Supporting Information

Interfacial electronic properties and tunable band offset in graphyne/MoSe₂ heterostructure with high carrier mobility

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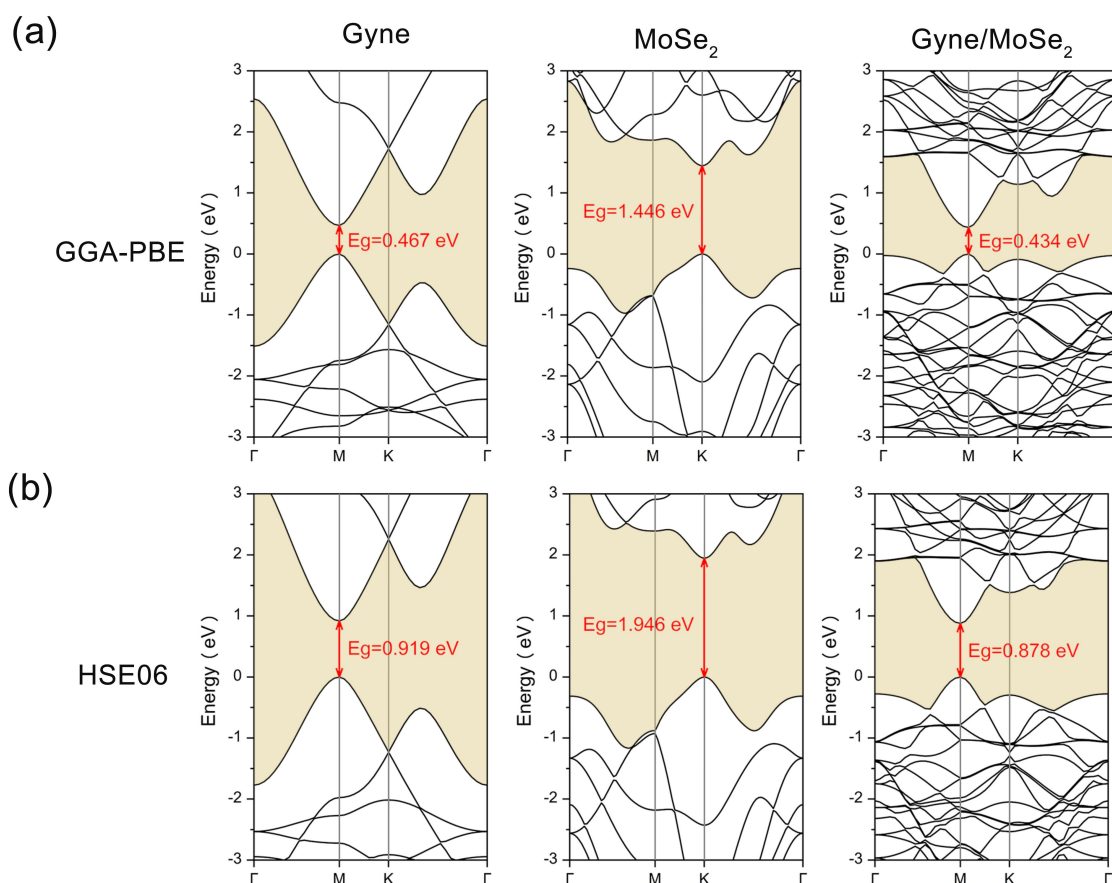[2]Department of Physics, McGill University, Montreal, Quebec H3A 2T8, Canada

Fig .S1. Band structures of the Gyne ML, MoSe₂ ML and Gyne/MoSe₂ heterostructure based on (a) PBE and (b) HSE06 method. Here, the Fermi levels are set to zero.
