Title	二次元材料のバレートロニクス特性の第一原理解析と実験的研究
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Abstract

It is known for many years that apart from the charge and spin degree of freedom, carriers have yet another degree of freedom known as valley degree of freedom. A per this degree of freedom, the charge carriers residing in the valleys of the band structure of certain materials behave opposite to each other. It also gave rise to a new branch of physics, namely, valleytronics. One of the physical quantity which is used to manipulate and control the valley degree of freedom of the carriers is the Berry curvature. Berry curvature can be understood as a pseudo-magnetic field in the reciprocal space which drives the carriers according to the direction of the Berry curvature resulting in valley current. However, the symmetry arguments of the Berry curvature require either time reversal symmetry or spatial inversion symmetry to be broken for the emergence of Berry curvature. Systems which preserve both these symmetries show no Berry curvature and hence cannot be used as a valleytronic material. Also, an ideal valleytronic material should possess two or more degenerate and in-equivalent valleys in its band structure.

Two-dimensional materials such as graphene and transition metal dichalcogenides, which are of great scientific interest these days have such valleys in their band structure. However, single layer graphene is centrosymmetric. Although AB-stacked bilayer graphene is widely considered to be symmetric, there have been several theoretical studies and experimental observations arguing about an inherent asymmetry persistent in ungated (AB-stacked)bilayer graphene due to electron-electron interaction at low temperatures. However, none of the experimental studies conducted so far have observed Berry curvature induced valley current in ungated (AB-stacked)bilayer graphene, which makes it vital to study the Berry curvature in ungated bilayer graphene. In this study, we observed a non-zero Berry curvature with opposite values at K and K$'$ valleys, validating the argumentation of the asymmetry persistent in ungated (AB-stacked)bilayer graphene. The asymmetry comes from the spontaneous charge transfer to one of the layers as a result of long-range Coulomb interaction between the electrons. This charge imbalance results in a layer asymmetry in the system. Application of an out-of-plane electric field (of the order of μV/nm) reduces the magnitude of the Berry curvature

and dies out at a threshold electric field. When the magnitude of the electric field is increased beyond the threshold value, the Berry curvature reappears but with a change in polarity at K and K$'$ valleys. This indicates that the polarity of the layer asymmetry also switches beyond the threshold electric field. However, application of higher electric fields (of the order of V/nm) shows a reduction in the magnitude of the Berry curvature with the increase in field strength. As for AA-stacked bilayer graphene, either ungated system or system under out-of-plane electric field did not show any Berry curvature owing to the symmetry present in the system.

Nonetheless, observation of valley current in ungated bilayer graphene is experimentally challenging as it requires ultra clean sample which is isolated from external perturbation. Thus we studied theoretically the possibility of breaking the symmetry in bilayer graphene with the use of hexagonal Boron Nitride (hBN) as a substrate or as an encapsulation layer. Although the role of hBN in breaking the layer symmetry in bilayer graphene and sublattice symmetry in single layer graphene is well known, the effect of the alignment and orientation of hBN layer on the emergence of Berry curvature in these systems is not studied in detail yet. The effect of the out-of-plane electric field is also studied in detail. In the case of bilayer graphene hBN systems the magnitude, as well as the polarity of the Berry curvature, greatly depends on the orientation of hBN layer to the bilayer graphene. This comes from the layer asymmetry induced by the hBN layer in bilayer graphene. Application of an out-of-plane electric field could manipulate the magnitude as well as the polarity of the Berry curvature in these systems. On the other hand, single layer graphene hBN systems are found to be rather insensitive to the configuration of the hBN layer. Although the magnitude of the Berry curvature depends on the alignment of the hBN layer, the orientation of the hBN layer or application of out-of-plane electric field does not impact the polarity of the Berry curvature.

Although the observation of valley current in ungated bilayer graphene which is completely isolated from the external perturbation is difficult, we can utilize the asymmetry induced by the substrate in bilayer graphene to observe valley current. We conducted experimental studies on bilayer graphene exfoliated on Si/SiO$_2$ substrate in order to detect valley current induced by Berry curvature. The non-local resistance measurement method is employed to detect the valley current. A non-zero non-local resistance was observed in ungated bilayer graphene. The Berry curvature induced valley current is an indication of asymmetry in the system. The asymmetry comes from the potential difference between the layers induced by the substrate. The Ohmic contribution to the non-local resistance was found to be negligible. From the temperature dependent measurements, it was confirmed that the bilayer graphene is gapped and the band gap is calculated to be around 20 meV. The band gap opening substantiates the asymmetry induced by the substrate. On the other hand, measurements conducted on

single-layer graphene did not show any valley current, implying the symmetry persistent in the system.

Keywords: Valleytronics, Berry curvature, Bilayer graphene, hBN, Valley current, Valley Hall effect.