Supplementary Information

Supplementary Table 1. The calculational lattice constants and band gap of monolayer MoS_2, along with the available experimental and theoretical data.

	present	experiment	GGA	HSE06	GW	QSGW
E_g (eV)	1.78	1.80 [1]	1.73 [7]	2.23 [7]	2.50 [3]	2.10 [6]
			1.90 [8]	2.12 [9]	2.78 [10]	
					2.76 [3]	
a (Å)	3.20	3.16 [2,5]	3.23 [2]			
			3.20 [3,4]			
			2.22 [5]			
$d_{Mo\text{-}S}$ (Å)	2.42	2.41[2]	2.45 [2]			
			2.42 [3,4]			
			2.44 [5]			
$d_{S\text{-}S}$ (Å)	3.15	3.19[2]	3.18 [2]			
			3.13 [3,4]			
			3.15 [5]			

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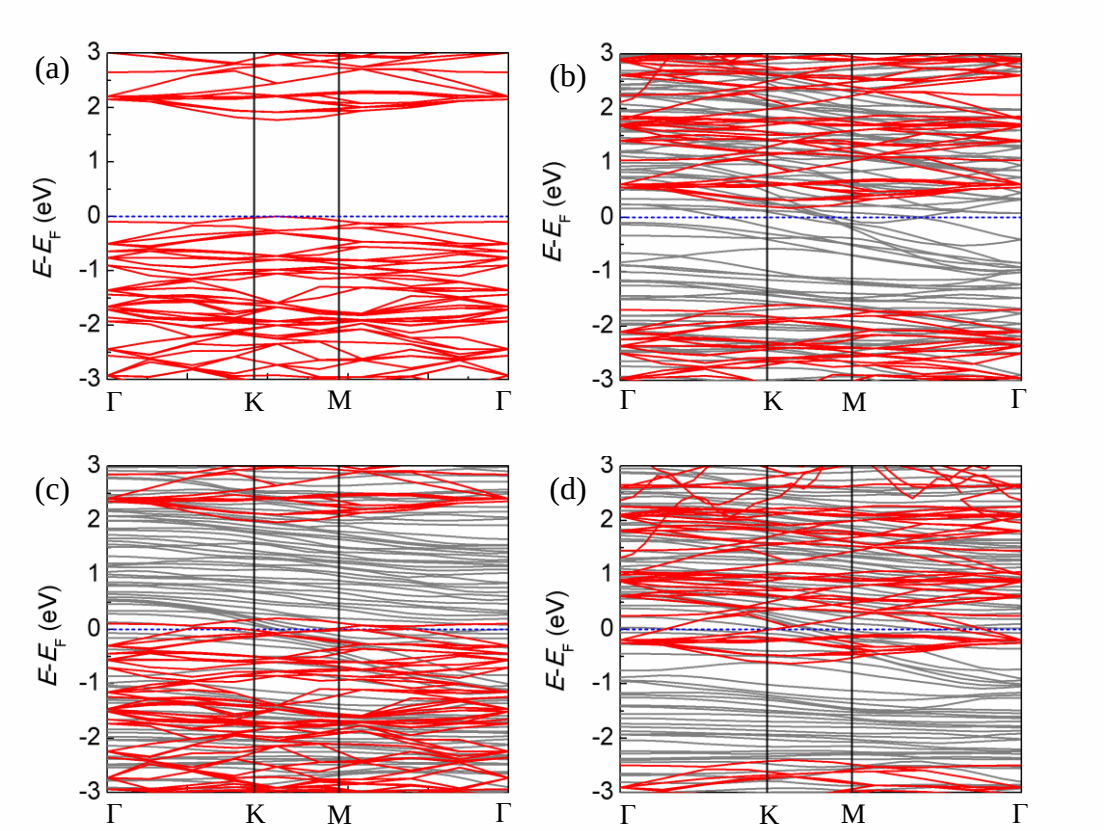
In this work, GGA method was adopted during calculations. The calculational lattice

constants and band gap of monolayer MoS_2 are listed in the Supplementary Table 1, along with the available experimental and theoretical data. The calculated band gap of monolayer MoS_2 is about 1.78 eV, which is consistent with the values of 1.73 eV [7] and 1.90 eV [8] obtained using GGA method, but lower than the values of 2.12-2.78 eV obtained by HSE06 [7, 9] and GW [3, 10]. The experimental value of 1.80 eV [1] may be rather an optical band gap because of the experimental methods used and the approximations applied in the treatment of the data. Hence, the band gap of monolayer MoS_2 obtained by the higher-level functionals of HSE06 [7, 9] and GW [3, 10] may be more close to the true experimental data. This is consistent with the expectation that the PBE Kohn-Sham gap usually underestimates the true band gap. Moreover, the calculated lattice constants of monolayer MoS_2 are in good agreement with the experimental values and previous GGA data [1-5]. Consequently, our results obtained by GGA are trustworthy.



Supplementary Figure 1. The band structures of intrinsic monolayer MoS_2 (a), perfect Mo-MoS_2 top contact (b), defective Mo-MoS_2 top contact with Mo-vacancy in monolayer MoS_2 (c), and defective Mo-MoS_2 top contact with S-vacancy in monolayer MoS_2 (d). The band structure of intrinsic monolayer MoS_2 is plotted for reference (red curves), which is superimposed on the new band structure (gray curves) so that old and new subbands align. The blue dash line is the Fermi energy of top contact system.