Anomalously polarised emission from MoS_2/WS_2 heterostructure

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Supplementary Information

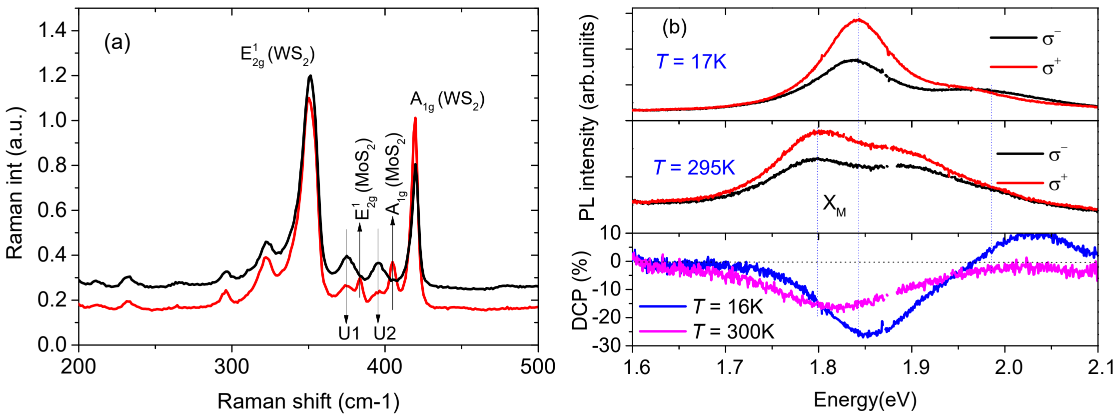

Figure S1. (a) Normalized Raman signal from the top (red) and edge (black) of the HS sample. (b) Helicity resolved PL spectra obtained from the MoS_2/WS_2 HS with 532 nm, circularly polarized (σ^-) excitation at $T = 17$ K (top panel) and $T = 295$ K (middle panel). Degree of polarization (DCP) at $T = 17$ K and $T = 295$ K (Bottom panel) obtained with σ^- excitation of the MoS_2/WS_2 HS with 532 nm light.

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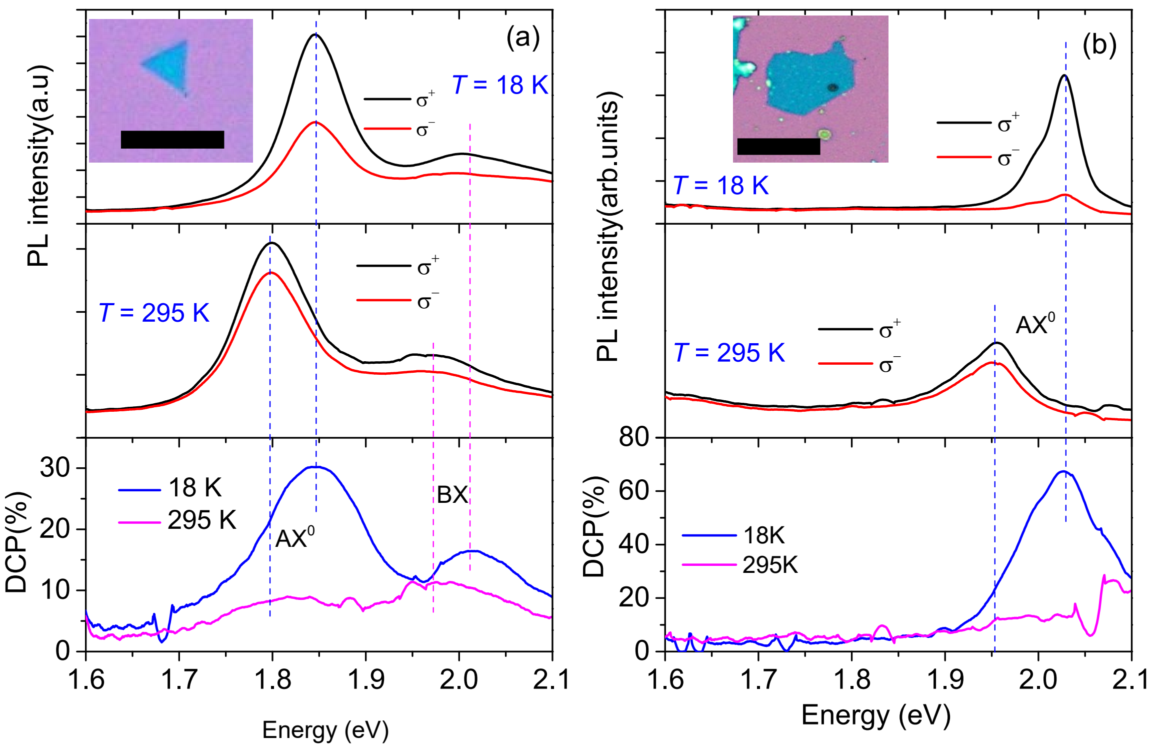

