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Student Paper

Single Layer MoS_2 Band Structure and Transport

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Introduction: Ultrathin two dimensional materials have significant potential for application in nano-electronic devices. Graphene is a popular two-dimensional material due to its intrinsic high mobility. However, Graphene does not have any band gap, which makes it hard to be used for field effect transistors (FET)[1]. On the other hand, monolayer Molybdenum Disulfide (MoS_2) is a thin two dimensional material with large intrinsic band gap. These characteristics and recent successful fabrication of transistors [1] make it a promising candidate for future device applications. In this paper, the band structure of monolayer MoS_2 is calculated by density functional theory (DFT) using the *abinit* [2] package with the local density approximation (LDA) and GW approximation. The newly computed GW band structure and effective masses are different from previously reported LDA results in the literature. Using the new band structure we simulate a short gate length field FET and report initial results.

Band structure calculation methodology and results: Monolayer MoS_2 has a hexagonal crystal structure as does the Brillouin zone (BZ). To perform the band structure calculations, we used DFT as implemented in the *abinit* software [2]. For LDA calculation a cutoff of about 500eV for the plane-wave expansion was used to converge. For BZ integrations, a 30x30x1 k-point mesh centered at Γ point was used. The GW approximation with a plane-wave expansion cutoff of 160eV for the dielectric function was applied to obtain the band structure. The LDA and LDA+GW computed band structure are shown in Fig 1. The LDA results are qualitatively identical to previously reported LDA calculation [3] and experimental value for band gap [4]. Recently, T. Olsen et al. used LDA+GW to calculate the band structure of monolayer MoS_2 [5]. Their results and experimental research [6] show the band gap which was measured before is from excitonic bands and the right band gap is *indirect* and about 2.3eV. Here also, the results by LDA and LDA+GW show a big difference between LDA and LDA+GW calculation. As it is shown in the Fig 2 the lowest conduction band is along $\Gamma \rightarrow K$. The LDA+GW band gap in our calculation is 2.14eV. The discrepancy between the calculated band gap and reported one in [5] is due to different approximation levels. In this research we used a higher cutoff energy for GW and smaller mesh size. The lowest conduction bands in the first BZ is shown in Fig 2. Six equivalent valleys along *K* direction can be seen in the conduction band contour on BZ in Fig 2. The calculated effective masses and valley degeneracy are shown in Table 1. The achieved dielectric constant for monolayer MoS_2 with *abinit* is between 6.8-7.3ε_0 which is close to the dielectric constant for bulk MoS_2 [7].

Device description and modeling method and results: The device structure is shown in Fig 3 with details described in the caption. A real-space quantum transport solver based on a self-consistent solution of the Schrödinger-Poisson equations [8] is used to compute the I_D-V_G and I_D-V_D shown in Fig 4. The current at 0.6V over drive is 1783μA/μm with I_{ON}/I_{OFF} in excess of 10^6. The achieved results are close to previously reported results [9][10], although our model predicts a heavier effective mass and a higher valley degeneracy factor.

Conclusion and provision: The band structure of monolayer MoS_2 is studied by LDA+GW and the effective masses and dielectric constant are extracted. The effective mass is used to model a short channel FET device. The simulated transport characteristics are similar to previously reported results even though our improved model indicates a heavier effective mass and higher valley degeneracy factor. The large band gap in this 2D material and high I_{ON}/I_{OFF} ratio in nominal and fabricated devices make it worthy to explore this material for device applications. More precise band structure is required to have a better understanding about this material. The band structure could be more precisely obtained by using larger mesh size and higher cut-off energy for plane wave expansions. More sophisticated device transport simulations tight binding model would be required to capture the confinement effects.

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Table 1. Effective masses computed here and reported earlier. The valley degeneracies (g_v) for different band structures are also shown.

