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Title: A theoretical investigation of oxygen vacancy defect in $SrTiO_3$, an insulating oxide

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$SrTiO_3$ is an insulating oxide which belongs to the intriguing class of compounds called perovskites and shows a wide range of useful properties. At low temperatures it becomes superconducting and also undergoes a ferroelectric phase transition. It has a large dielectric constant and hence is used in high voltage capacitors. Besides this it often serves as an excellent substrate for epitaxial growth of oxide based thin films. In this work we present first principles calculations of oxygen vacancy (V0) defect which is known to be an important defect in this material. Since density functional theory (DFT) in the local density approximation (LDA) is known to underestimate band gaps we compute the electronic structure using the Heyd, Scuseria, and Ernzerhof hybrid functional popularly known as the HSE functional. This gives excellent agreement to the experimental band gap of 3.01 eV for $SrTiO_3$. On creating an oxygen vacancy a defect level appears at about 0.6 eV below the conduction band edge. We find this level to be comprised mainly of the neighboring Ti orbitals which point directly towards the vacancy site, namely the Ti dz2 orbitals and partly the Ti 4pz and 4s orbitals. From the charged state calculations (V0+ and V0++) we find the V0++ state to be more stable than the neutral and V0+ state. From the calculated formation energy and the charge neutrality condition we also estimate the concentration of this defect in $SrTiO_3$.