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Adsorbate-Induced Ferroelectricity Nanostructures¹ \mathbf{in} JONATHAN SPANIER, Drexel University, ALEXIE KOLPAK, ILYA GRINBERG, University of Pennsylvania, JEFFREY URBAN, LIAN OUYANG, WANSOO YUN, Harvard University, ANDREW RAPPE, University of Pennsylvania, HONGKUN PARK, Harvard University, DREXEL UNIVERSITY TEAM, UNIVERSITY OF PENNSYLVANIA TEAM, HARVARD UNIVERSITY TEAM — We discuss recent progress in understanding the size-dependent evolution of ferroelectricity in perovskite nanostructures and ultrathin films obtained via variable-temperature scanning probe microscopy investigations of individual nanorods and other ferroelectric nanostructures. We propose a mechanism in which the surface polarization charge is passivated by molecular adsorbates. A combination of density functional theory simulations, modified phenomenological Landau theory, and thermodynamic analysis demonstrates that the experimental behavior is well described by this mechanism.

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