

Abstract Submitted
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Polarization effect on the growth of Pt thin films on PbTiO₃ (100) surfaces¹ MIGUEL ANGEL MENDEZ POLANCO, ILYA GRINBERG, WISSAM AL-SAIDI, ANDREW RAPPE, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6323, USA — Results of Density Functional Theory calculations performed on Pt thin films grown on PbTiO₃ (100) Ferroelectric (FE) ideal surface terminations are discussed. We analyze the effect of the ferroelectric polarization on the metal-oxide interface and how this in turn influences the growth of Pt thin films on PbTiO₃. Our results suggest a preferential stacking ordering for the Pt layers that depends on the polarization of the surface: The *hollow*-top-hollow... arrangement is preferred over the *top*-hollow-top... registry for the positive (P⁺) polarization surface; however, this predilection is reversed for the negative (P⁻) polarization surface. The effect of strain in the adsorption of Pt layers will also be discussed. This polarization-dependent preference for the adsorption of Pt layers onto FE surfaces could be of interest in understanding the mechanism of polarization fatigue.

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