Novel hBN/In(Ga)Te Heterostructures For Wide Spectrum Light Absorbers

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In recent years, enormous attention given to the exploration and researching of two-dimensional materials has started a whole new era in materials science and countless possibilities for novel devices emerged. Two dimensional group III monochalcogenides have recently attracted quite attention for their wide spectrum of optical and electric properties, being promising candidates for optoelectronic and novel electrical applications[1]. However major obstacle in using them in various application arises from the fact they are strongly sensitive and vulnerable to oxygen in air in their pristine form, especially as thin films or single layer. Many studies reveal that monolayers are oxidized fast, almost instantly, after exposure to the air[2,3.] Here we present two newly designed vdW heterostructures based on hBN (hexagonal boron nitride) and GaTe or InTe monolayer, in order to make them more robust and resistant to mechanical influences while enhancing their optoelectronic properties. Using density functional theory we investigate electronic and optical properties of those heterostructures. Our study reveals them as an excellent candidates for various optoelectronic devices with great capabilities of absorption from visible light to far UV part of spectrum, being exceptionally good for absorbing the UV light. The hBN layer is beneficial[4] for mechanical protection of sensitive and vulnerable single layers of monochalcogenides like InTe and GaTe, while as we showed, in our heterostructures, electronic and optical properties are not only preserved but even enhanced**.** Importantly, we demonstrate type of stacking does not affect properties of the heterostructure, making them convenient for experimental realization.

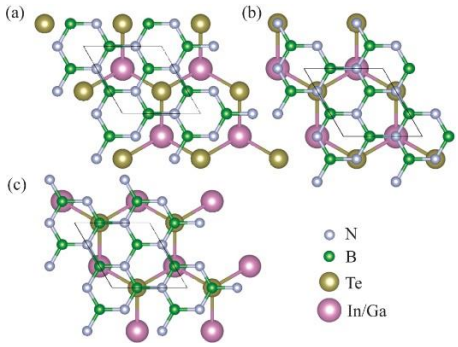

FIG 1. hBN/In(Ga)Te heterostructures. Top view of three possible stacking types, (a) H-top, (b) N-top and (c) B-top

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