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Supporting Information

Valley splitting in the antiferromagnetic heterostructure $MnPSe_3/WSe_2$

Bing-Jie Wang[1,ξ], Yu-Yun Sun [1,ξ], Ju Chen[1], Weiwei Ju[4], Yi-Peng An[5], Shi-Jing Gong[1,2,3,*]

[1]*Department of optoelectrics, School of Physics and Electronic Science, East China Normal University, Shanghai, 200241, China*

[2]*Collaborative Innovation Center of Extreme Optics, Shanxi University, Taiyuan, Shanxi, 030006, China*

[3]*Shanghai Institute of Intelligent Electronics & Systems, Fudan University, Shanghai 200433, China*

[4]*College of Physics and Engineering and Henan Key Laboratory of Photoelectric Energy Storage Materials and Applications, Henan University of Science and Technology, Luoyang, 471023, China*

[5]*School of Physics and Henan Key Laboratory of Boron Chemistry and Advanced Energy Materials, Henan Normal University, Xinxiang, 453007, China*

[ξ] *B –J Wang and Y-Y Sun contributed equally to this work*

** E-mail: sjgong@ee.ecnu.edu.cn*

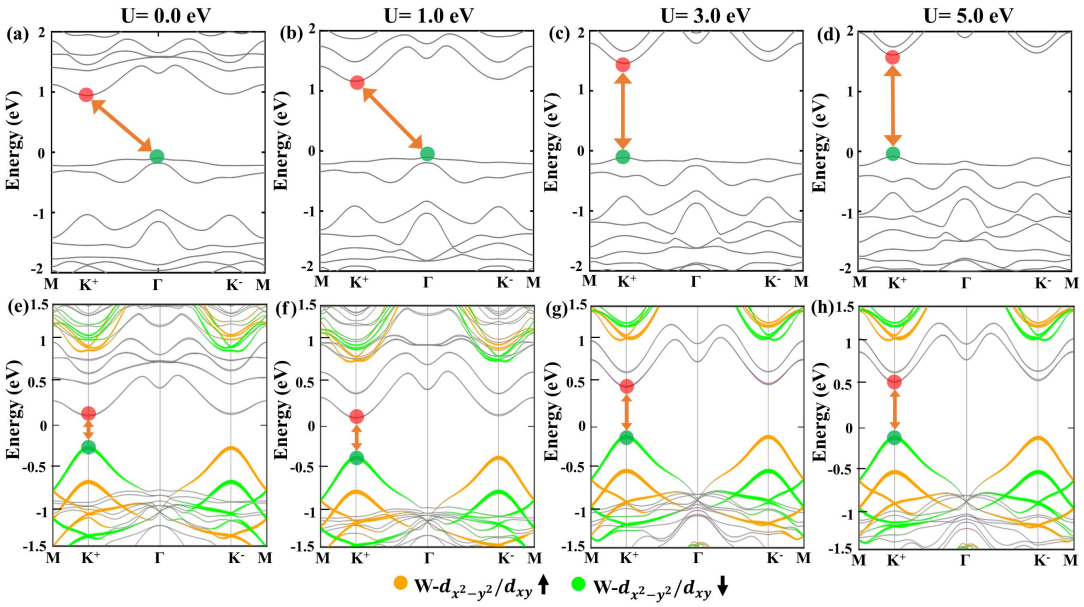

Fig. S1 Band structures of (a-d) $MnPSe_3$ monolayer and (e-h) $MnPSe_3/WSe_2$ heterostructure with spin orbit coupling (SOC), which are all based on GGA+U method with (a, e) U=0.0 eV, (b, f) U=1.0 eV, (c, g) U=3.0 eV and (d, h) U=5.0 eV.

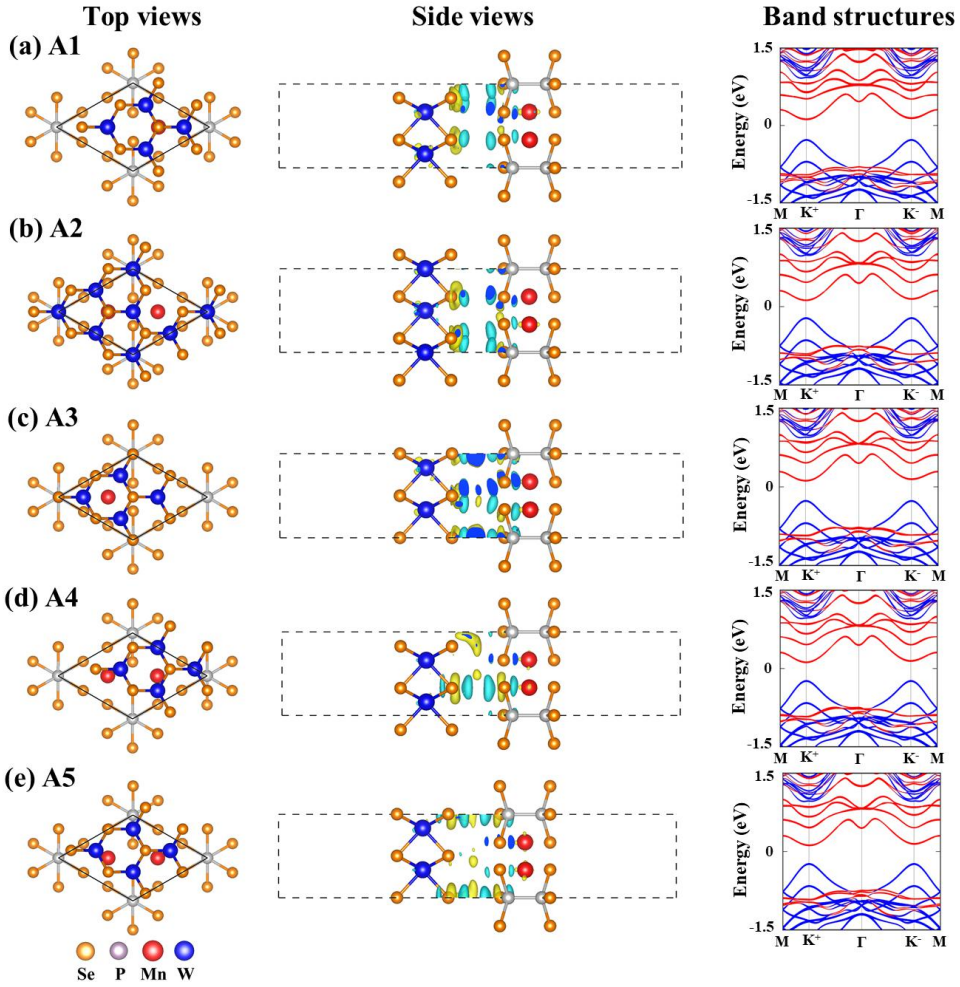

Fig. S2 Structures and side views of the charge density difference of $MnPSe_3/WSe_2$ heterostructures. Yellow (blue) regions represent the net charge gain (loss), and the isosurface value is 1.2 e/nm^3. The corresponding band structures are shown in the right figures, in which blue and red lines represent the states of WSe_2 and $MnPSe_3$ layers, respectively.

Table S1. Calculated binding energy E_b (meV), the interlayer distance d (Å) and valley splitting (meV) of $MnPSe_3/WSe_2$ heterostructures with different stacking models.

Stacking models	A1	A2	A3	A4	A5
d (Å)	3.500	3.507	3.468	3.447	3.439
E_b (meV)	-634.5	-613.9	-646.3	-629.0	-629.4
Valley splitting (meV)	35.4	35.0	40.0	37.0	36.9