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"Structural and electronic properties of $(TiO_2)_{10}$ cluster with impurities"

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We report the structural, energetics, and electronic properties of free-standing binary clusters (TiO2)10 with substitutional metallic and non-metallic impurities. The selected (TiO2)10 cluster has tetrahedral symmetry and is the putative low energy structure for this size. The substitutional impurity can be located at a vertex (4 sites) or at an edge (6 sites). The former has a binding energy only 0.03 eV/atom less than the latter, so they can be considered as almost degenerate. A total of 28 impurities are considered in the present report. We study the edge substitutional place since this environment is very similar to the corresponding one in the bulk, which makes these system a possible model for the bulk-like structures. Another advantage of the cluster considered here is that its energy gap is as large as the one presented in the bulk phases (anatase and rutile). This system allows us to mimic the bulk behavior without the use of intrasite Coulomb corrections (U) which are generally applied as parameters to fit the real energy gap observed in bulk (TiO2) systems. We show results for the formation energies, energy gaps and magnetism suggesting a way to control the band gap by means of the use of the appropriate impurity used in the substitution. The impurity case of a vacancy in an oxigen site is also considered and compared with experiment result for bulk systems.

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