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Computational study of oxygen vacancy defects in perovskite oxides, SrTiO₃ and LaAlO₃

CHANDRIMA MITRA, CHUNGWEI LIN, University of Texas at Austin, JOHN ROBERTSON, Cambridge University, ALEXANDER DEMKOV, University of Texas at Austin — Insulating perovskite oxides, SrTiO₃ (STO) and LaAlO₃ (LAO) have attracted a lot of attention due the observed two dimensional electron gas at the interface of these two insulating oxides. Oxygen vacancies, which are easily incorporated in these oxide systems during various processes such as growth, annealing and redox reactions, form an n-type defect in these systems. Hence they are responsible for modifications of various physical properties such as conductivity and optical properties to name a few. As such, there is still a lack of comprehensive theoretical understanding of these important defects in these materials. In this work we present first principles calculations of neutral (V^0) and charged (V^+ , V^{++}) oxygen vacancies in STO and LAO. Density functional theory within the local density approximation proves insufficient in reliably predicting the defect levels due to their well know band gap problem. We therefore employ the Heyd, Scuseria, and Ernzerhof (HSE) hybrid functional to study these defects. Band gaps of 3.01 eV and 5.0 eV are obtained for bulk STO and LAO which are in excellent agreement to experimental values. In STO we find a localized V^0 defect state at 0.7 eV below the conduction band edge (CBE) while in LAO it is a deep lying level at 2.13 eV below the CBE. A band alignment of the defect levels in these two materials shows that upon stabilizing the singly ionized state, charge transfer could take place from the V^+ LAO state to the V^+ STO state which lies at 1.19 eV below the former.

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