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 MoX2 nanoflowers: By controlling the time and temperature of hydrothermal reaction, we obtained MoX2 nanoflower materials. Three kinds of MoSe2 were obtained at 12 h by setting the preset temperature at 180 °C, 220 °C and 260 °C, respectively. At 220 °C, two MoSe2 materials were obtained by changing the reaction time, in which the reaction time was 12 h and 24 h respectively. MoS2 was prepared under reaction conditions of 24 h and 200 °C. At 200 °C, MoTe2 was obtained by setting the reaction time to 24 h and 48 h respectively.

1.2 MoX2@ZnO composite materials: MoSe2@ZnO composite was obtained at 60W and 0.5h, and sputtering time was set at 100 °C, 200 °C and 300 °C, respectively, in which MoSe2 was prepared at 200°C and 24h. Under the conditions of 1 h and 150 °C, MoS2@ZnO composite material was obtained by changing the sputtering power, in which the power was 50 W, 100 W and 150 W, respectively. MoTe2 obtained at 200 °C and 24 h was used as the base. MoTe2@ZnO composite was prepared at 60 W and 150 °C with sputtering time of 0.5 h, 1 h and 1.5 h, respectively.

In this paper, MoSe2 obtained at 220 °C, 24 h and MoSe2@ZnO prepared at 100 °C were selected as the research objects. The MoS2 obtained at 200 °C, 24 h and MoS2@ZnO prepared at 100 W sputtering power were studied. The MoTe2 prepared at 200 °C, 24 h and MoTe2@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 state and (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.