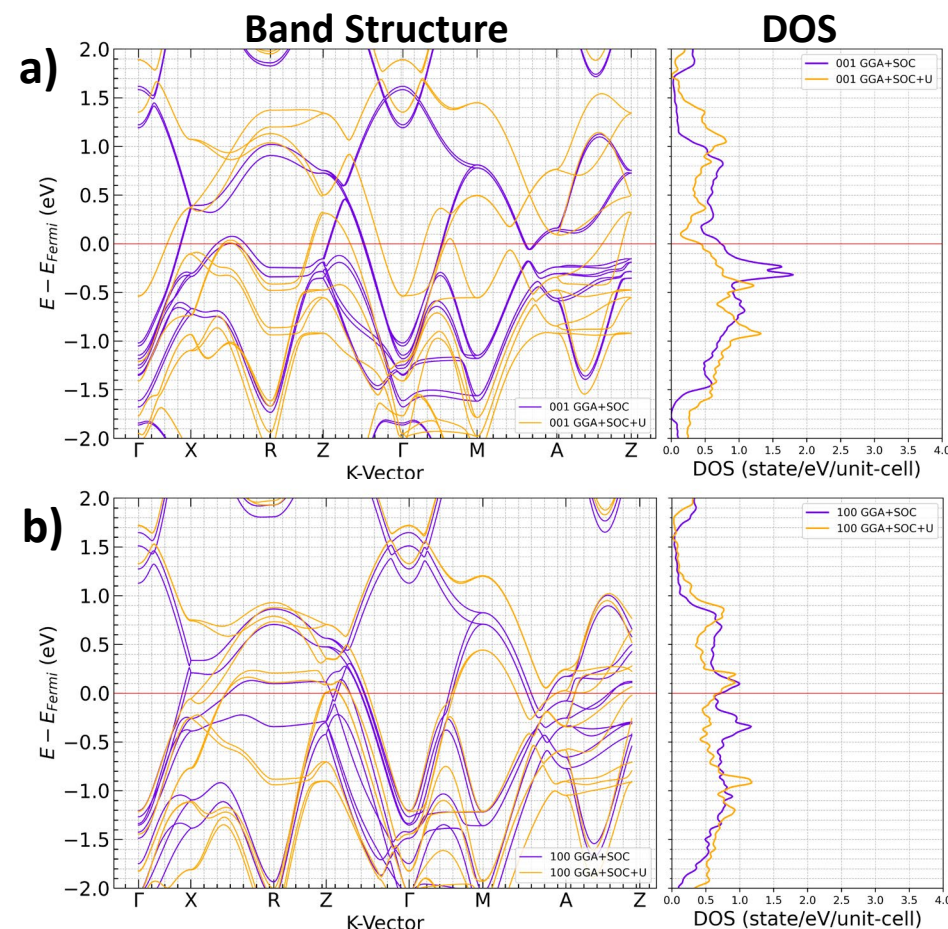


Ab Initio Studies of the Electronic Structure and Electrical Transport in Epitaxially Strained RuO₂ Thin Films

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Recent discovery of strain-induced superconductivity in rutile RuO₂ thin films has attracted considerable attention. Superconducting behavior of RuO₂ films has been linked to the changes in the electronic structure of strained RuO₂ crystal lattice resulting in significant increase of the density of states at the Fermi level. Ab initio density functional computational methods were applied to study the influence of epitaxial strain and doping on the electronic and transport properties of RuO₂ thin films grown on TiO₂ substrates. The emergence of flat bands in the electronic structure of RuO₂ and their potential role in mediating superconductivity was investigated by applying biaxial epitaxial strain along the (001) and (100) crystal orientations of rutile RuO₂. The results of this study suggest that the combined influence of strain and doping may offer a viable route to the stabilization of superconducting phases in RuO₂ thin films.



Calculated band structures and density of states of strained (a) (001) and (b) (100) RuO₂ thin films grown on TiO₂ substrate.