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Imaging Charged Domain Walls in a 2D Ferroelectric

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Two-dimensional (2D) ferroelectrics such α-In_2Se_3, have recently garnered interest for their applications in nanoscale electronics, memory storage, and quantum devices [1-3]. In particular, the structure, orientation, and local charge at ferroelectric domain walls are key factors governing ferroelectric switching and interfacial emergent phenomena [4]. Here, we study the atomic structure and electronic properties of ferroelectric domain walls in α-In_2Se_3, an out-of-plane 2D ferroelectric. Using a combination of aberration-corrected scanning transmission electron microscopy (STEM), 4D-STEM, piezoelectric force microscopy (PFM), and density functional theory (DFT), we show that mechanical deformation can be used to create and localize domain walls in α-In_2Se_3. We observe two types of domain boundaries: electrically neutral transverse domain walls (TDWs) and strongly charged lateral domain walls (LDWs), which respectively are oriented perpendicular and parallel to the basal plane. These domain walls are readily identified through either atomic resolution imaging or 4D-STEM. We show that, while transverse domain walls can be atomically sharp, the head-to-head and tail-to-tail LDWs have a finite 1-2 nm width. Using 4D-STEM supported by DFT and Bloch wave simulations, we directly image the charged layers at the lateral domain walls in α-In_2Se_3. Our methods should be useful for understanding the atomic and nanoscale interplay between mechanical deformations, ferroelectric polarization, and ferroelectric switching in 2D ferroelectrics [5].

References:

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