Supplementary information for

The interaction between vacancy defects in gallium sulfide monolayer and a new vacancy defect model

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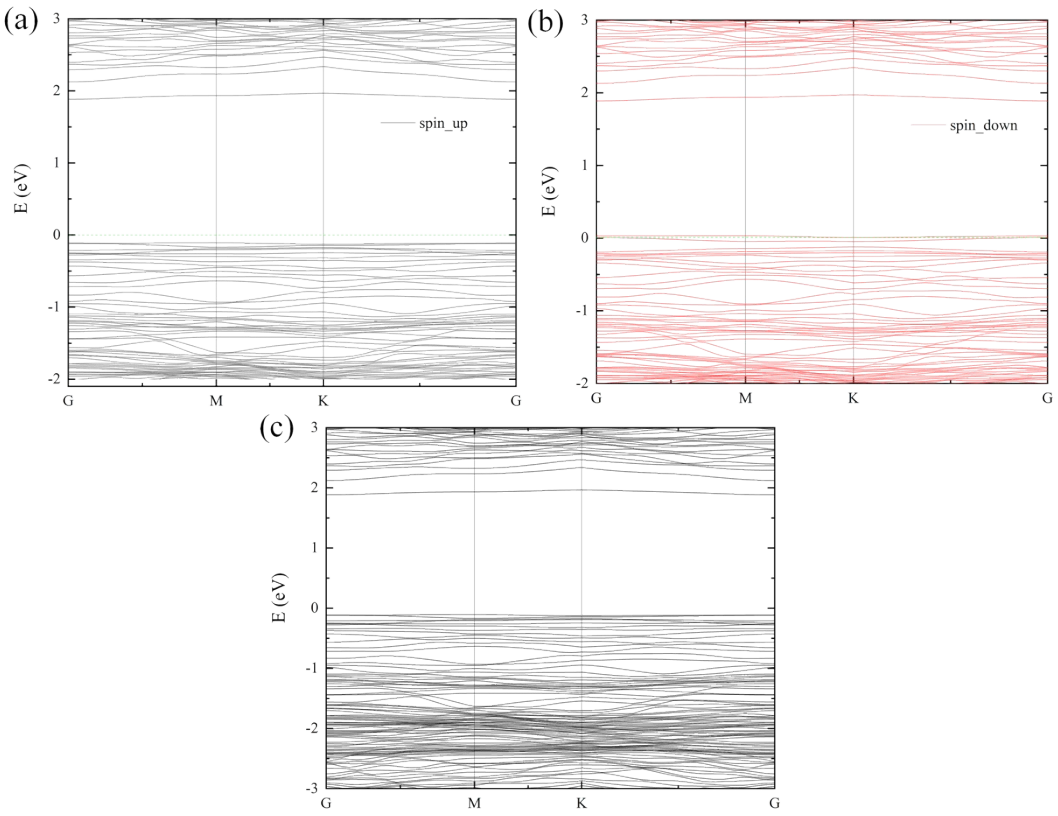

Fig. S1 Band structure of (a)-(b) 4×5×1 GaS monolayer with a Ga vacancy and (c) 4×5×1 pristine GaS monolayer. The Fermi level is set to zero.

