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Electronic and Transport Properties of Vertical Heterostrucrure of h-BN and Black Phosphorus

Recently, considerable attention has been paid to the electronic structure, electric, and thermoelectric properties of black phosphorus (BP) in monolayer or few-layers, due to their potential applications in areas such as the nanoscale optoelectronic, photovoltaic, and chemical sensing devices [1-3]. Recentl y, to protect BP from the chemical degradation in the atmosphere, the air-stable hexagonal boron nit ride (h-BN) encapsulated BP devices have been suggested and demonstrated [4-7]. However, many d etails about the electric and thermoelectric transport properties of semiconductor heterostructure consis ting of h-BN and BP are still lacking. In this work, based on the density functional theory (DFT) cal culation, we investigate the electronic structure and transport properties of vertical heterostructure of 2 D h-BN and BP. In particular, we estimate the carrier mobility and the relaxation time at room temp erature using the deformation potential (DP) theory proposed by Bardeen and Shockley [8]. In additio n, we also obtain the electrical conductivity at room temperature by adopting the semi-classical Boltz mann transport theory [9]. Detailed discussion of those properties of h-BN/BP heterostructure will be given.

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