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RESEARCH ARTICLE

Van der Waals epitaxy of type-II band alignment $CsPbI_3$/TMDC heterostructure for optoelectronic applications

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Supporting Information

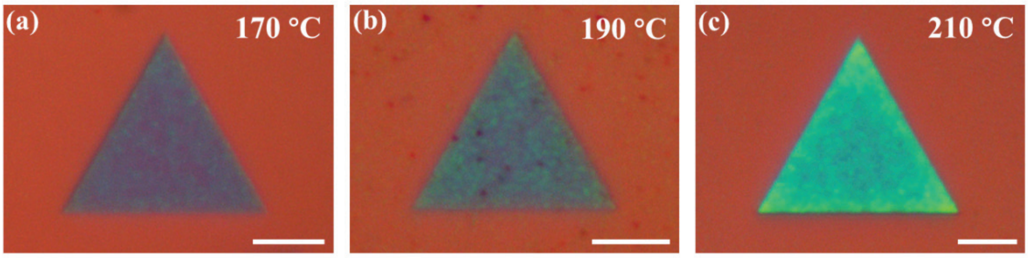

Fig. S1 Temperature dependent morphology evolution of $CsPbI_3$ on monolayer WSe_2 at growth temperature of **(a)** 170 °C; **(b)** 190 °C; **(c)** 210 °C. Scale bars are 10 μm in (a–c).

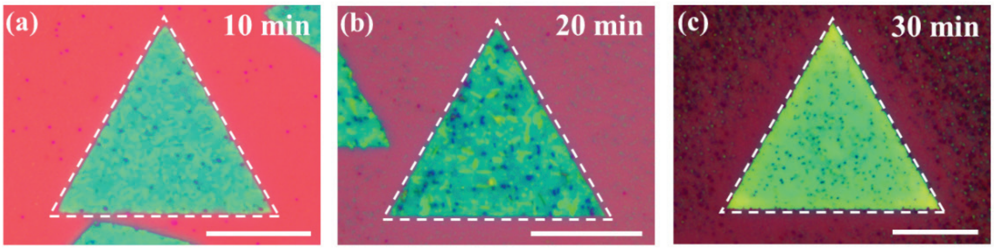

Fig. S2 Time dependent morphology evolution of $CsPbI_3$ on monolayer WSe_2 at growth time of **(a)** 10 min; **(b)** 20 min; **(c)** 30 min. Scale bars are 20 μm in (a–c).

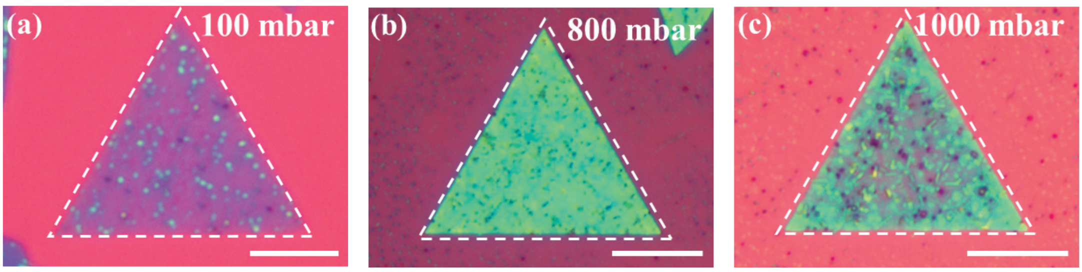

Fig. S3 Pressure dependent morphology evolution of $CsPbI_3$ on monolayer WSe_2 at growth pressure of **(a)** 10 kPa; **(b)** 80 kPa; **(c)** 101 kPa. Scale bars are 10 μm in (a–c).

The layered structure of the WSe_2 substrate exhibits sixfold in-plane symmetry with a lattice constant of 3.286 Å. For cubic $CsPbI_3$ nanowire, lattice constant of *a* and *b* equals to 6.289 Å. Here the lattice mismatch between $CsPbI_3$ and WSe_2 is defined as the factor $f = (1 - d_{substrate}/d_{overlayer}) \times 100\%$[1], where d is the plane distance. For zigzag grown $CsPbI_3$ nanowires, we find that

21*WSe_2[$\bar{1}100$]≈11*$CsPbI_3$[001] and 6*WSe_2[$11\bar{2}0$] ≈5*$CsPbI_3$[110]. Thus, the obtained lattice mismatch factor along and perpendicular to the zigzag direction is calculated to be 0.2% and 2.3%, respectively. For armchair grown $CsPbI_3$ nanowires, we find that 5*WSe_2[$11\bar{2}0$]≈3*$CsPbI_3$[001] and 4*WSe_2[$\bar{1}100$] ≈3*$CsPbI_3$[110]. Therefore, the obtained lattice mismatch factor along and perpendicular to the armchair direction is calculated to be 0.5% and 1.4%, respectively.

