Effect of Electric Field on Optoelectronic Performance of 1T-ZrS2

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**Abstract**. The present study employs density functional theory calculations to investigate the effect of an external electric field on the electronic and optical properties of bilayer ZrS2. With each step, the electric field is increased by 0.2V/Å in a direction perpendicular to the layers, from 0 V/Å to 1.4 V/Å. Bilayer ZrS2 is found to have an indirect bandgap that continuously decreases as an external electric field is applied, eventually reaching a value of 0.03 eV (at 1.4 V/Å) from 0.81 eV (at 0 V/Å). The effect of spin-orbit coupling is also studied and the value of Eg varies from 0.77eV to -0.06eV. Thus, a rise in the electric field leads to the observation of a semiconductor to metal transition. Moreover, almost every optical parameter, including reflectance, absorption coefficient and others, exhibits a red shift in the spectra when the electric field increases. The values of static reflectance and refractive index show a clear shift. Our research shows that ZrS2 properties can be adjusted to suit a variety of applications.

References:

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