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Theoretical study of growth of Pt on $BaTiO_3$ slabs KURT FREDRICKSON, AGHAM POSADAS, The University of Texas at Austin, CATHERINE DUBOURDIEU, JOHN BRULEY, IBM T.J. Watson Research Center, ALEXANDER DEMKOV, The University of Texas at Austin — $BaTiO_3$ (BTO) is a well-known ferroelectric perovskite, which is tetragonal at room temperature. As BTO has potential as a component of a ferroelectric field-effect transistor (Matthews *et al.*, Science **276**, 238 (1997)), development of metal electrodes is of crucial importance. We investigate Pt deposition on (001) BTO. The metal is deposited in ultra-high vacuum in the molecular beam epitaxy reactor and characterized using transmission electron microscopy and in situ photoemission. Using density functional theory we calculate the surface energies of Pt(001), (011), and (111), and BTO (001) and investigate the wetting conditions of Pt(001) and (011) on TiO_2-terminated BTO(001). We use transmission electron microscopy to examine the interfaces of epitaxially grown Pt on BTO and compare the sizes of the islands with the sizes predicted by theory. In addition, we examine the dependence of ferroelectricity on the sample thickness. Results of our photoemission experiments are compared with first principles spectra.

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