Figure S2. (a) Helicity resolved PL spectra obtained from the ML MoS_2 with 532 nm, circularly polarized (σ^+) excitation at T = 18 K (top panel) and T = 295 K (middle panel) and the corresponding degree of polarization (DCP) (Bottom panel). (b) Data, same as in (a), obtained for the 3L WS_2 sample. The insets of the top panels show the optical images of the flakes. The scale bar is 10 µm.

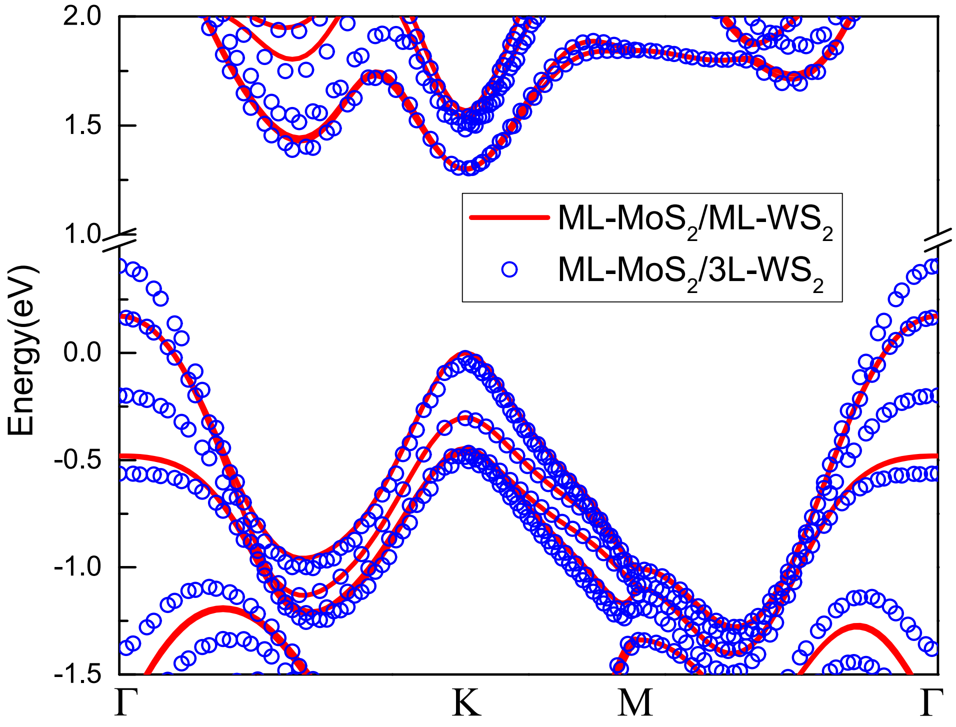

Figure S3. Calculated band structure of heterostructures with ML MoS_2-ML WS_2 (red line) and ML MoS_2-3L WS_2 (blue open symbols).

