Supporting Information

Defects and interfacial/surface synergistically Modulated electron transfer and nonlinear absorption properties in MoX2 (X=Se, S, Te) @ZnO Heterojunction

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1. Experimental parameters of sample preparation

1.1 MoX_2 nanoflowers： By controlling the time and temperature of hydrothermal reaction, we obtained MoX_2 nanoflower materials. Three kinds of $MoSe_2$ were obtained at 12 h by setting the preset temperature at 180 ℃, 220 ℃ and 260 ℃, respectively. At 220 ℃, two $MoSe_2$ materials were obtained by changing the reaction time, in which the reaction time was 12 h and 24 h respectively. MoS_2 was prepared under reaction conditions of 24 h and 200 ℃. At 200 ℃, $MoTe_2$ was obtained by setting the reaction time to 24 h and 48 h respectively.

1.2 MoX_2@ZnO composite materials： $MoSe_2$@ZnO composite was obtained at 60W and 0.5h, and sputtering time was set at 100 ℃, 200 ℃ and 300 ℃, respectively, in which $MoSe_2$ was prepared at 200℃ and 24h. Under the conditions of 1 h and 150 ℃, MoS_2@ZnO composite material was obtained by changing the sputtering power, in which the power was 50 W, 100 W and 150 W, respectively. $MoTe_2$ obtained at 200 ℃ and 24 h was used as the base. $MoTe_2$@ZnO composite was prepared at 60 W and 150 ℃ with sputtering time of 0.5 h, 1 h and 1.5 h, respectively.

In this paper, $MoSe_2$ obtained at 220 ℃, 24 h and $MoSe_2$@ZnO prepared at 100 ℃ were selected as the research objects. The MoS_2 obtained at 200 ℃, 24 h and MoS_2@ZnO prepared at 100 W sputtering power were studied. The $MoTe_2$ prepared at 200 ℃, 24 h and $MoTe_2$@ZnO prepared at 1 h sputtering time were analyzed.

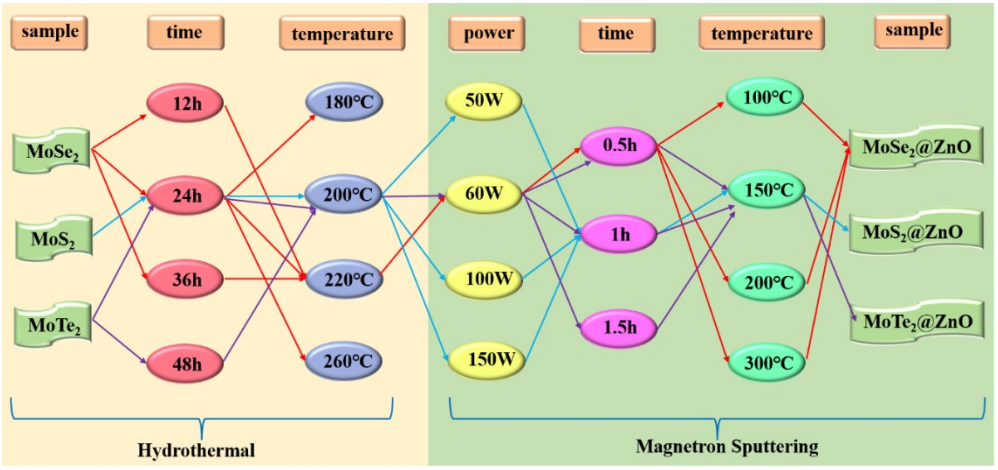

Fig. S1 Experimental parameters of MoX_2 and MoX_2@ZnO.