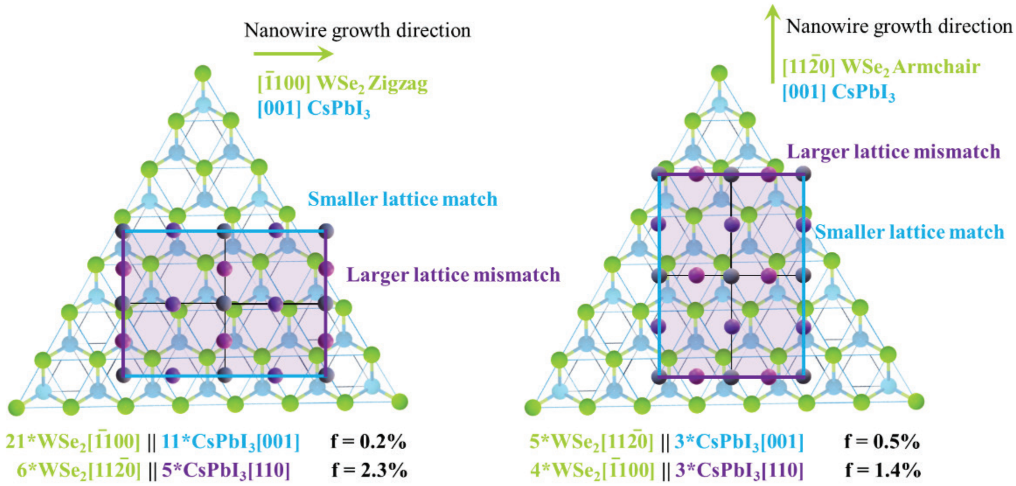

Fig. S4 Atomic model of lattice mismatch between the $CsPbI_3$ nanowire and the WSe_2 surface along different directions.

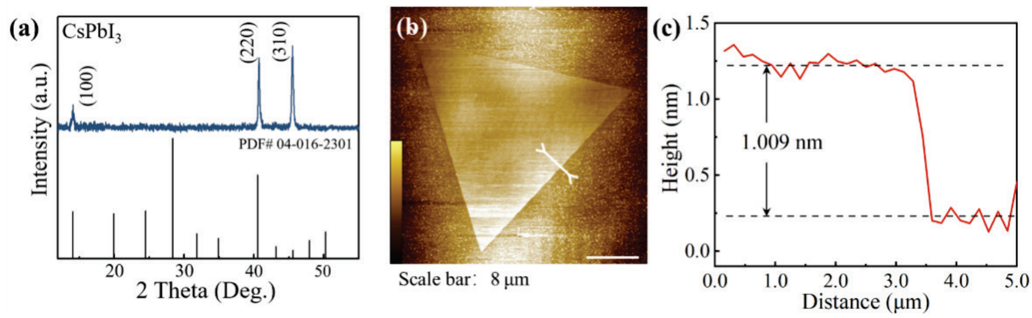

Fig. S5 (a) XRD spectrum of as-grown $CsPbI_3$ on WSe_2. Standard XRD pattern for cubic phase of $CsPbI_3$ is inserted at the bottom. **(b)** AFM image and **(c)** height profile of the as-grown monolayer WSe_2.

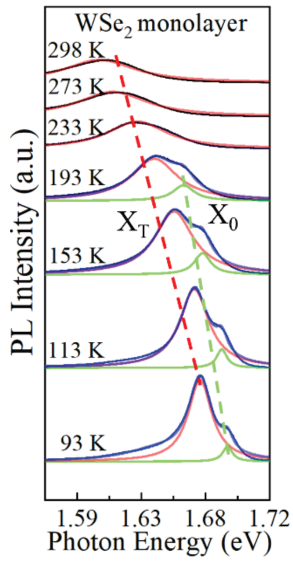

Fig. S6 Temperature-dependent PL spectra of a monolayer WSe_2.

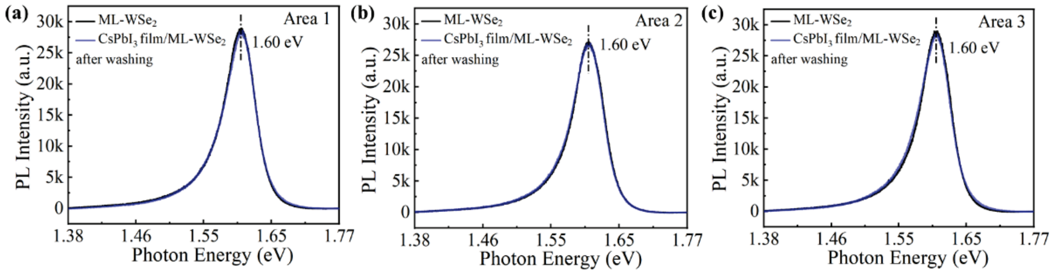

Fig. S7 PL emission comparisons of monolayer WSe_2 before $CsPbI_3$ growth and $CsPbI_3$ nanofilm/WSe_2 heterojunction after removing $CsPbI_3$ by water washing. PL spectra in **(a–c)** are collected at three different areas.

