Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Penta-MX_2(M = Ni, Pd and Pt, X = P and As) monolayers: direct band-gap semiconductors with high carrier mobility

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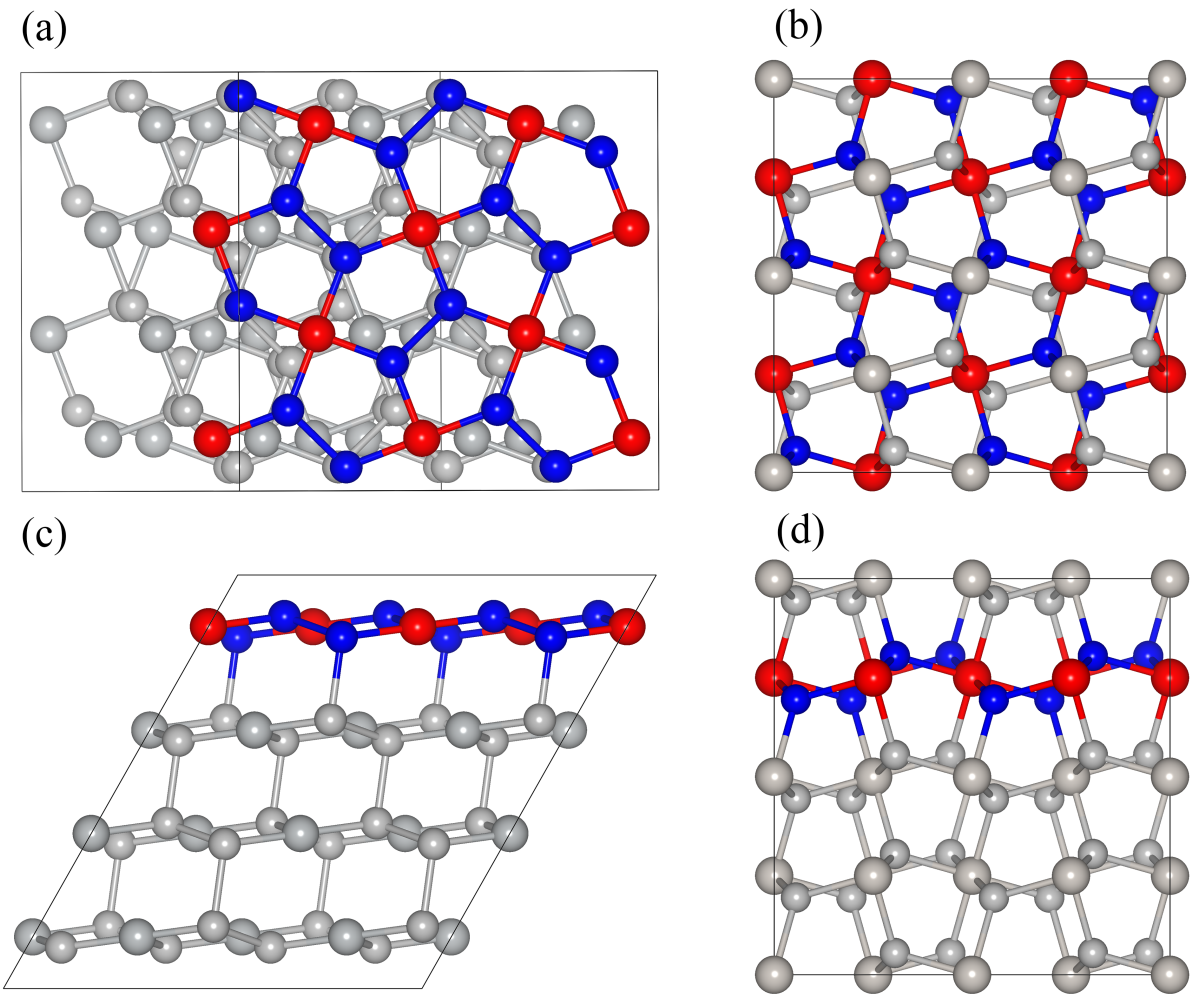

FIG. S1: Structure of bulk NiP_2 and PdP_2 in space group of C2/c (a) and bulk PtP_2, $NiAs_2$, $PdAs_2$and $PtAs_2$ in space group of $Pa\overline{3}$ (b). Red and blue balls represented the metal and P/As atoms in a layer, respectively.

