Berry Curvature Study of hBN-Bilayer Graphene Heterostructure

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Introduction of Berry's phase and related effects has led to the study of yet another degree of freedom in electrons i.e. valley degree of freedom and a brand new branch of research, Valleytronics [1]. This degree of freedom gives scope for a novel information carrier for electronic devices, apart from the charge and spin degree of freedom [2-3]. Berry phase has given rise to various physical properties such as Berry curvature and orbital magnetic moment. Berry curvature, which can be described as a pseudo-magnetic field in the reciprocal space drives the carriers to the opposite edges of the materials according to the direction of the curvature in the presence of an in-plane electric field. This phenomenon is called Valley Hall Effect (VHE). There have been several studies on the valleytronics properties of bilayer graphene (BLG). However, the valleytronic properties of hBN-bilayer graphene heterostructure are not studied extensively. hBN is widely used as a clean and uniform dielectric layer for bilayer graphene. Thus, herein, we study the valleytronics properties of the hBN-BLG heterostructure.

The *ab initio* calculations are performed using the LCAO method implemented in SIESTA [4] based on van der Waals exchange-correlation functionals. A vacuum layer of thickness 25 Å was used to avoid the interaction between adjacent bilayers. A fine Monkhorst-Pack grid of 40 x 40 x 1 and a mesh cut off of 500 Ry were used in all the calculations. Berry curvature was calculated using Wannier90 [5].

In order to study the effect of hBN on the valleytronic properties of bilayer graphene, we put hexagonal boron nitride under bilayer graphene (Fig. 1a) and carried out the Berry curvature calculation. A non-zero Berry curvature with opposite polarity at the adjacent corners of the Brillouin zone was observed (Fig. 1b). The polarity of the Berry curvature can be reversed with the application of an out-of-plane electric field (Fig. 1c). We have also studied the effect of encapsulation of bilayer graphene with hBN layers (Fig. 1d). The hBN-BLG-hBN heterostructure did not show any Berry curvature (Fig. 1e). However, application of an out-of-plane electric field can induce Berry curvature in hBN-BLG-hBN heterostructure (Fig. 1f).

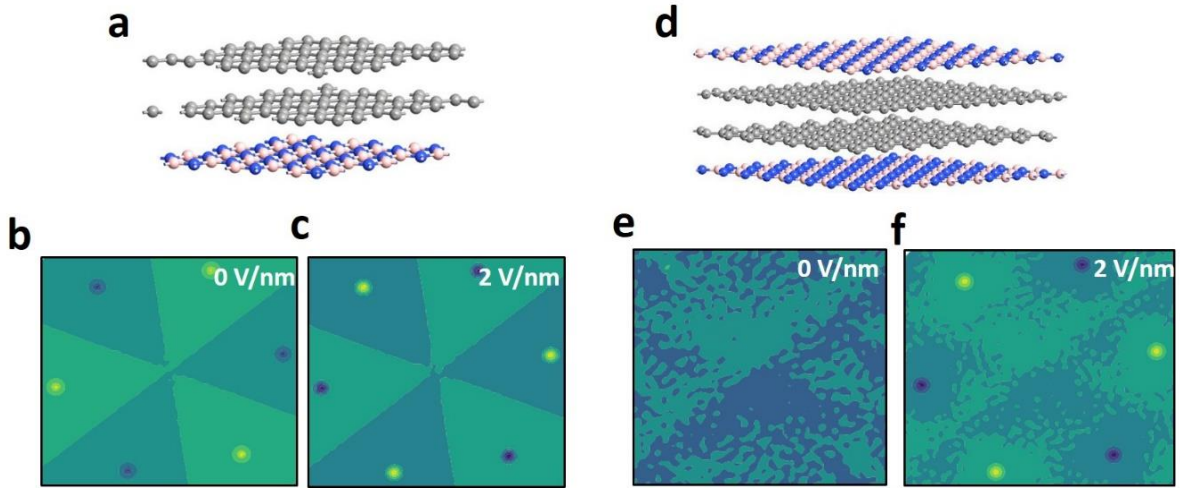

Figure. 1: (a) Schematic diagram of the hBN-BLG heterostructure. Berry curvature plot in the reciprocal space for hBN-BLG heterostructure at (b) 0 V/nm and (c) 2 V/nm. (d) Schematic diagram of hBN-BLG-hBN heterostructure and its Berry curvature plot at (e) 0 V/nm and (f) 2 V/nm

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