Electronic Supplementary Material (ESI)

Atomically thin semiconducting penta- PdP_2 and $PdAs_2$ with ultrahigh carrier mobility

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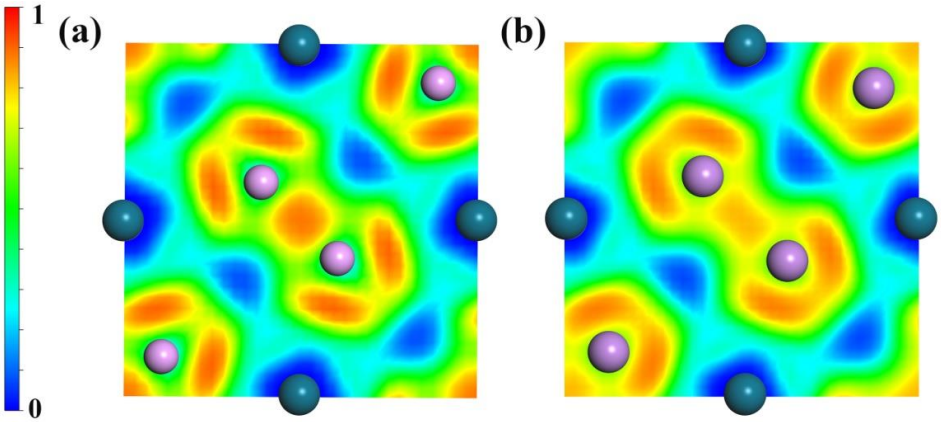

Fig. S1 Electron localization functions (ELFs) for (a) penta-PdP_2 and (b) penta-$PdAs_2$.

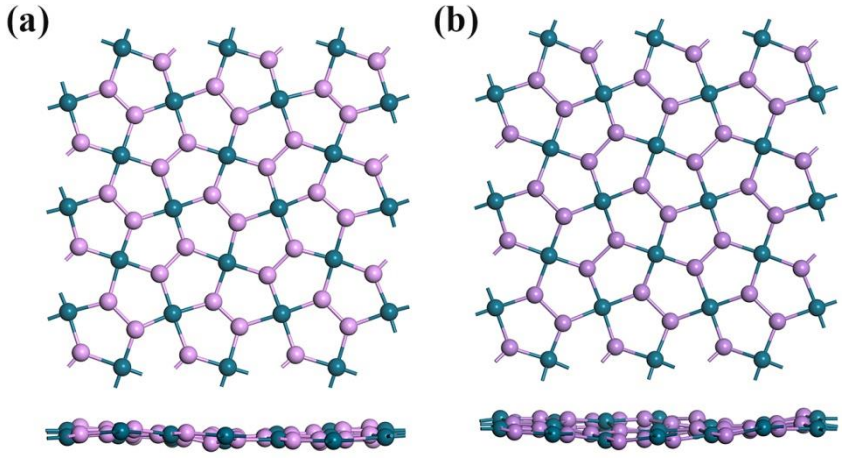

Fig. S2 Snapshot of AIMD simulations at 300 K for (a) penta-PdP_2 and (b) penta-$PdAs_2$.

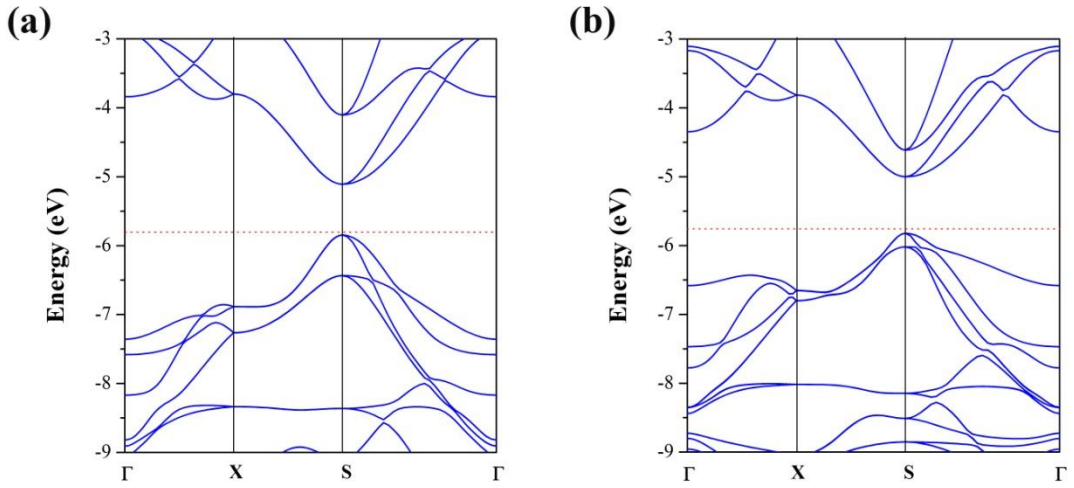

Fig. S3 HSE band structure with SOC for (a) penta-PdP_2 and (b) penta-$PdAs_2$.

