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Thermoelectric transport across graphene/phosphorene/graphene heterostructures

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New features have been observed recently across the plane in the heterostructures made from layered two-dimensional materials, of which, graphene based heterostructures, e.g. graphene/hBN, graphene/MoS_2, graphene/hBN/graphene (GhBNG), have gained a lot of attention. In this work, we investigate the thermoelectric transport across the stacked graphene/phosphorene/graphene (GPG) heterostructure coupled to semi-infinite gold leads by using the non-equilibrium Green's function (NEGF) method within a first-principles framework. The obtained resistance extracted from the current-voltage characteristics is about 1 $\Omega/\mu m^2$, much lower than that of GhBNG, which indicates energy barrier in GPG structures are lower than in GhBNG. The nonlinear Peltier coefficient of GPG is calculated at finite currents, while a value of S=4.76 $\mu V/K$ is obtained at zero bias. A sign change of the Peltier coefficient is observed at a current of ~3.8 $A/\mu m^2$ corresponding to a bias of 1.7V. This indicates a transition of hole to electron current as the bias is increased. The reason is elaborated by referring to the projected density of states of different layers. In addition, the effect of the number of layers of the central phosphorene has been investigated. For multilayers of phosphorene in the GPG structure, there is no significant difference observed in the I-V curve compared with that in the monolayer case, indicating that up to 5 phosphorene layers the system is still in the ballistic regime.