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First Principle Ab-initio Study of TiO_2[1] CHINEDU EKUMA, MARK JARRELL, JUANA MORENO, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA, DIOLA BAGAYOKO, Southern University and A&M College, Baton Rouge, LA 70803, USA — We report results from first principle computations of electronic properties of rutile TiO_2 within the local density functional approximation (LDA). Our first principle, non-relativistic and ground state calculations employed a local density functional approximation (LDA) potential and the linear combination of atomic orbitals (LCAO) – utilizing a self-consistently obtained, optimized basis set. 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 calculated band structure shows that there is significant O_2p-Ti_3d hybridization in the valence bands. These bands are well separated from the conduction bands by an indirect band gap of 2.95 eV, from Γ to R. Consequently, this work predicts that rutile TiO_2 is an indirect band gap material, as all other gaps from our calculations are larger than 2.95 eV. A slightly larger, direct band gap of 3.05 eV is found at the Γ point, in excellent agreement with experiment. Our structural optimization led to lattice parameters of 4.65 Å and 2.97 Å for a_o and c_o, respectively, with a u parameter of 0.3051, and a bulk modulus of 215 GPa.

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