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Ferroelectric properties of nm-scale barium and lead titanate films Y. -H. TANG, M. -H. TSAI, National Sun Yat-Sen University, Kaohsiung 80424 Taiwan — The first-principles calculations of the total energies of nm-scale barium titanate ($BaTiO_3$) and lead titanate ($PbTiO_3$) films with respect to the off-center Ti ion displacement, d_{Ti}, have been carried out to understand ferroelectric properties of these films. Since the driving force of ferroelectricity is the attractive total dipole-dipole interactions associated with the collective off-center displacements of the transition metal ions in the octahedrons [1], the ferroelectric properties of nm-scale films is expected to be different from those of thick films because of the drastic reduction of the number of available dipoles. Thus, it is interesting to know whether the nm-scale films retain ferroelectricity. The calculated total energies as a function of d_{Ti} along the (110) direction show a potential well at about 0.17 and 0.15Å for $BaTiO_3$ and $PbTiO_3$, respectively. By symmetry, the potential well is the same for – d_{Ti}. The existence of double potential wells is a characteristic of ferroelectricity. Thus, the total energy result shows that nm-scale $BaTiO_3$ and $PbTiO_3$ films retain ferroelectricity and resultant dipoles are parallel with the films.

[1] M. –H. Tsai**, Y. –H. Tang**, and S. K. Dey, J. Phys.: Condens. Matter **15**, 7901 (2003).

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