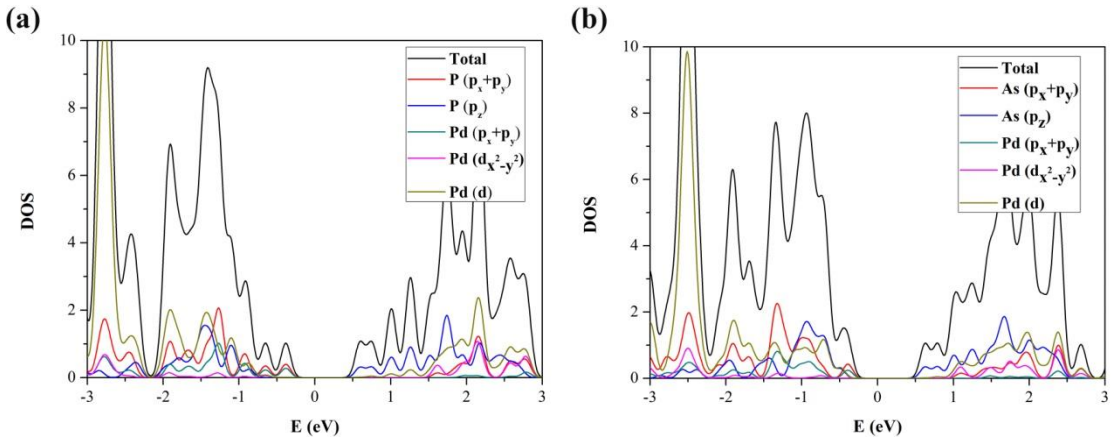

Fig. S4 Total and partial density of states (DOS) of (a) penta-PdP_2 and (b) penta-$PdAs_2$ monolayers.

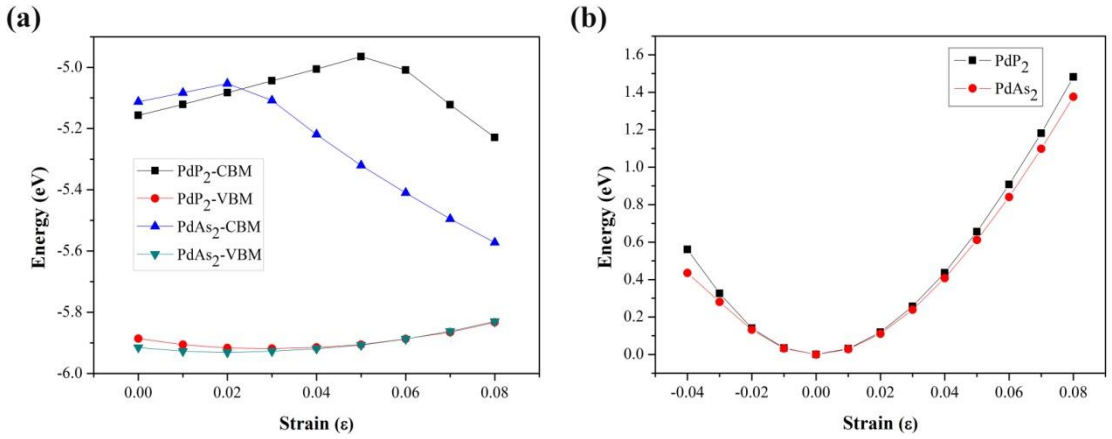

Fig. S5 (a) Evolution of band edges of penta-PdX_2 under tensile strain. (b) Change of total energy of penta-PdX_2 under biaxial strain.