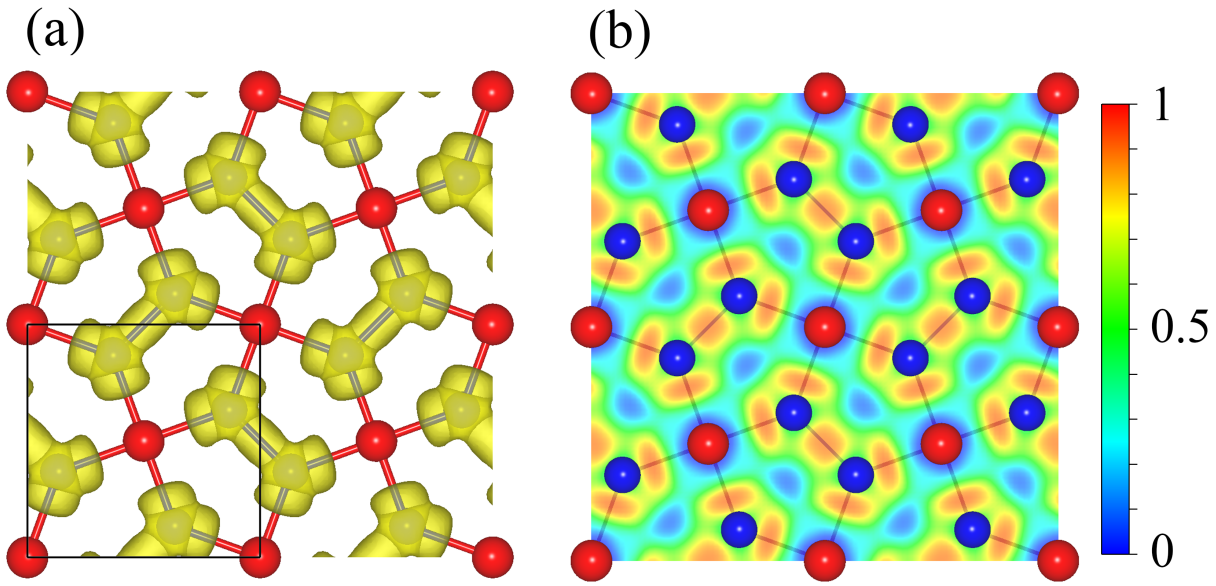

FIG. S2: (a)3D ELF of NiP_2 with isosurface value of 0.7. (b) 2D ELF of NiP_2 in (001) plane.

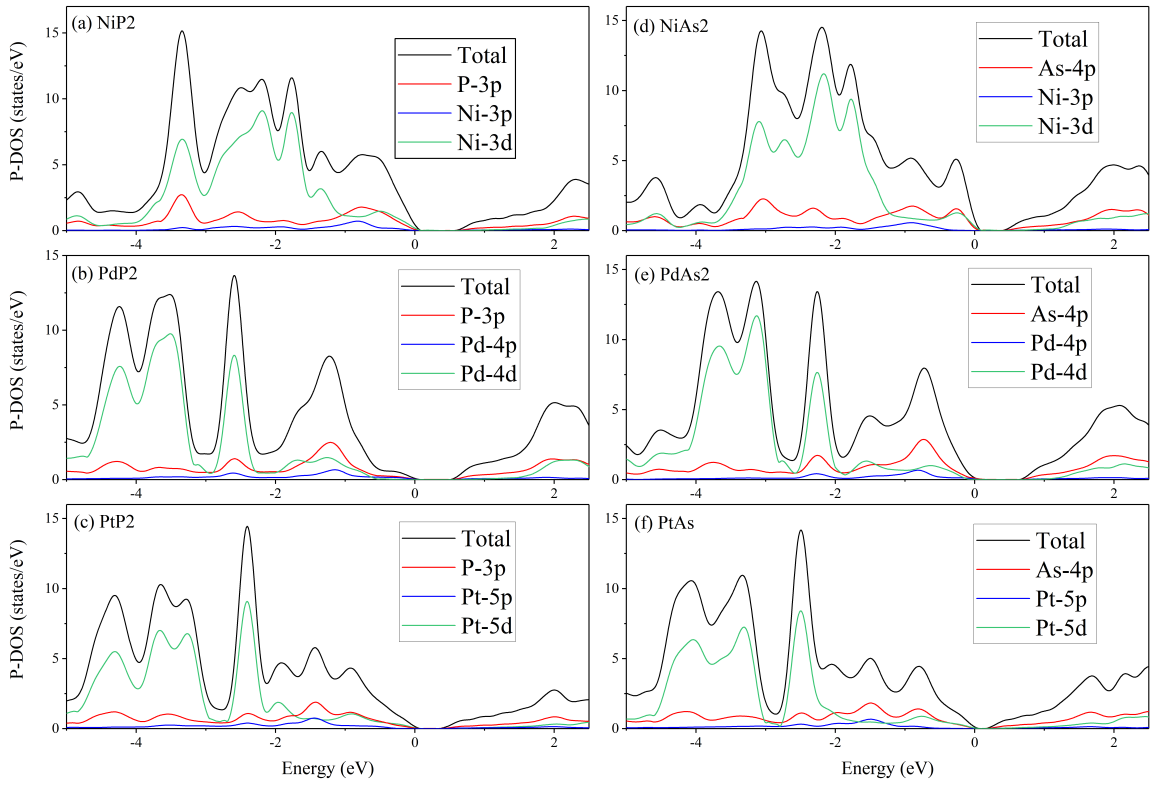

FIG. S3: The projected DOS of MX_2.

