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Polarizing-Depolarizing fields competition on $PbTiO_3$ nanocapacitors[1] MIGUEL ANGEL MENDEZ POLANCO, ILYA GRINBERG, ANDREW RAPPE, University of Pennsylvania, Department of Chemistry — We analyzed the stability of various interfacial atomic arrangements in $PbTiO_3$ (PTO) based nanocapacitors, using density functional theory (DFT). We observed that particular constructions induce a large polarization enhancement via a net field depolarizing-to-polarizing swap within the PTO layers, as revealed by analysis of electrostatic potential profiles. In contrast to those with a dominant depolarizing field, possessing a polarization below that of the bulk, the polar structures are stable in the thin-film regime. Interface atomic relaxation is also observed to be a key factor in determining the overall stability of the different capacitor configurations. This boosted charge screening capacity along with appropriate engineering of the interface chemistry, are potential how-to pointers to alleviate the critical thickness in ferroelectric-based nanocapacitors.

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