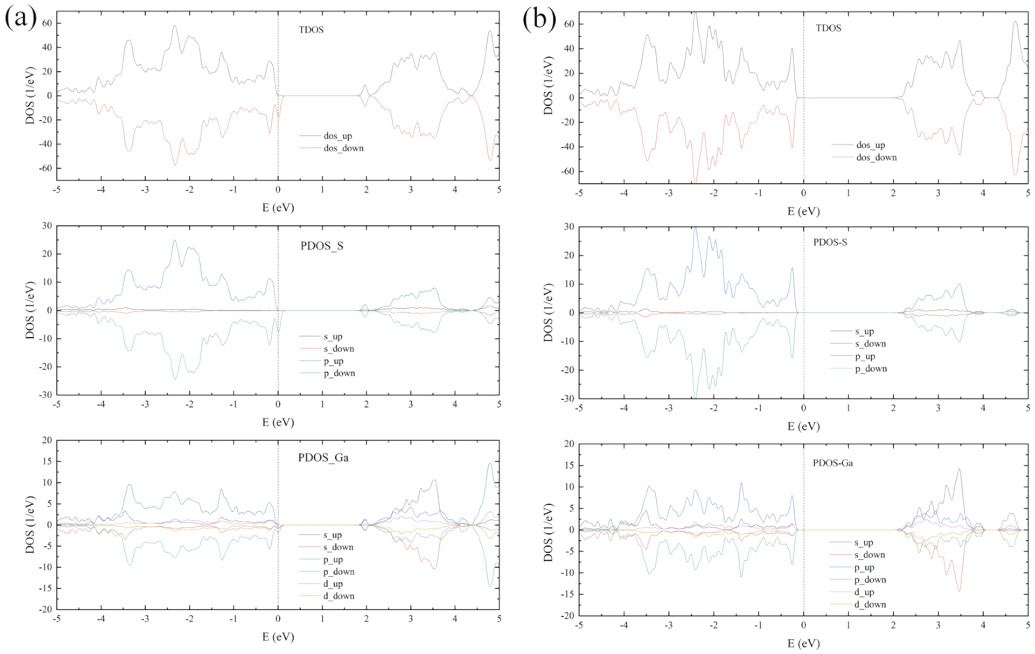

Fig. S2 Density of states of (a) 4×4×1 GaS monolayer and (b) 4×4×1 GaS monolayer with a Ga vacancy.

