First-Principle Study of Bilayer Graphene Valley States

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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). Thus herein we study the evolution of Berry curvature with out-of-plane electric field ($E_\perp$) in bilayer graphene.

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 20 Å was used to avoid the interaction between adjacent bilayers. A fine Monkhorst-Pack grid of 36 x 36 x 1 and a mesh cut off of 400 Ry were used in all the calculations. Berry curvature was calculated using Wannier90 [5].

Fig. 1(a) shows the band structure of bilayer graphene along the high symmetry points. The energy values are shifted so as to keep the Fermi level at 0 eV. Fig. 1(b) shows the Berry curvature at K and K' high symmetry points for pristine bilayer graphene and bilayer graphene at an out-of-plane electric field ($E_\perp$) 1600 μV/nm. A sign reversal for the Berry curvature is observed with the application of the electric field. The non-zero Berry curvature is attributed to the asymmetry in the system. Whereas the sign reversal is due to the change in potential experienced by the two layers as a result of the applied electric field. Further details will be discussed in the presentation.

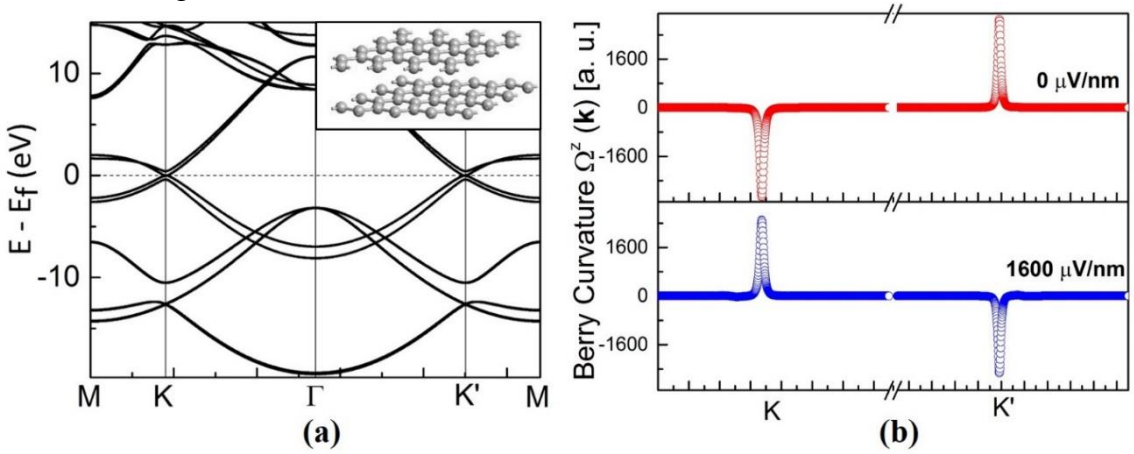

Figure. 1: (a) Band structure of bilayer graphene. Inset: Bilayer graphene crystal structure. (b) Berry curvature at K and K' valleys of pristine bilayer graphene and bilayer graphene at an out-of-plane electric field ($E_\perp$) 1600 μV/nm.

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Acknowledgements: This research was supported by the Grant-in-Aid for Scientific Research No. 18H03861 and 18K04260 from Japan Society for the Promotion of Science (JSPS).