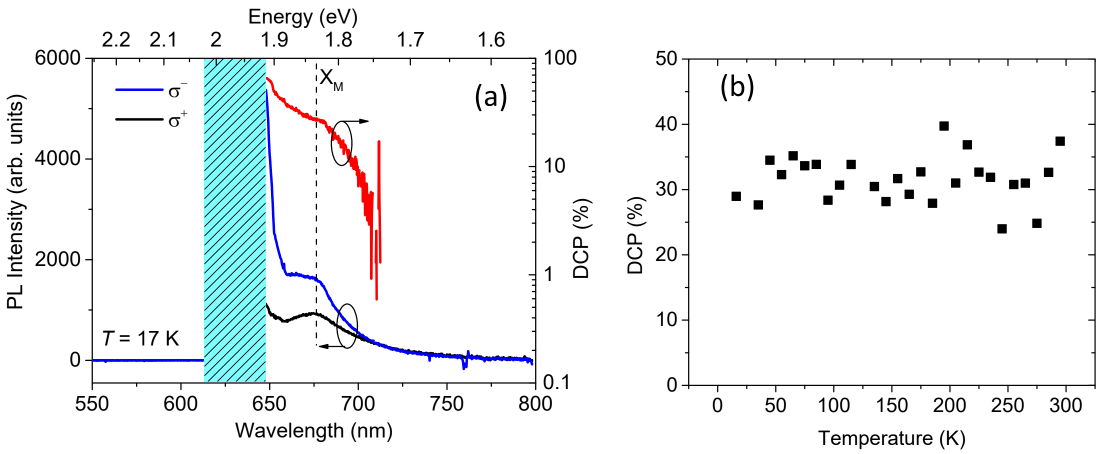

Figure S4. (a) Helicity resolved PL spectra and degree of polarization (DCP) obtained from the MoS_2/WS_2 HS with 633 nm, circularly polarized (σ^-) excitation at T = 17 K. The shaded blue region indicated the stopband of the filter used to block the laser light from reaching the detector. (b) DCP near the X_M obtained from the HS with 633 nm excitation as a function of temperature.

Supplementary Note 1:

Fully relativistic calculations within the density functional theory (DFT) were employed using the Quantum-ESPRESSO package. [1] The calculations were performed with the projector-augmented wave (PAW) scheme.[2]The Perdew-Burke-Ernzerhof (PBE) [3] parameterization of the generalized gradient approximation (GGA) was used for the exchange-correlation potentials with a plane-wave cutoff of 400 eV and a 12×12×1 *k*-point mesh. The van der Waals interactions were taken into account through the DFT- D2 dispersion correction.[4][5] The spin-orbit interaction was also included in the calculation. A vacuum of 20 A^o thickness was added in the vertical direction to avoid spurious interactions between adjacent slabs. The structural optimization was continued until the residual forces have converged to less than 2.57 x 10^{-2} eV/A^o and the total energy to less than 1.36x10^{-3} eV.

Supplementary References:

[1] Giannozzi P, Baroni S, Bonini N, Calandra M, Car R, Cavazzoni C, Ceresoli D, Chiarotti G L, Cococcioni M, Dabo I, Dal Corso A, De Gironcoli S, Fabris S, Fratesi G, Gebauer R, Gerstmann U, Gougoussis C, Kokalj A, Lazzeri M, Martin-Samos L, Marzari N, Mauri F, Mazzarello R, Paolini S, Pasquarello A, Paulatto L, Sbraccia C, Scandolo S, Sclauzero G, Seitsonen A P, Smogunov A, Umari P and Wentzcovitch R M 2009 QUANTUM ESPRESSO: A modular and open-source software project for quantum simulations of materials *J. Phys. Condens. Matter* **21** 395502

[2] Kresse G and Joubert D 1999 From ultrasoft pseudopotentials to the projector augmented-wave method *Phys. Rev. B* **59** 1758–75

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[4] Grimme S 2006 Semiempirical GGA-type density functional constructed with a long-range dispersion correction *J. Comput. Chem.* **27** 1787–99

[5] Barone V, Casarin M, Forrer D, Pavone M, Sambi M and Vittadini A 2009 Role and effective treatment of dispersive forces in materials: Polyethylene and graphite crystals as test cases *J. Comput. Chem.* **30** 934–9