Properties of 3*d* transition metal point defects used to stabilize hexagonal $BaTiO_3$ at room temperature

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Chromium doped hexagonal barium titanate is studied from first-principles density functional theory using the generalized gradient approximation as the exchange and correlation energy functional. The results are compared with experimental data available from electron paramagnetic resonance (EPR), X-ray diffraction (XRD) and optical absorption spectra and from literature. The probable site for the impurity atom occupancy in the lattice, their probable charge states and the role of oxygen vacancies in their stabilization are investigated. Defect formation energy is used to analyse the role of electronic- and ionic-compensation mechanisms in stabilizing the point defect. Various atomic positions for the oxygen vacancy surrounding the impurity atom are taken into consideration in order to compare with some of the conclusions derived from experiments. Our results on the substitutional site preference and the location of oxygen vacancy in the next-neighbor surrounding of the impurity Cr is in good agreement with experiments.

References

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