Size Effect of Symmetric and Asymmetric Ferroelectric Tunnel Junctions: Combining First-Principle Calculation and Phenomenological Modeling

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Ferroelectric size effect of $BaTiO_3$ tunnel junctions with Pt and/or $SrRuO_3$ electrodes has been comprehensively investigated combining first-principle calculation and phenomenological modeling. A vacuum layer is included in the supercell, so that full-relaxations are achieved without artificial strain constraint. The characteristics of atomic structure, polarization, charge density and electrostatic potential for ten possible types of tunnel junctions are revealed. It shows that the ferroelectric stability of tunnel junctions depends significantly on the details of the interfaces, which present specific short- and long-range properties, e.g., local bonding environment, electronic screening and built-in field, etc. To quantitively reproduce the size effect of ferroelectric tunnel junctions, we present a modified phenomenological model with parameters determined from the results of first-principle calculations. Our study provides a comprehensive picture of the ferroelectric size effect in BTO tunnel junctions as a function of electrode/ferroelectrics interfaces, and should have valuable implications for future studies and applications.

Keywords: Ferroelectric tunnel junction, Size effect, First-principle calculation, Phenomenological model