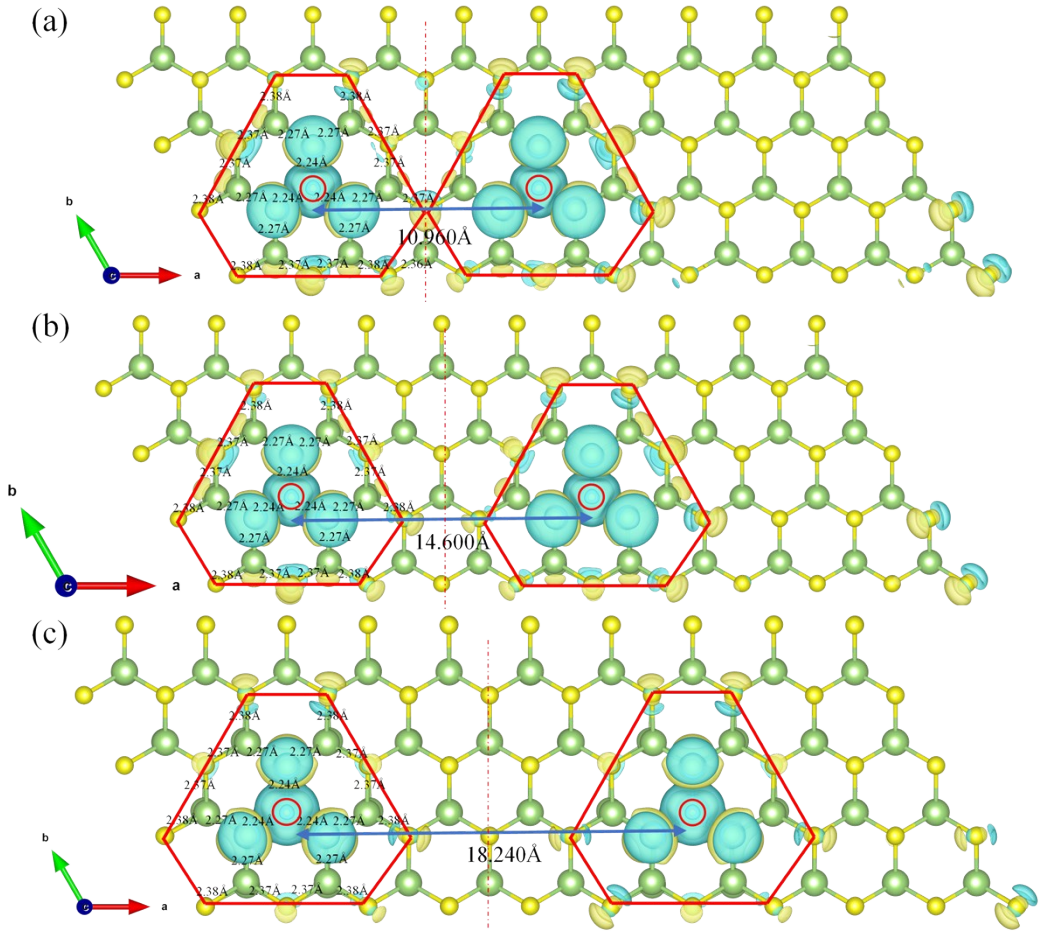

Fig. S3 Charge density difference of 4×10×1 defective GaS monolayer. The relative distance of vacancies is (a) 10.960 Å, (b) 14.600 Å, (c) 18.240 Å. The isoface value is set to 0.005 e/Å^3.

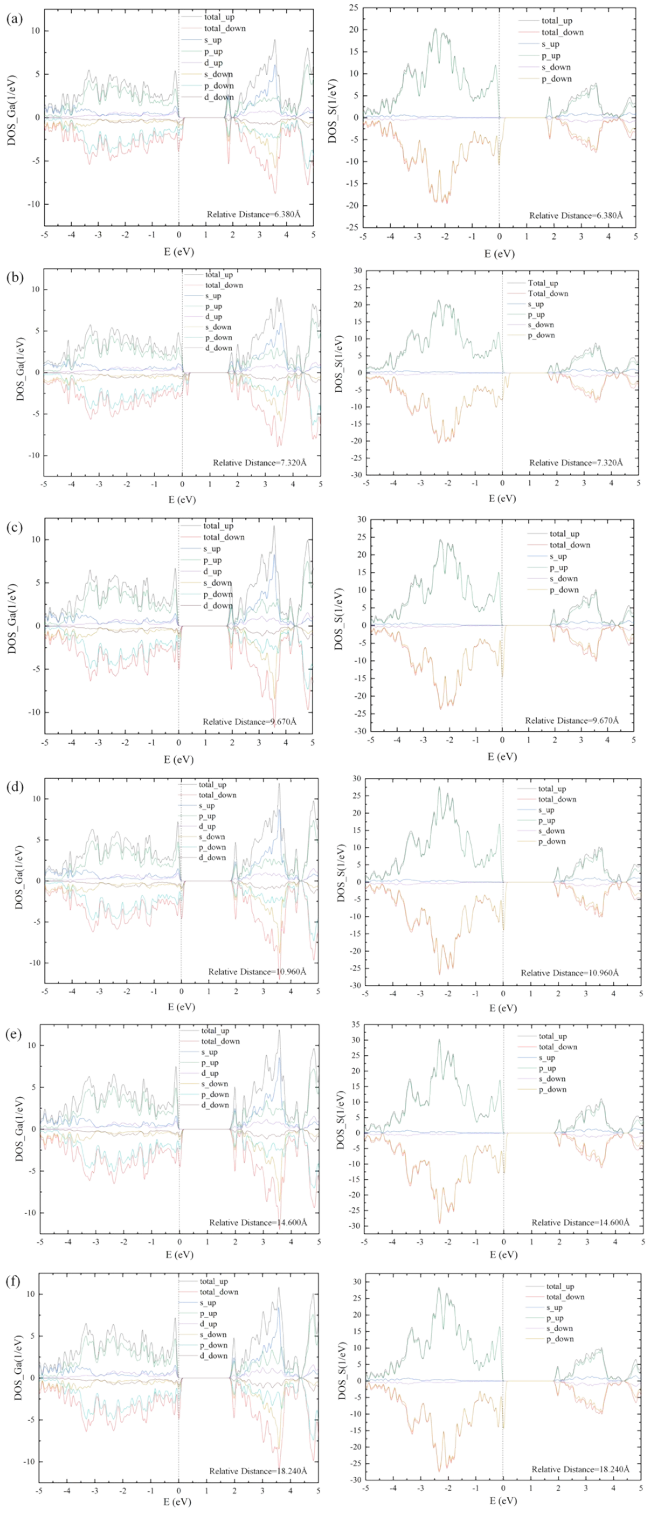

Fig. S4 Projected density of state (PDOS) of Ga atoms and S atoms in red box under different RDVs-Ga. The relative distance of Ga vacancies is (a) 6.380 Å, (b) 7.320 Å, (c) 9.670 Å, (d) 10.960 Å, (e) 14.600 Å and (f) 18.240 Å, respectively. The vertical dash line indicates the E_F.

