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Calculated Electronic Properties of Rutile TiO_2 and Cubic SrTiO_3 CHINEDU EKUMA, Louisiana State University, Baton Rouge, LA, DIOLA BAGAYOKO, Southern University and A&M College, Baton Rouge, LA — We present preliminary, calculated, electronic properties of rutile titanium dioxide (TiO_2) and of cubic strontium titanate (SrTiO_3). Our computations employed local density approximation (LDA) and generalized gradient Approximation (GGA) potentials for TiO_2 and SrTiO_3 , respectively. We implemented the linear combination of atomic orbitals (LCAO) within the framework of the Bagayoko, Zhao, and Williams (BZW) method. In doing so, we solved, self-consistently, both the Kohn-Sham equation and the equation giving the ground state charge density in terms of the wave functions of the occupied states. Our preliminary findings indicate that TiO_2 has an indirect band gap of 2.95 eV, from Γ to R. The direct gap at Γ is 0.10 eV larger. The indirect band gap of SrTiO_3 , from L to Γ or X, is 3.05 eV.

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