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A First-Principles Study of TiX_2 ($X =$ S, Se, and Te) Compounds Optical Properties under the Effect of Externally Applied Electric Field and Strain

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Optical properties of titanium dichalcogenide compounds, TiX_2 ($X =$ S, Se, and Te) have been calculated by first-principles calculations using density functional theory as implemented in SIESTA code. The unit cell of each of these compounds was optimized and the calculations were performed to obtain the optical properties. Further, external electric field (along Z direction) and biaxial strain (along X and Y directions) was employed to study their effect on these properties. The effect of biaxial strain on the geometry of the compounds is also studied. The optical properties are investigated for polarized light along the Z direction (c axis). This include the calculation of real and imaginary parts of dielectric function, absorption coefficient, reflectance, optical conductivity, and refractive index in $0-25$ eV energy range. Various modulations of these properties are observed including the blue shifts and red shifts of energies with highest peaks in the visible region and also shifting of energies to other regions of the electromagnetic spectrum. Hence, due to the tunable diverse optical properties, the compounds can be useful in the field of optoelectronics and in making various optical devices.

Keywords: density functional theory, electric field, biaxial strain, optical properties.