Investigation of the Gauss Model on Improvement of Permittivity and Optical Absorption of TMDC Monolayers in the Visible Spectrum

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Abstract

Two-dimensional layers of transition metal dichalcogenids (TMDCs) with direct band gap in the visible and infrared range have shown an open horizon in photonics and optoelectronics. Among TMDC family, MoSe₂, WSe₂, MoS₂ and WS₂ monolayers have shown special optical properties. In this paper, the permittivity constant of the aforementioned monolayers are calculated based on Lorentz, Lorentz- Gauss and Lorentz-Drude-Gauss models with quite acceptable consistency to their experimental values. The optical absorption response of these photovoltaic monolayers is similar to imaginary component of their permittivity. In addition, based on investigation of optical absorption in the presence of substrates, it is found that absorption decreases which is more pronounced while the refractive index of substrates increases. Such thin layers with absorption efficiency above 10% with thickness below 1 nm are suitable candidates for solar cell and photovoltaic applications.

Keywords: Permittivity, Absorption, Transition metal dichalcogenids, Photovoltaic, Lorentz model, Drude model and Gauss model