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Electronic and magnetic properties of Ba_2CoWO_6: First principal investigation

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Abstract : We report an investigation of the structural; electronic and magnetic properties of a new double perovskite Ba_2CoWO_6 by means of density functional calculations (DFT); within the generalized gradient approximation (GGA). The lattice constants of Ba $_2CoWO_6$ was obtained and found toagree very well with published experimental reports. The total and partial density of state are calculated and discussed. The results reveal that the Ba_2CoWO_6 has stable antiferromagnetic character. Our results predicts that Ba_2 $CoWO_6$ have metallic nature.

Keywords : ab initio, FP-LAPW, Electronic structure, Double perovskite