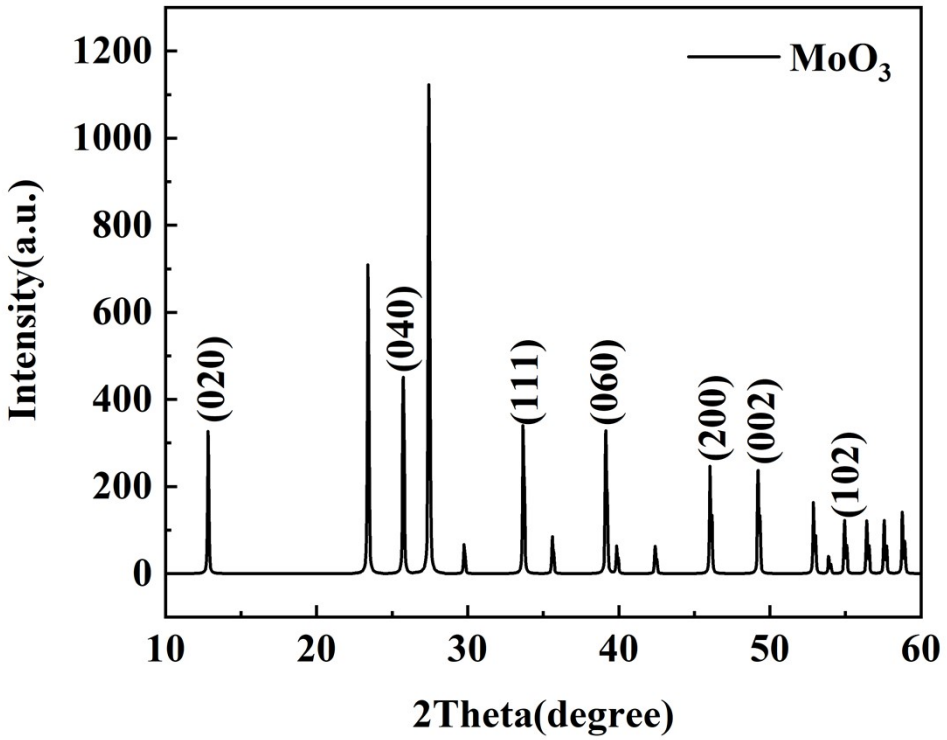

Fig. S2 XRD pattern of MoO_3 (JCPDS card number 1-706).

