Supporting Information

Electronic and optical properties of a novel two-dimensional semiconductor material $TlPt_2S_3$: a first-principles study

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The phonon dispersion curve, the AIMD and the work function of bilayer $TlPt_2S_3$ have shown in Fig.S1. It can be seen that any negative phonon frequency is complete absence in the phonon dispersion curve of bilayer $TlPt_2S_3$, and neither phase transitions nor significant structural distortions is observed during the AIMD process, which indicates that the structure of bilayer $TlPt_2S_3$ is thermo-dynamically stable. The work function of the bilayer $TlPt_2S_3$ (4.98 eV) in the vacuum environment shows it is also chemical stability.

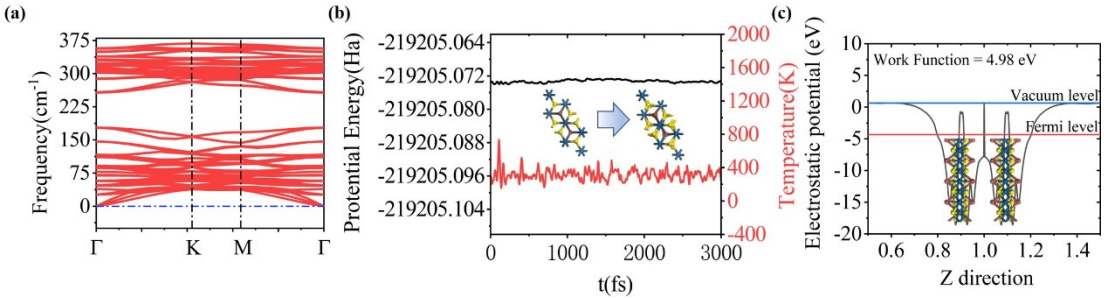

Fig. S1 (a) Phonon-dispersion spectrum for bilayer $TlPt_2S_3$. (b) Energy variations during the AIMD simulation under a temperature of 300 K. Inset plots show the bilayer $TlPt_2S_3$ structure before and after simulation. (c) Work function and electrostatic potential along the direction perpendicular to the plane.

Table S1 summarizes the corresponding values of μ^{2D}, C_{2D}, m^*/m_0 and E_d of the bilayer $TlPt_2S_3$. The electron mobility along the armchair direction is 13635.04 cm^2 V^{-1} s^{-1}, whereas along the zigzag direction it is calculated to 12332.20 cm^2 V^{-1} s^{-1}. The hole mobility along the armchair and zigzag direction are 3531.33 cm^2 V^{-1} s^{-1} and 858.55 cm^2 V^{-1} s^{-1}, respectively. It can be found that these electron and hole mobilities are much higher than that of the monolayer $TlPt_2S_3$.

Table S1 Effective mass m^*/m_0, DP constant E_d (eV), in-plane stiffness C_{2D} ($N \cdot m^{-1}$) and carrier mobility μ ($cm^2 \cdot V^{-1}s^{-1}$) for electrons and holes of bilayer $TlPt_2S_3$.

Carrier type		m^*/m_0	E_d (eV)	C_{2D} ($N \cdot m^{-1}$)	μ ($cm^2 \cdot V^{-1}s^{-1}$)
Electron	arm	0.78	0.57	108.45	13635.04
	zig	0.55	0.72	107.96	12332.20
Hole	arm	0.69	1.15	108.45	3531.33
	zig	0.75	2.23	107.96	858.55