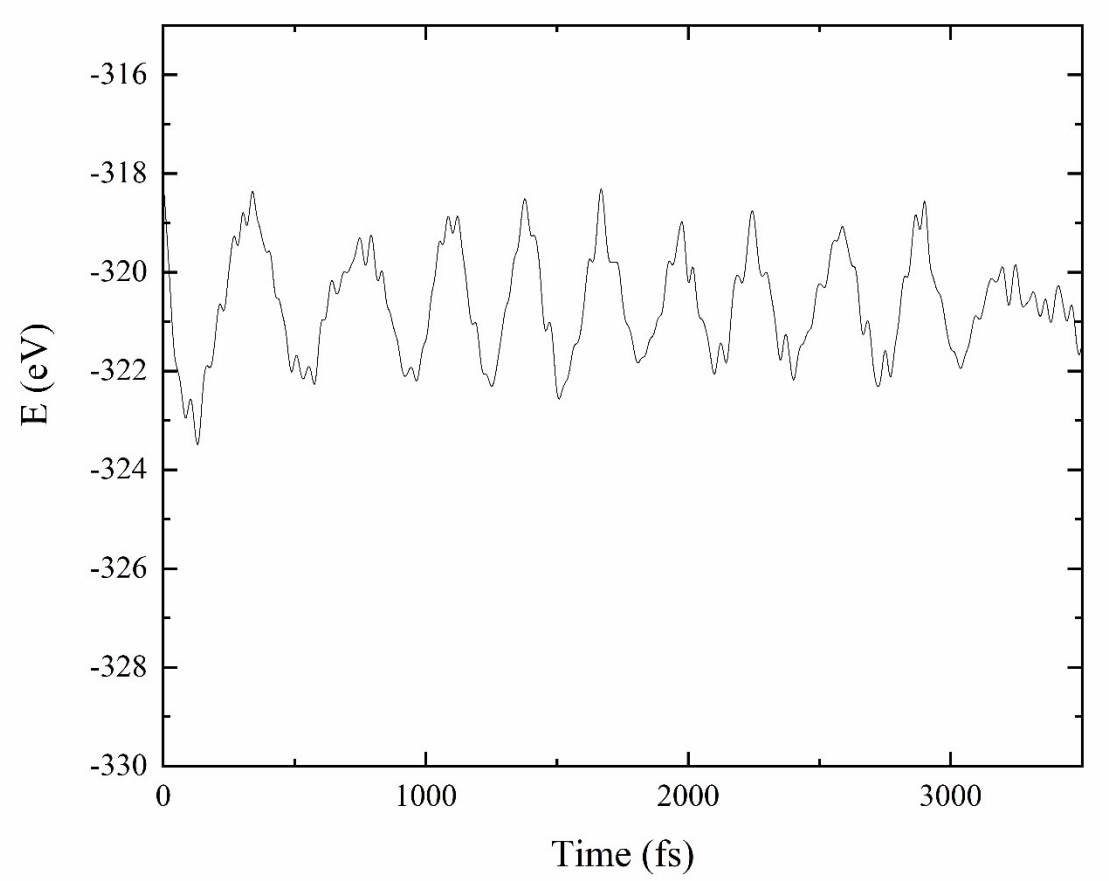

Fig. S5 Ab initio molecular dynamic simulation of 4×5×1 V_{Ga} defected GaS monolayer under T=600K.

Table S1. The bandgap of different vacancy defect model.

□	traditional concentration model		VDCM (4%)				VDCM (3%)	TB model (3%)
vacancy location	3×4-V_1(4%)	4×4-V_1(3%)	V_1-V_2^1-V_3^1	V_1-V_2^1-V_3^2	V_1-V_2^2-V_3^1	V_1-V_2^3-V_3^1	-	-
bandgap	1.042	1.116	0.892	0.899	0.946	1.005	0.916	0.75