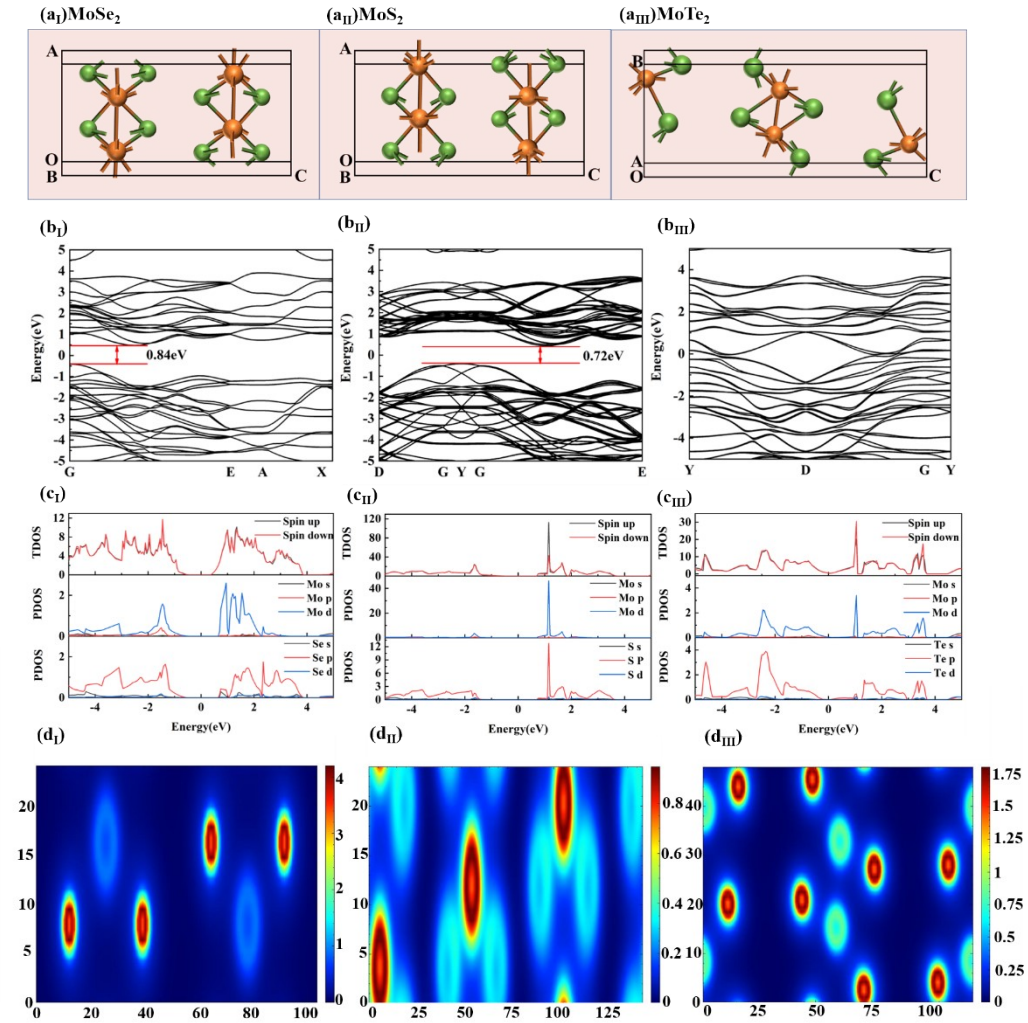

Fig. S3 (a) Original cell model of the electronic structure of MoX_2, (b) energy band, (c) density of stateand (d) charge density.

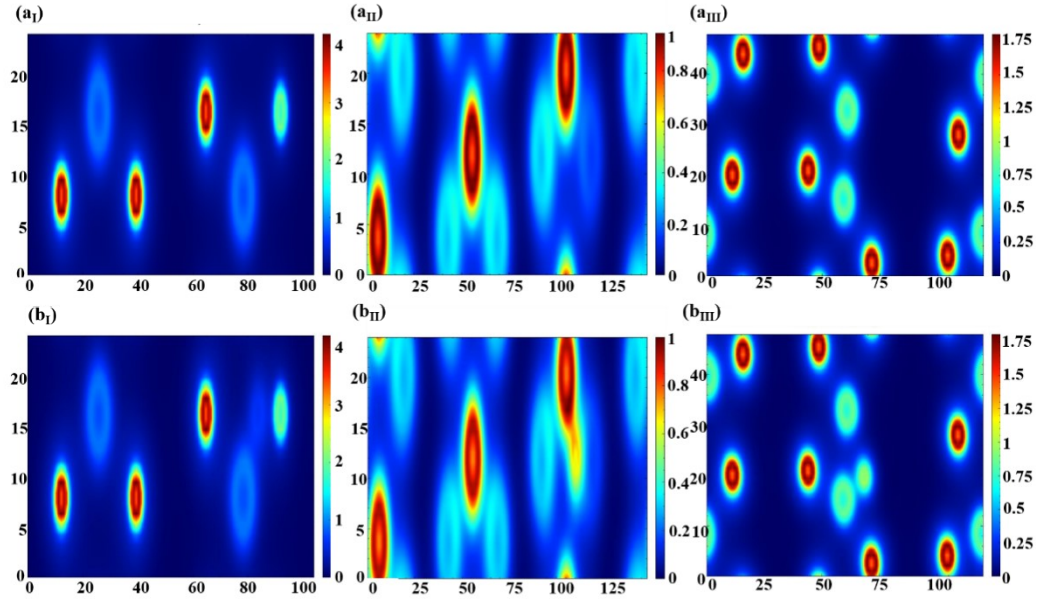

Fig. S4 (a) The charge density of the electronic structure of MoX_2 with chalcogenide vacancy defects.

(b) The charge density of the O atom entering the electronic structure of the MoX_2 lattice.