Correlation between band gap and electronegativity of substituted atoms in the TiO_2 crystalline structure

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The electronic structure of TiO_2 has been extensively studied through a variety of experimental and computational methods. Its properties range from thin film photovoltaic cells to optics. TiO_2 provides an excellent model to study computationally due to the wealth of experimental data and its inexpensive computational cost. Our hypothesis is that the electronegativity of a substituent changes the band gap of crystalline TiO_2. Atoms of different electronegativities were selected for substitution into the three polymorphic forms of TiO_2, which are rutile, anatase, and brookite. Our computational approach utilizes the linearized-augmented plane-wave approach of density functional theory in the WIEN2k computational software, and includes the incorporation of the modified Becke-Johnson potential, to determine the band gap and density of states for each case. Initial results showed that fluorine substitution in a 2x2x2 rutile supercell resulted in a slight decrease in the band gap.