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Effect of interface structure on Schottky barrier height in $SrRuO_3/SrTiO_3$ heterojunctions VEMULAVADA SAMPATH KUMAR, MANISH NIRANJAN, Indian Institute of Technology Hyderabad — Complex oxide heterostructures are highly promising for technological applications as they offer novel device concepts and functionalities. One of the fundamental parameters that influence the characteristics of the metal/oxide heterostructure is the Schottky barrier formed at the interface. The Schottky barrier height (SBH) is strongly influenced by the atomic structure of the interface and is of fundamental interest as an intrinsic property of the system. The SrRuO3/SrTiO3 (001) heterostructure is a prototypical system to study SBH at the oxide metal/dielectric interface. In recent years, the SRO has attracted a lot of attention as an electrode material for ultrathin ferroelectric films. Using *ab-initio* calculations, we have studied the *p*-type SBH and its dependence on the interface structure in SRO/STO heterostructure. In addition, we have estimated the *p*-SBH using semi-empirical Metal-Induced-Gap-States (MIGS) model. In particular we have considered three types of interfaces: RuO2/SrO/TiO2, RuO2/BaO/TiO2 and MnO2/SrO/TiO2 the *ab-initio* estimate of *p*-SBH comes out to be 1.27, 1.33 and 0.78 eV for respective interfaces. We find that semi-empirical MIGS model overestimate the p-SBH by $\sim$2 eV.

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