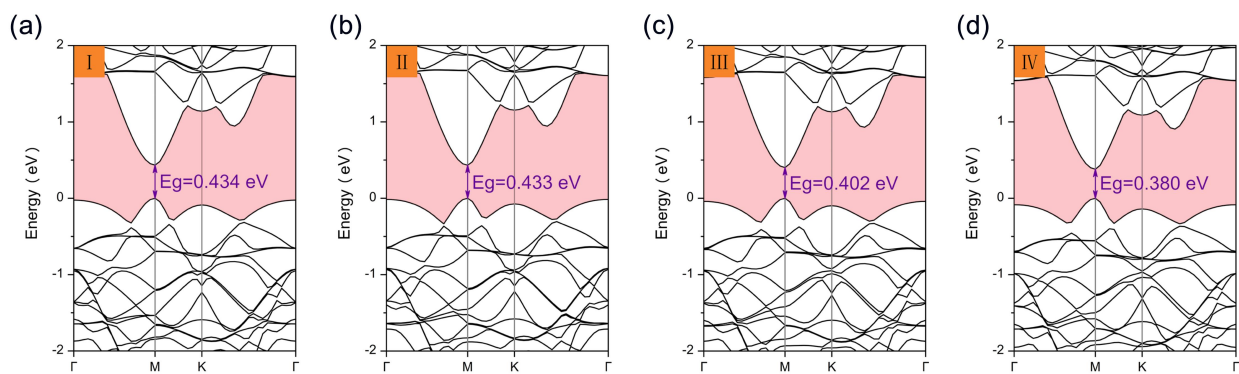
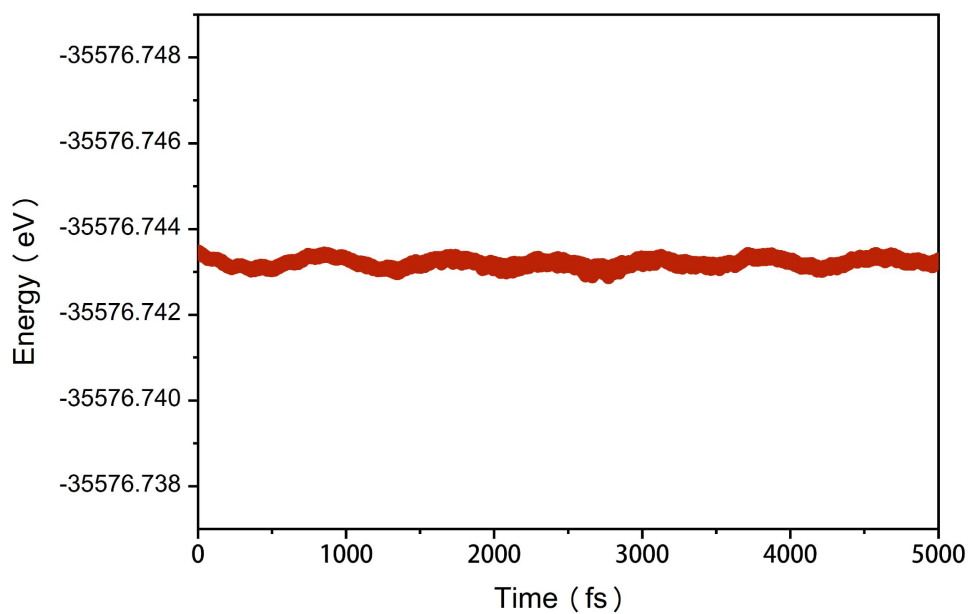**Fig .S2.** The band structures of four stackings of Gyne/MoSe$_2$ heterostructure.

Fig. S3. The calculated AIMD snapshots of the Gyne/MoSe$_2$ heterostructure at 300K with 5ps.
