

Abstract Submitted  
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**Crystal structure, electronic and magnetic properties of SrRuO<sub>3</sub> under epitaxial strain**<sup>1</sup> ALEXEY ZAYAK, KARIN RABE, Rutgers University, 136 Frelinghuysen Rd., Piscataway 08854, New Jersey, XIANGYANG HUANG, RJ Mears, LLC 1100 Winter Street, Suite 4700, Waltham, MA 02451, JEFFREY NEATON, The Molecular Foundry, Material Science Division, Lawrence Berkeley National Laboratory, Berkeley CA 94720 — Using density functional theory, properties of SrRuO<sub>3</sub> have been investigated. We focused both on general properties of the orthorhombic distortion in SrRuO<sub>3</sub> and the effects of applying epitaxial constraints, whereby the influence of large in-plane strain resulting from coherent epitaxy have been isolated and investigated. The overall pattern of the structural relaxations revealed coherent distortions of the oxygen octahedra network which are sensitive to the magnetic order. The magnetic parameters exhibit substantial changes allowing us to discuss possibilities of magneto-structural tuning of the SrRuO<sub>3</sub>-based thin film structures.

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