ペロブスカイト及び関連酸化物の電子状態計算（7）

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Electronic State Calculations of Perovskite and Perovskite-related Oxides (7)

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We have studied the ferroelectricity disappearance phenomenon in $BaTiO_3$ thin films using the Discrete Variational-Xα molecular-orbital method. This study have configured calculation model of $BaTiO_3$ with electrodes. We have calculated electronic states of the $BaYiO_3$ by using the model, and evaluated the change of Ti 3d-O 2p overlap population against film thickness. As a calculated result, we have found that the changes of external field and film thickness influence the magnitudes of spontaneous polarization field, and then they influence presence ferroelectricity of a $BaTiO_3$.