoclinic CuCl_2 multiferroic system AMBESH DIXIT, Indian Institute of Technology Jodhpur — Materials with simultaneous magnetic and ferroelectric ordering are getting attentions and are widely investigated to understand the strong lattice-charge-spin coupling in these systems. Also, the strong coupling among different degree of freedoms in these systems may give rise to the novel magnetoelectric phenomenon. Recent experimental studies on monoclinic CuCl_2 system suggest that system undergoes antiferromagnetic transition ~ 25 K in conjunction with ferroelectric ordering simultaneously. The helimagnetic ordering of Cu ions ($S = 1/2$) along c-axis causes the onset of ferroelectric ordering along b-axis, breaking spatial inversion symmetry. We investigated the ground state magnetic and ferroelectric properties of copper chloride in its monoclinic structure (space group $C2/m$) using density functional theory. The spin dependent calculations are carried out to understand the magnetic structure and ferroelectric polarization was calculated along different axis. The correlation of magnetic structure and the onset of polarization in CuCl_2 system will be discussed in the context of magnetoelectric coupling in this system.

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