

Electronic structure and magnetism of SrRuO₃ under epitaxial strain

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Using density functional theory, properties of SRO under epitaxial conditions have been investigated. Focus was on the role of Ru-Oxygen octahedra tilting with special interest to the magnetic properties of the Ru ions. We isolated and studied effects of large in-plane strain resulting from coherent epitaxy. These strains result in the changing of the tilting parameters of the Ru-Oxygen octahedral network, whereby the spin states of the Ru⁴⁺ ions exhibit substantial changes. We discuss a possibility of different electronic (magnetic) configurations of SRO. In effect of the epitaxial boundary conditions with lattice mismatch, it is important to what extent the tilting degrees of freedom in SRO are compatible on the interfaces. This approach allows us to discuss experimental observations where properties of STO/SRO thin films show rather unexpected thickness dependence [1]. We consider a possibility of additional ways to control properties of ferroelectric thin films in epitaxial heterostructures with SrRuO₃.

[1] Feizhou He *et al.* Phys. Rev. B **70**, 235405 (2004).