ABSTRACT

AB INITIO STUDIES OF THE ELECTRONIC STRUCTURE
AND SUPERCONDUCTING PROPERTIES OF
RuO_2 THIN FILMS
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The discovery of strain-induced superconductivity in rutile RuO_2 thin films has attracted considerable attention from the scientific community. The superconducting behavior of the RuO_2 films has been linked to changes in the electronic structure of the strained RuO_2 crystal lattice, resulting in a significant increase in the density of states at the Fermi level. We applied ab initio density functional computational methods to study the influence of epitaxial strain on the electronic and transport properties of RuO_2 thin films grown on TiO_2 substrates. Our calculations were performed using the PBE exchange-correlation functional with the inclusion of Hubbard correction and spin-orbit coupling. The emergence of flat bands in the electronic structure of RuO_2 and their potential role in mediating superconductivity were investigated by applying biaxial epitaxial strain along the crystal orientations (100) and (001) of rutile RuO_2. Additionally, we examined the impact of epitaxial strain on the superconducting properties of RuO_2, focusing on the phonon dispersion and Eliashberg spectral function conditions favorable for superconductivity. Our results suggest that the influence of strain may offer a viable route to stabilize superconducting phases in RuO_2 thin films.