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Ferroelectricity in Ultrathin Perovskite Films in Metal-Ferroelectric-Metal Junctions C. DUAN, R. SABIRIANOV, W.-N. MEI, Department of Physics, University of Nebraska-Omaha, S.S. JASWAL, E. TSYMBAL, Department of Physics and Astronomy, University of Nebraska-Lincoln —
We present first-principles studies of electronic and ferroelectric properties of Metal/Ferroelectric/Metal junctions. We consider $KNbO_3$ as the ferroelectric, while strontium ruthenite, $SrRuO_3$, and platinum, Pt, as metals. These materials have a match in the lattice constants, which eliminates the appearance of stresses and misfit dislocations. We utilize the projector augmented plane wave method to perform the first principles calculations. The fully relaxed geometry of the structure is obtained assuming that the substrates have bulk lattice parameters away from the interface. We use the Berry phase formalism to obtain the polarization of the ferroelectric layer. The calculation of the electric polarization requires a proper subtraction of the Berry phase for the reference paraelectric structure from that for a distorted structure. We show the existence of ferroelectricity in these heterostructures at ferroelectric thickness of 0.22nm. We find that for the case of asymmetric leads, i.e. for the $SrRuO_3/KNbO_3/Pt$ junction, the electrostatic potential profile across the ferroelectric layer is asymmetric with respect to the direction of the electric polarization suggesting a change in transport properties with switching the electric polarization. This work is supported by Nebraska Research Initiative and National Science Foundation.

Renat Sabirianov
University of Nebraska at Omaha

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