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p-Electron Magnetism in anion doped $BaTiO_{3-x}X_x$ (X=C,N,B) CHRISTOPH GRUBER, PEDRO OSVALDO BEDOLLA VELAZQUEZ, JOSEF REDINGER, PETER MOHN, Vienna University of Technology, MARTIJN MARSMAN, University of Vienna — We present VASP calculations using the HSE functional for carbon, nitrogen, and boron doped $BaTiO_{3-x}X_x$ (X=C,N,B). We calculate a 40-atom supercell and replace one oxygen atom by C,N, or B. For all three substituents we find a magnetically ordered groundstate which is insulating for C and N and halfmetallic for B. The changes in the electronic structure between the undoped and the doped case are dominated by the strong crystal field effects together with the large band splitting for the impurity p-bands. Using an MO picture we give an explanation for the pronounced changes in the electronic structure between the insulating non-magnetic state and the as well insulating magnetic state for doped $BaTiO_3$. p-element doped perovskites could provide a new class of materials for various applications ranging from spin-electronics to magneto-optics.

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