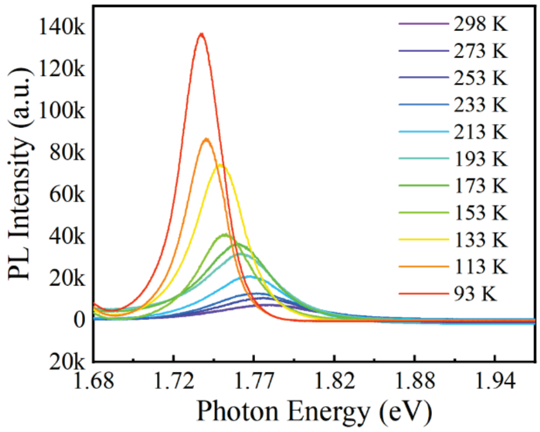

Fig. S8 Temperature-dependent PL spectra of armchair oriented $CsPbI_3$ NW/WSe_2.

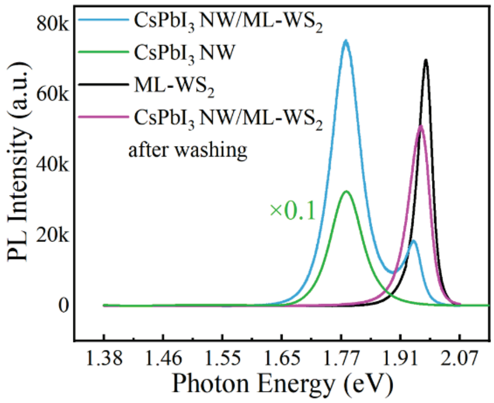

Fig. S9 PL emission comparisons of $CsPbI_3$/WS_2 heterojunction, $CsPbI_3$ NW, WS_2 and $CsPbI_3$/WS_2 heterojunction after removing $CsPbI_3$ by water washing.

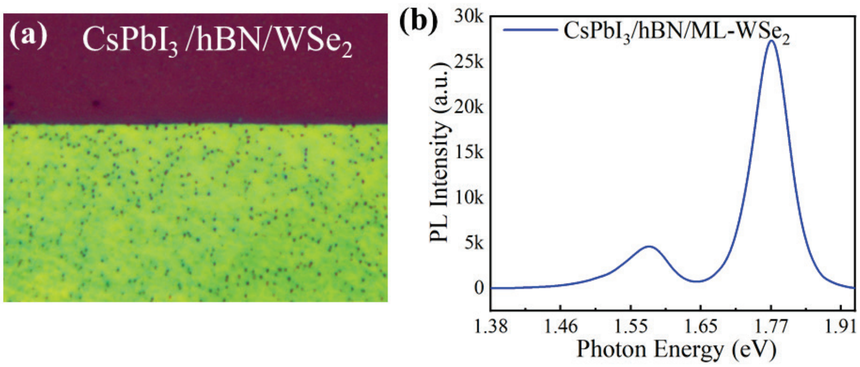

Fig. S10 Formation of $CsPbI_3$ nanostructure on the surface of transferred hBN on monolayer WSe_2. PL spectra of as grown $CsPbI_3$ film on the surface of transferred h-BN on monolayer WSe_2.

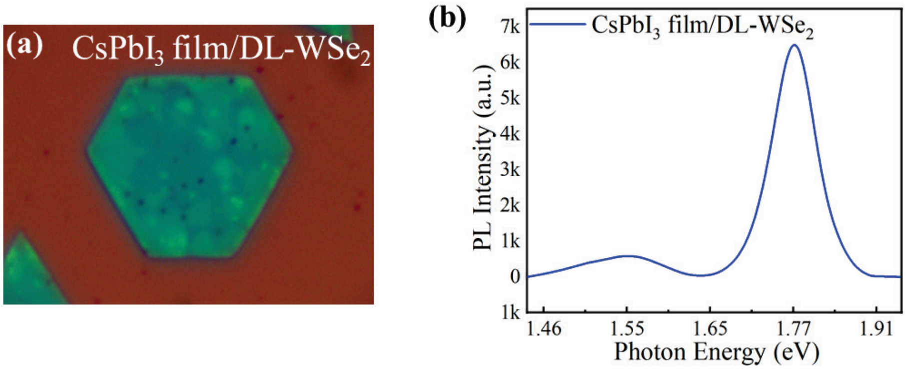

Fig. S11 (a) Formation of $CsPbI_3$ nanostructure on -bilayer WSe_2. **(b)** PL spectra of as grown $CsPbI_3$ film on the surface of double layers WSe_2.

References

1. A. Trampert, O. Brandt, and K. Ploog, Crystal Structure of Group III Nitrides, Elsevier, p. 167, 1997