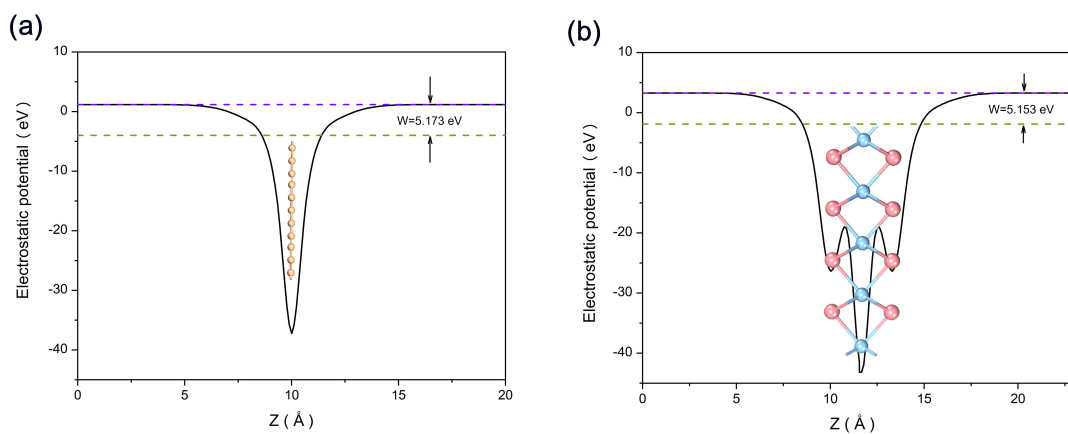

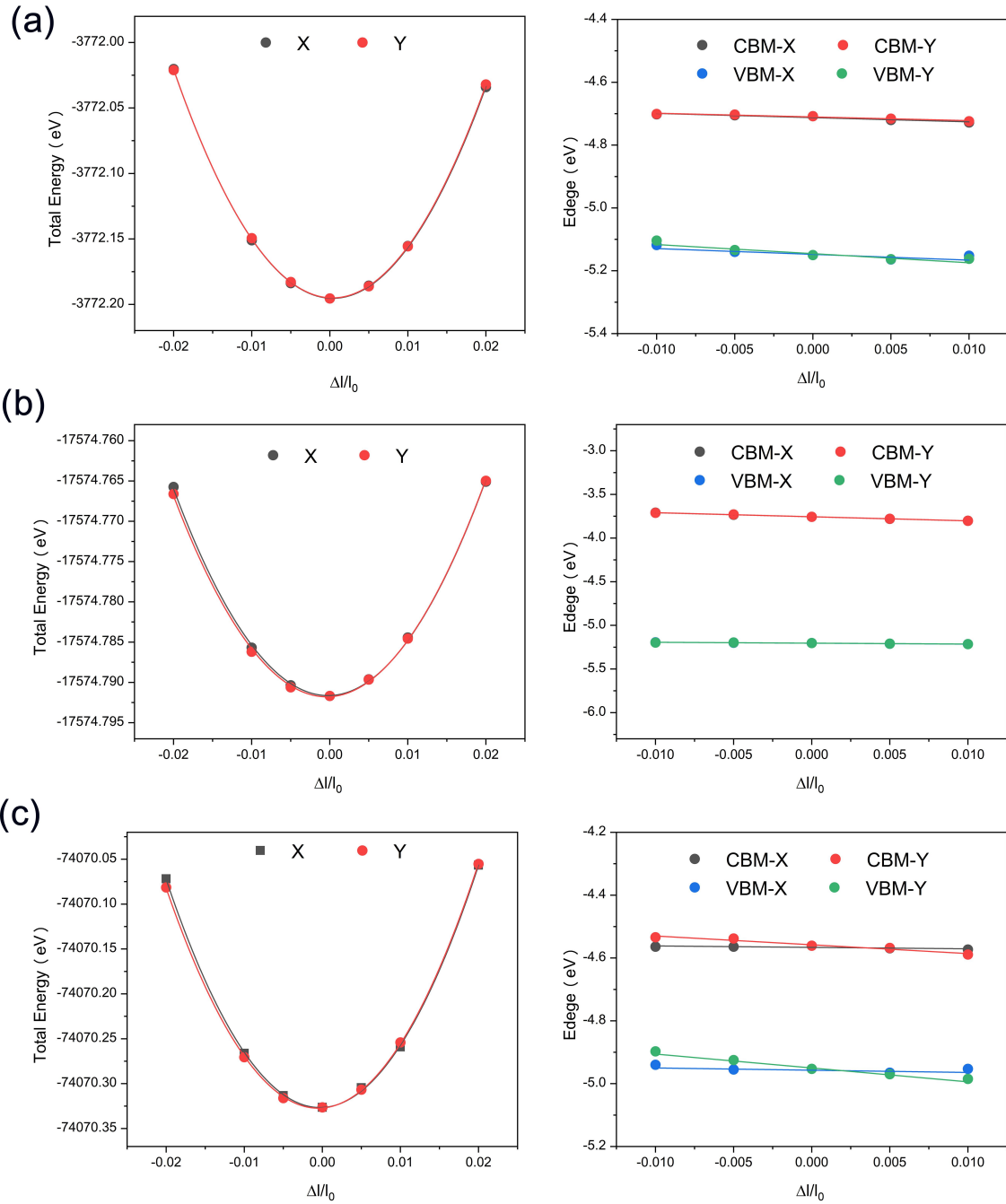**Fig .S4.** The work functions of (a) Gyne and (b) MoSe$_2$ monolayer.

