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Electron hybridization and anharmonic thermal vibration effect on structure transition of SrTiO₃ at high-pressure and low-temperature

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Abstract

We execute electron density analysis of SrTiO₃ at low temperatures up to 80 K and high pressures up to 11.88 GPa using X-ray single-crystal diffraction and *ab initio* quantum chemical molecular orbital (MO) calculation. By changing pressures, the cubic SrTiO₃ with perovskite structure goes through a antiferroelastic distortion to tetragonal symmetry above the critical pressure $P_c = 7$ GPa with $c/a < 1$ and decreasing with increasing pressure. On the other hand, by changing temperatures, the tetragonal distortion occurs below the critical temperature $T_c = 105$ K with $c/a > 1$ and increasing with lowering temperature.

Difference Fourier (D-F) synthesis experimentally proves the residual electron densities $\Delta\rho(xyz)$ are associated with two different effects: electron hybridization bonding electron and anharmonic thermal vibration atoms. The *d-p- π* hybridization between Ti(3*d*) and O(2*p*) orbitals is confirmed in the residual electron density, which is deformed from the ideal spherical density conducted by the atomic scattering factor *f*_i using Hartree-Fock (HF) approximation. MO calculation also reveals the electron hybridization. Anharmonic thermal vibration of atoms yields a large effect to the structure transition. Mulliken charges analysis of MO calculation indicates much smaller charges than their formal ionic charges. Their ionicity increases from cubic to tetragonal above P_c and below T_c .

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