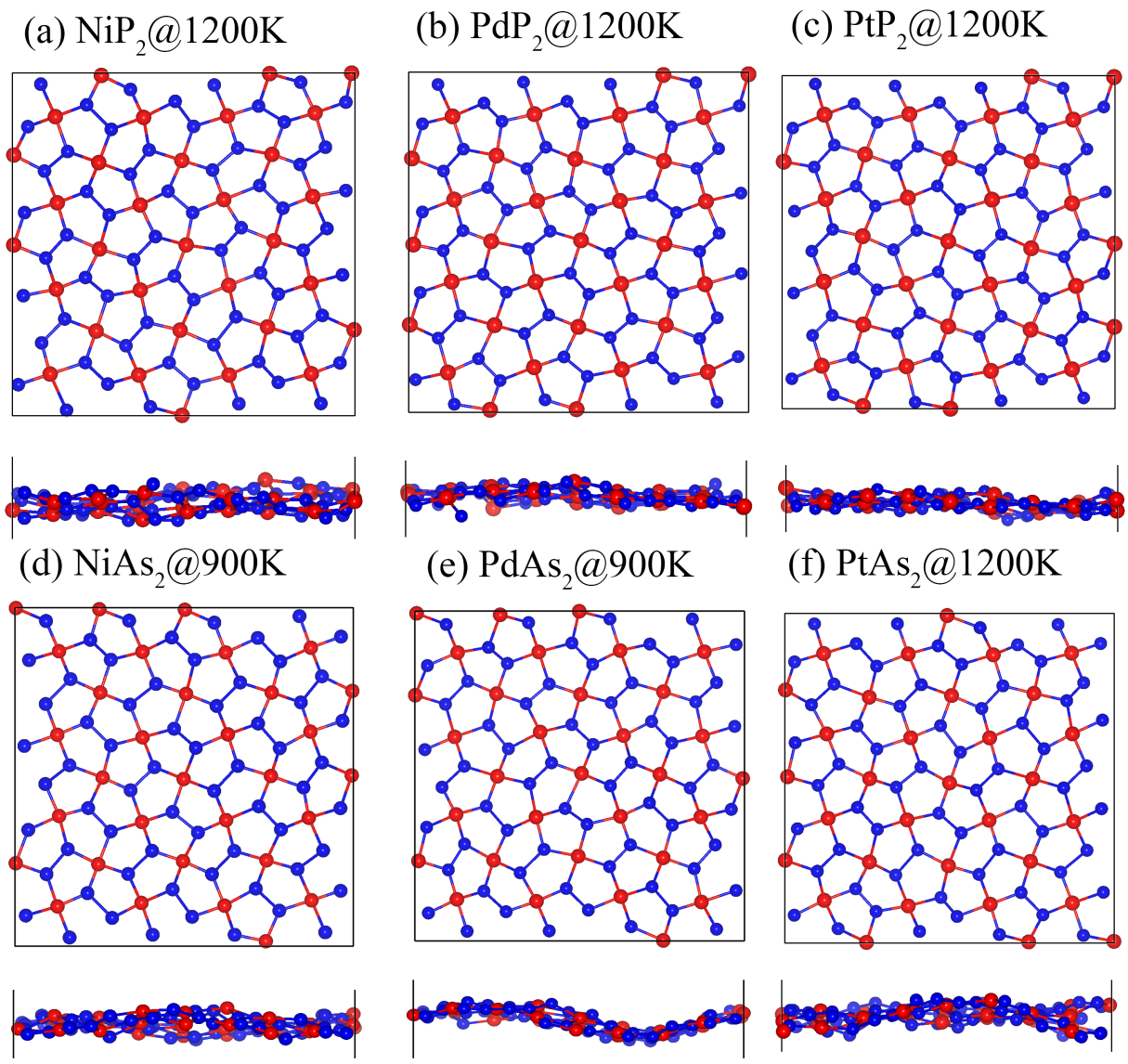

FIG. S4: Snap shots of the final frame of each molecular dynamic simulation using NVT.