Reference	Method	Values	g_v
Ref [9]	Based on LDA results in [3]	$m^* = 0.45m_0$	2
Ref [10]	GGA	$m_l^* = 0.5788m_0$	2
		$m_t^* = 0.5664m_0$	
This paper	LDA+GW	$m_l^* = 0.87m_0$	6
		$m_t^* = 0.58m_0$	

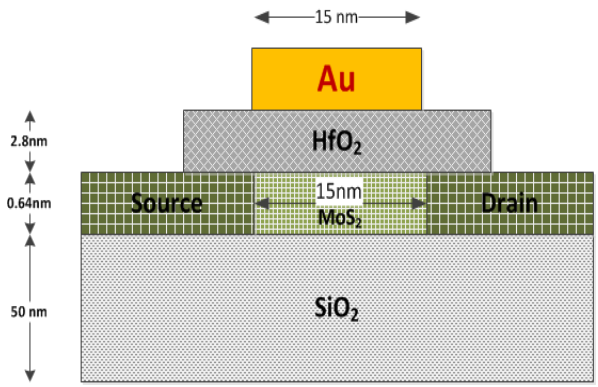

Figure 3. Schematic structure for monolayer MoS_2 transistor. Nominal device parameter in simulation: Gate length (15nm), top gate insular HfO_2 (ε=25), V_{DD}=0.4V, and a grid size of 0.1nm for constructing Hamiltonian long transport direction. Transport direction is along K.

(b)

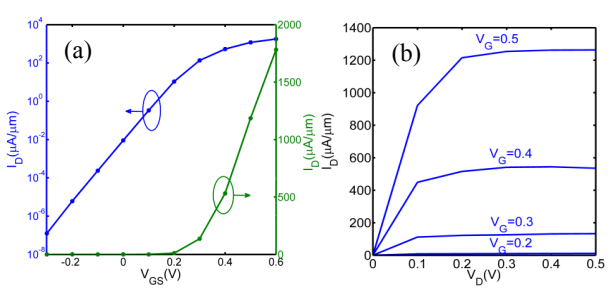

Figure 4. (a) Achieve I_D-V_G characteristics for the nominal device at V_D=0.4V. (b) I_D-V_D characteristics for V_G=0.2, 0.3 and 0.4 V. The current at 0.6V over drive was 1783μA/μm. The maximum achieved I_{ON}/I_{OFF} in the range of simulation was more than 10^6.

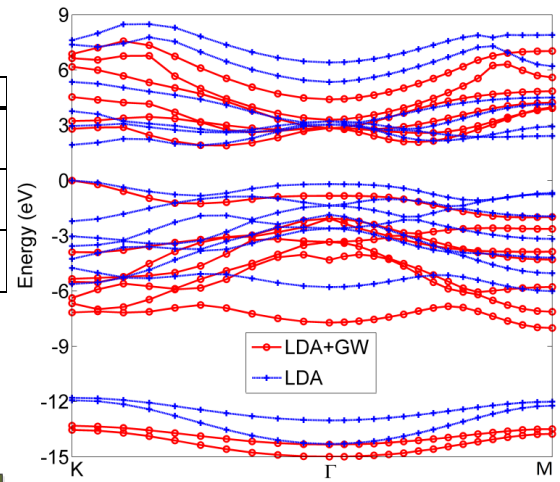

Figure 1 . Calculated band structure by LDA and LDA+GW approximation. LDA band structure is direct band gap in K point while LDA+GW is indirect along Γ→K. The band gap in LDA is 1.9eV and for LDA+GW is 2.14eV.

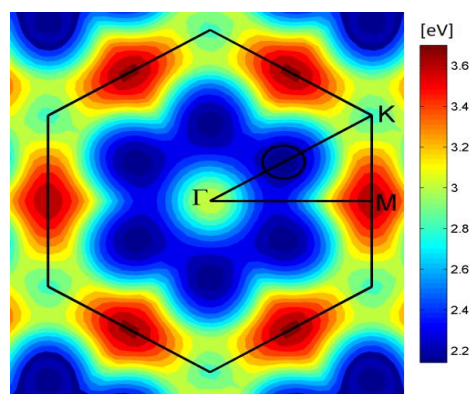

Figure 2. The lowest conduction band in the first BZ. It is shown clearly in the figure, the lowest value is along Γ→K. There are six valleys. For transport, six valleys are split into two groups: two folded and four folded valleys.