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Antiferromagnetism and insulating nature of ultrathin films of SrRuO3 PRIYA MAHADEVAN, S.N. Bose National center for Basic Sciences, F. ARYASETIAWAN, Chiba University, A. JANOTTI, Materials Department, UCSB, T. SASAKI, NIMS — Metallic oxides form an integral part of oxide-based technologies, constituting the connecting electrode material. In this context SrRuO3 is a material that has been widely studied as it in addition to being metallic is also ferromagnetic. Recent experiments have found that ultrathin films of $SrRuO_3$ are insulating and hence 5-6 monolayers are required before metallic character is observed. In this work we theoretically examine the origin of the insulating state with first principle GGA+U calculations. The value of U is calculated from first principles. Ru has a formal configuration of d^4 in $SrRuO_3$. In bulk $SrRuO_3$ this translates into a low spin state with an electronic configuration of $t_{2g\uparrow}t_{2g\downarrow}$. Hence at the surface/ultrathin film limit one expects the observed insulating nature to come from a transition into the nonmagnetic state with the lowest crystal-field levels contributed by d_{yz} and d_{xz} orbitals being completely filled. However one finds that the system undergoes an unusual structural distortion which is accompanied by a spin state transition. This spin state transition is accompanied by a transition into an antiferromagnetic state which drives the system insulating.

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