Valleytronics in Biased Bilayer MoS_2

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Valleytronics is the study of the valley degree of freedom where the valley refers to the minima in the electronic band structure of the materials [1-2]. The charge carriers residing in these valleys have a geometrical phase associated with them called Berry's phase [3]. Berry phase gives rise to various physical properties such as Berry curvature and which has opposite values in the adjacent valleys in inversion asymmetric materials. Thus, 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). Monolayer MoS_2 is widely studied for valleytronics properties due to its inversion asymmetry. Although bilayer MoS_2 is symmetric, an out-of-plane electric field can render asymmetry in the system. Thus herein we study the Valleytronics of biased bilayer MoS_2.

The *ab initio* calculations are performed using the LCAO method implemented in SIESTA [4] based on GGA exchange-correlation functionals. A fine Monkhorst-Pack grid of 36 x 36 x 1 and a mesh cut off of 500 Ry was used in all the calculations. Berry curvature was calculated using Wannier90 [5].

Bilayer MoS2 is a wide bandgap semiconductor (Fig. 1a) with inbuilt inversion symmetry, which makes it not useful for valleytronic studies as it gives zero Berry curvature (Fig. 1c). However, the application of an out of plane electric field reduces the bandgap and renders asymmetry in the system. This, in turn, results in a non-zero Berry curvature with opposite values at K and K' high symmetry points of the Brillouin zone (Fig. 1d). In order to confirm the asymmetry in the system, we calculated the charge density difference for the unbiased (Fig. 1e) and biased (Fig. 1f) bilayer MoS2. While the unbiased case shows symmetric charge distribution for the top and bottom layer, the biased case shows an asymmetry around the top and bottom sulfur atoms, confirming the asymmetry in the system.

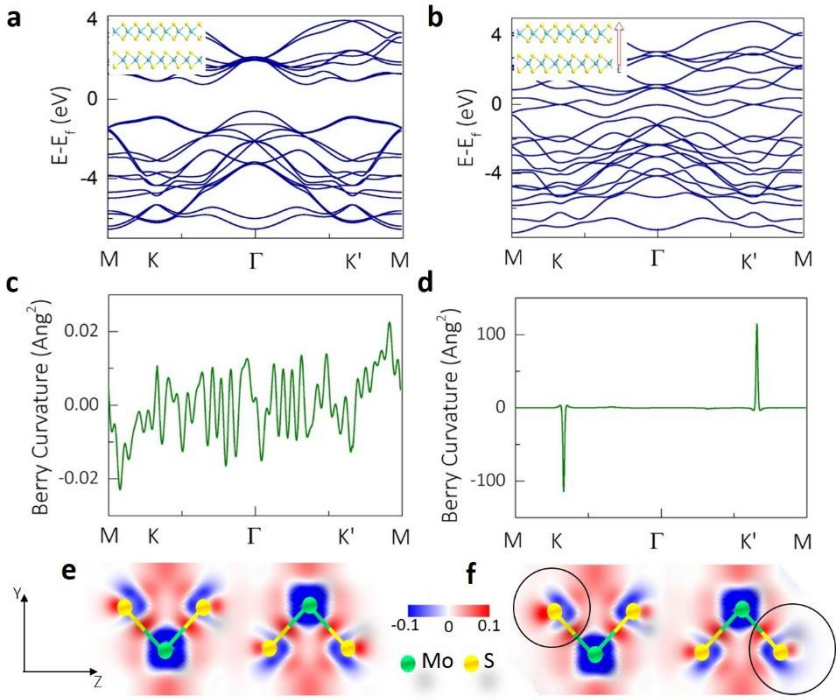

Figure. 1: (a) Band structure of the unbiased Bilayer MoS2 with a large bandgap. (b) The application of an out-of-plane electric field reduces the bandgap. (c) Unbiased bilayer MoS2 shows zero Berry curvature which makes it not useful for valleytronic studies. (d) Bilayer MoS2 under an out-of-plane electric field shows a non-zero Berry curvature with opposite values at K and K' high symmetry points of the Brillouin zone. Charge density difference for the (e) unbiased and (f) biased bilayer MoS2.

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