Dependence of Critical Thickness on particle-Size for Ferroelectricity in $BaTiO_3$ by *Ab Initio* Calculations

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Particle-size effects on the critical thickness on the ferroelectric properties of nanoscale $BaTiO_3$ particles are investigated using a first-principles molecular orbital method and population analysis for the next change and overlap population. A series of models composed of a $Ba_8Ti_7O_6$ cluster and point charges surrounding the cluster are employed for calculations of the electronic structures of the $BaTiO_3$ particles, with the size of the model defined by the size of the point charge array. Results of the calculations show that the critical thickness for the ferroelectric-to-paraelectric transition for nanoscale $BaTiO_3$ particles decreases as the area of the base of the rectangular particles decreases.