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Elucidating the optical properties of $MoTe_2$/InN heterostructures for photovoltaic applications[1] ALEXANDRE ROCHA, CESAR E.P. VILLEGAS, Univ Estadual Paulista-UNESP — Recently, two-dimensional (2D) atom-thick hexagonal crystals have drawn both experimental and theoretical interest due to their fundamental properties and potential applicability in electronics and optoelectronics. While most studies are focused on 2D crystals with gap in the visible electromagnetic spectrum, the ones with gaps in the near infrared region have not been explored yet. Motivated by this and considering the individual properties of transition metal dichalcogenides and group III-V compounds, we carry out density functional theory (DFT) calculations combine with the GW-Bethe-Salpeter (GW-BSE) methodology to study the optical properties and the power conversion efficiency of $MoTe_2$/InN heterostructures. First, we study the geometric and electronic structure of three heterostructures based on different stacking. Secondly, we use the GW-BSE methodology to study the optical spectrum and estimate the power conversion efficiency of the device. Our results indicates that the photoexcited exciton are originated in the range of 1.12 to 1.5 eV. In addition, we estimate the exciton recombination time finding values in the nanosecond range. Finally, we estimated the short-circuit current and power conversion efficiency of the 2 nm thick device.

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