Metallic-like to Nonmetallic Transitions in a Variety of Heavily Oxygen Deficient Ferroelectrics

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The coupling between ferroelectric distortions and electron transport is an important factor in understanding ferroelectric/noncentrosymmetric materials with metallic conductivities and ferroelectric-based thermoelectrics. Here, multiple d0 ferroelectrics with a variety of crystal structures are doped via oxygen deficiency, resulting in metallic-like conduction in the paraelectric state. It is found that most of the studied systems show a metallic-like to nonmetallic transition near the paraelectric-ferroelectric-ferroelectric transition. The metallic-like to nonmetallic transition temperature can be shifted using mechanisms that shift the paraelectric-ferroelectric transition temperature. It was found that the metallic-like to nonmetallic transition temperature could be shifted from 373K to 273K by varying (Ba1xSrx)TiO3d from x.0 to x.0.3 and x.1. The most probable mechanism for ferroelectric-electron transport coupling was determined to be Anderson localization associated with polarization with short-range order.