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A new class of atomic-layer-thick ferroelectric films on silicon ALEXIE KOLPAK, SOHRAB ISMAIL-BEIGI, Center for Research on Interface Structures and Phenomena, Yale University — As a result of depolarizing field effects, the behavior of nanoscale ferroelectrics often suffers from the suppression of the ferroelectric phase transition temperature, as well as the polarization magnitude, with respect to that of the bulk ferroelectric. Using density functional theory, we design a novel class of ferroelectric heterostructures that, in contrast, display ferroelectric behavior only in the limit of atomically thick films. These heterostructures are composed of a single layer of epitaxial MX_2 on a Si(001) substrate, where MX_2 is a transition metal chalcogenide or pnictide with a bulk layered crystal structure (*e.g.*, CdI_2, pyrite). We discuss the chemical and mechanical interactions that stabilize the two polarization states in these materials, and we demonstrate that continuous switching between these states is possible. Our work may thus lead to the realization of new applications based on nanoscale ferroelectrics. We acknowledge financial support by the NSF under MRSEC DMR 0520495, as well as computational support from the NCSA TeraGrid and Yale HPC.

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