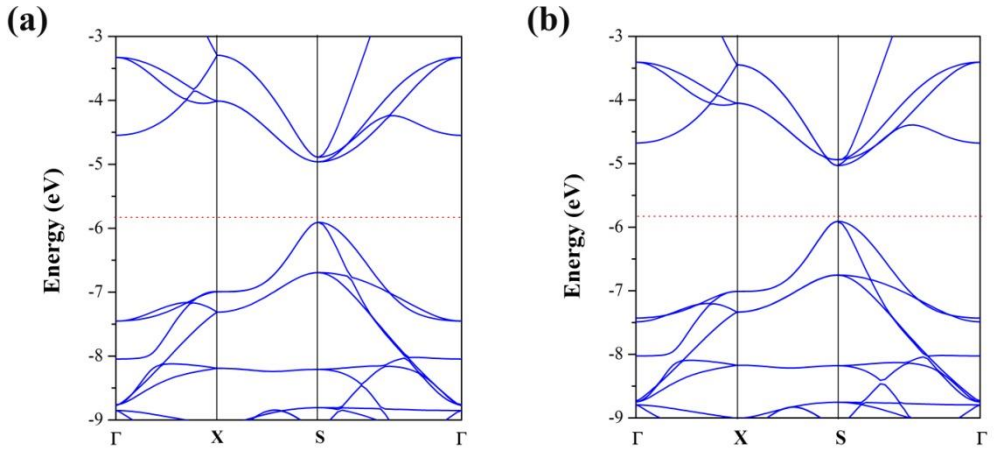

Fig. S6 Band structures of penta-PdP_2 monolayer under (a) 5% and (b) 6% biaxial strain.

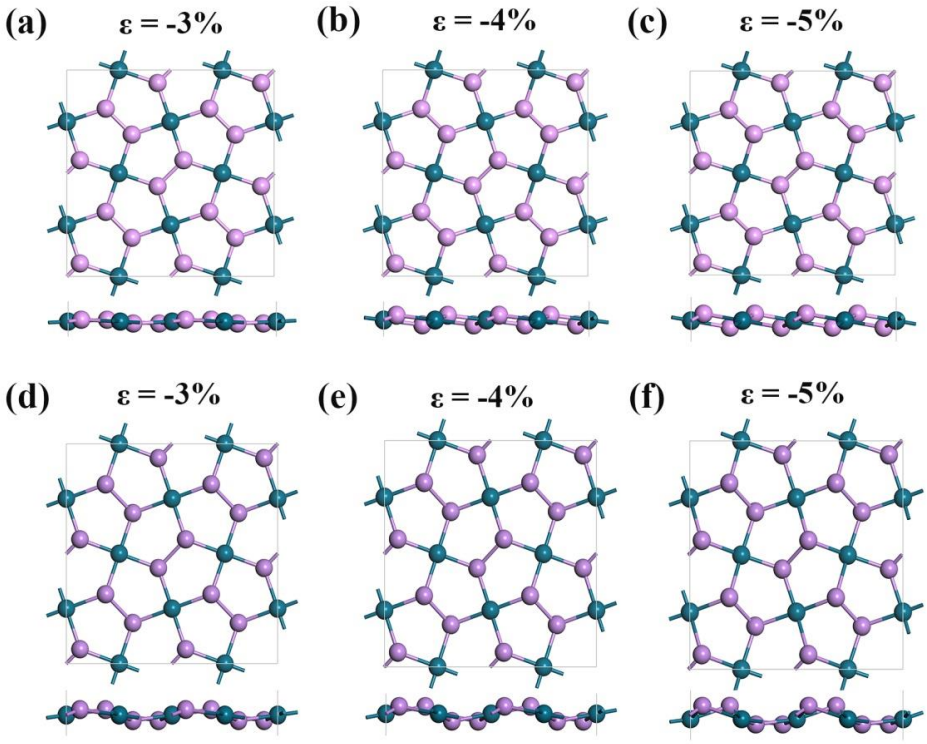

Fig. S7 Top and side views of compressed (a)-(c) penta-PdP_2 and (d)-(f) penta-$PdAs_2$ monolayers.

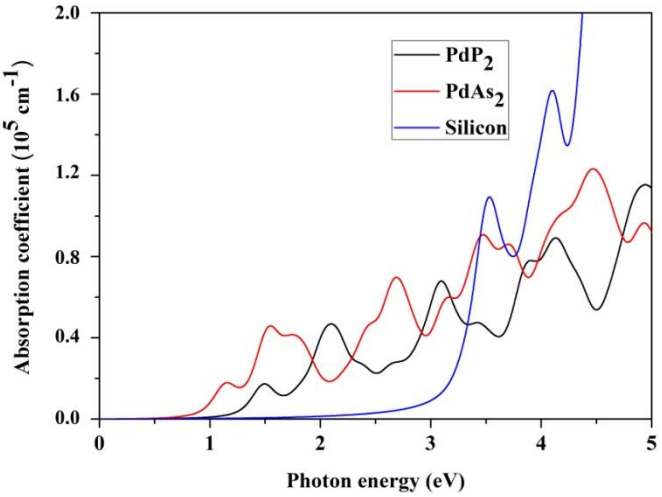

Fig. S8 Calculated absorption coefficient of penta-PdX2 monolayers and silicon at HSE06 level..