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## **[233] Role of the surface structure in determining ferroelectric polarization direction**

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Interest in ferroelectric perovskites is due to their applications in electronics, and thin films are especially relevant. However, bulk properties, such as ferroelectricity itself, can be compromised at reduced scale. In this work, ferroelectric lead titanate (PTO) thin films are investigated.

Experimental (second harmonic generation) and computational (density functional theory) methods were employed to study thin films of PTO(100). It was found that the polarization in the film is strongly influenced by the geometric and electronic structure of the surface. A stoichiometric PTO(001) surface has a strongly reduced polarization which can be restored by the deposition of adsorbates [1, 2].

### **References**

- [1] D. D. Fong *et al.*, Phys. Rev. Lett., 96:127601 (2006).
- [2] M. Stengel, Phys. Rev. B, 84:205432 (2011).

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