Fig. S5. Elastic modulus (left) and deformation potential constant (right) evaluation for (a) Gyne ML, (b) $MoSe_2$ ML, and (c) $Gyne/MoSe_2$ heterostructure.
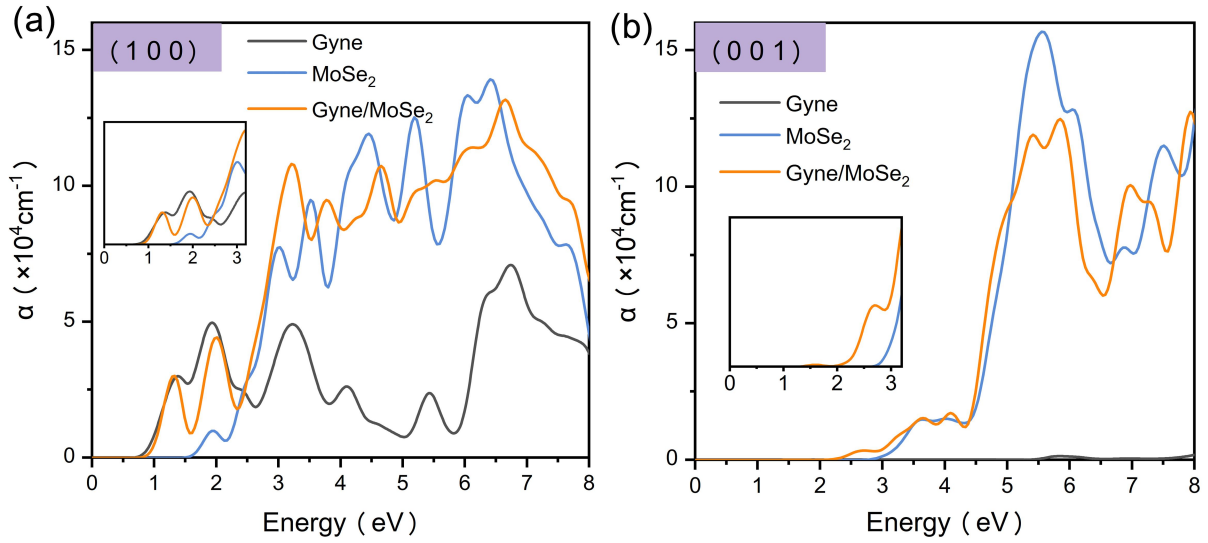
Fig. S6. The optical absorption of Gyne ML, MoSe$_2$ ML, and Gyne/MoSe$_2$ vdW heterostructure in the (a) (100) and (b) (001) directions under HSE06 function, and the insets are the optical absorption in micro-region.