TABLE S1: Calculated values for elastic modulus tensor C_{ij} (in Nm^{-1}) and the in-plane Young's modulus (Y) (in Nm^{-1}) of MX_2

	C_{11}	C_{12}	C_{66}	Y
NiP_2	124.2	28.1	39.3	117.9
PdP_2	114.9	34.8	28.4	104.4
PtP_2	143.3	40.4	35.9	131.9
$NiAs_2$	103.3	27.8	29.4	96.0
$PdAs_2$	92.6	32.4	23.7	81.2
$PtAs_2$	107.4	27.6	34.8	100.3

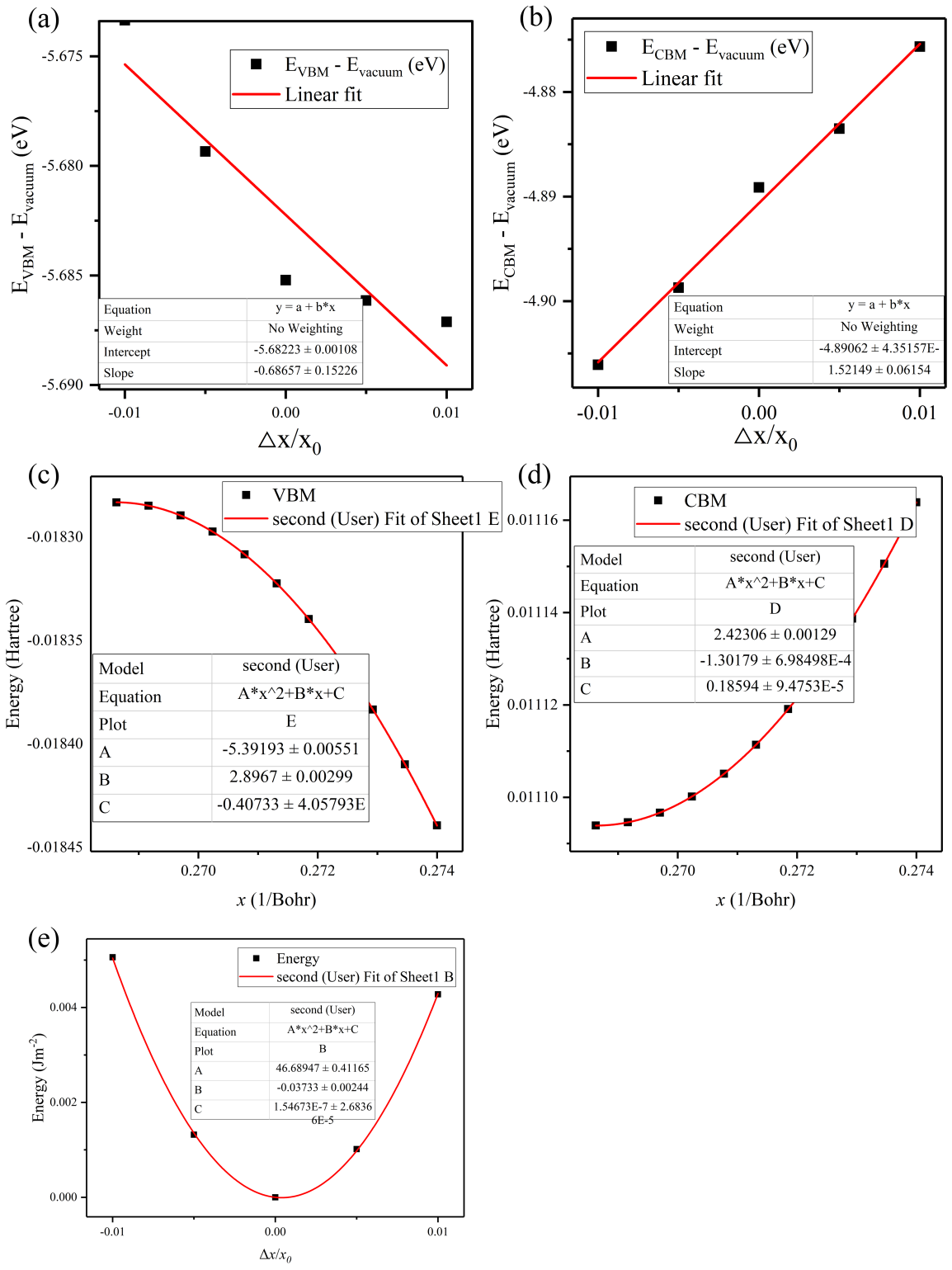

FIG. S5: Band energy of the VBM (a) and CBM (b) of $PdAs_2$ with respect to the vacuum energy as a function of lattice dilation. Band structure near the VBM(c) and CBM(d) of $PdAs_2$. Total energy-strain curve of $PdAs_2$. Red solid lines are the fitting curves.