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The contact barrier of 1T′/2H MoS_2 heterophase bilayer and its modulation by adatom and strain: A first-principle study

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1. The effective mass of MoS_2 in the related systems.

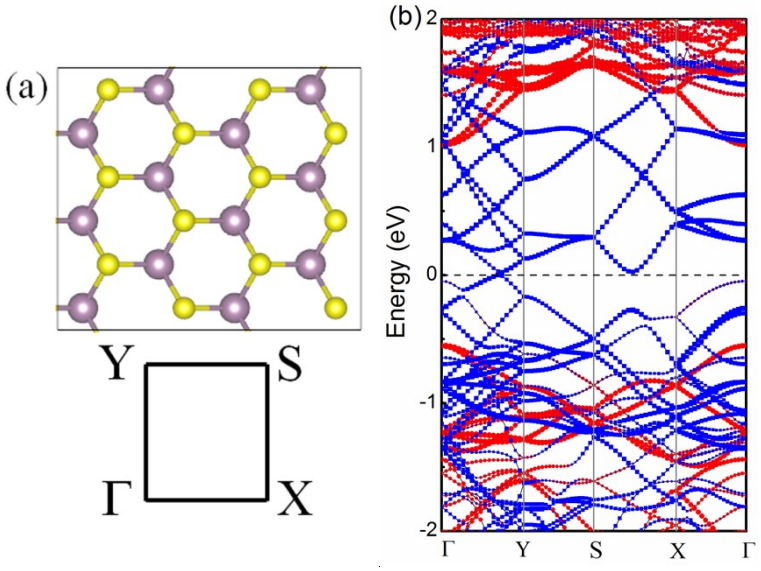

Figure S1. (a) 2×3 supercell of 2H-MoS_2 (b) the electronic band structure of 1T′/2H MoS_2.

Table S1. Effective masses of the electron and hole along high symmetry points of each system.

	Γ-X		Γ-Y	
	m_e^* (m_0)	m_h^* (m_0)	m_e^* (m_0)	m_h^* (m_0)
2H-MoS2	0.43	0.57	0.48	0.67
1T′/2H MoS_2	0.45	0.61	×	0.51
Li	0.47	×	×	×
Na	0.47	×	×	×
Mg	0.48	×	×	×
Al	0.49	×	×	×

The effective mass of MoS_2 in the related systems is evaluated from the band structure $m^* = \hbar^2 \left(d^2E/dk^2 \right)^{-1}$. Here, a 2×3 supercell of 2H-MoS_2 and 1T′/2H MoS_2 is adopted as shown in Figure S1 (a). Figure S1 (b) is the corresponding band structure of 1T′/2H MoS_2 system. The effective mass along high symmetry points of each system is given in Table S1. Some values are not given because it is hard to obtain from the projected band structure. We can see from Table S1 that the effective mass of both electrons (m_e^*) and holes (m_h^*) along Γ-X of MoS_2 in 1T′/2H MoS_2 system are slightly enlarged compared with that in pure 2H-MoS2 system. However, m_h^* along Γ-Y of MoS_2 in 1T′/2H MoS_2 system is reduced compared with that in pure 2H-MoS_2 system. As for 1T′/2H MoS_2 system with metal atoms adsorption, m_e^* along Γ-X of MoS_2 is increased according to order of m_e^*(Al)> m_e^*(Mg)> m_e^*(Na) =m_e^*(Li).

2. The projected band structure of adatoms adsorbed on the top layer of 1T′/2H MoS_2 heterophase bilayer.

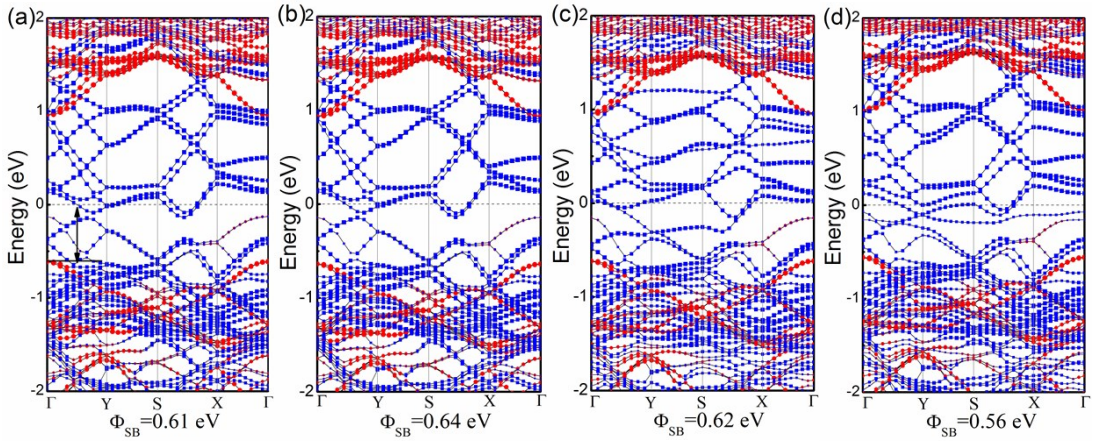

Figure S2. The projected band structure of adatoms adsorbed on the top layer of 1T′/2H MoS_2 heterophase bilayer.