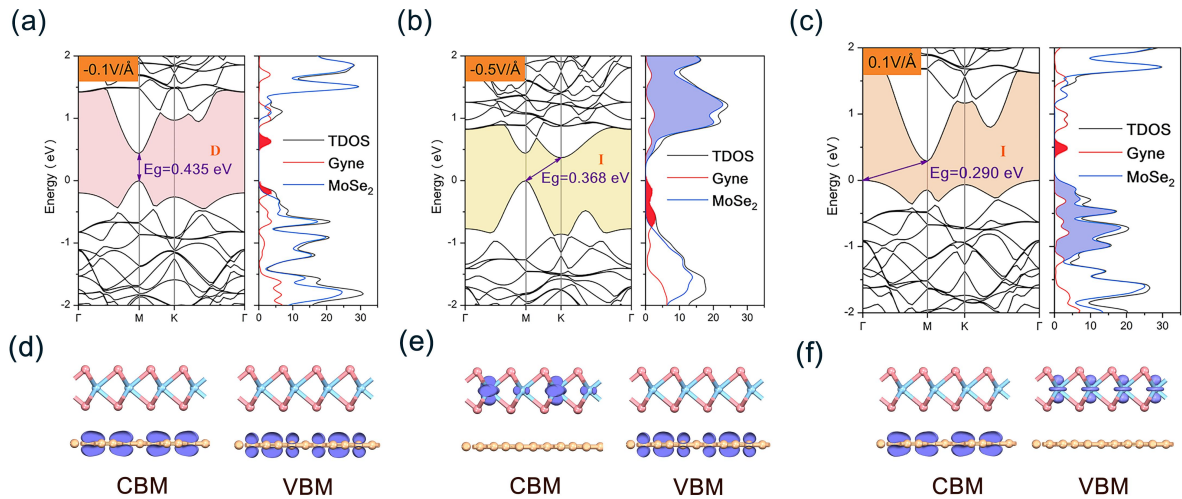

Fig .S7. Band structures, density of states and side views of band decomposed charge density CBM and VBM of the Gyne/MoSe$_2$ heterostructure under the external electric field of (a)-0.1V/Å, (b)-0.5V/Å and (c) 0.1V/Å. The Fermi levels are set to zero.
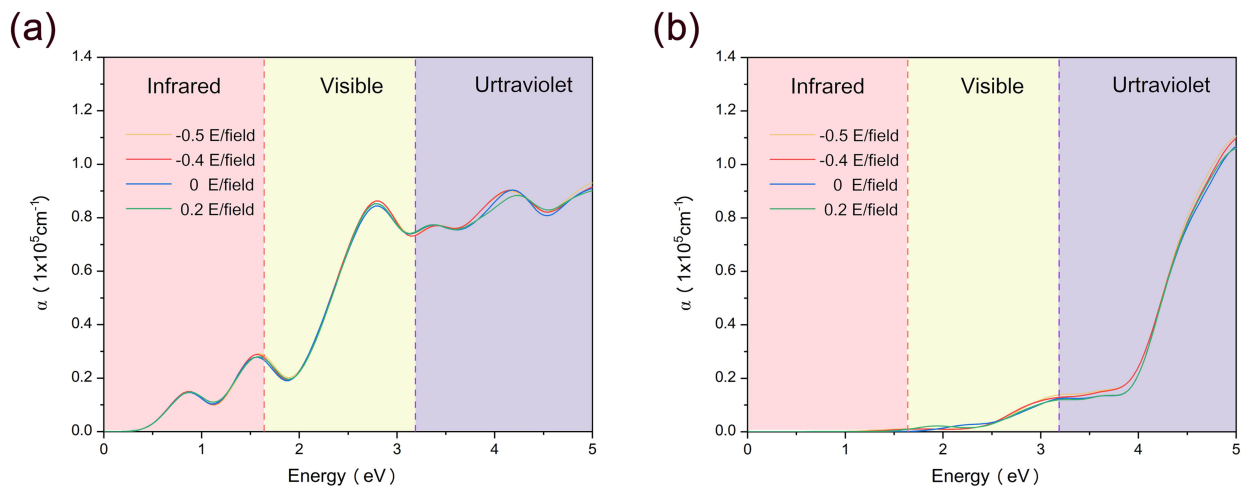
Fig .S8. The optical absorption Gyne/MoSe$_2$ heterostructure under the external electric field in the (100) (a) and (001) (b) directions.