Synthesis of 2D $MoS_{2(1-x)}Se_{2x}$ Semiconductor Alloy by Chemical Vapor Deposition Supporting Information

Experiments: The growth of $MoS_{2(1-x)}Se_{2x}$ sheets was performed in a three-temperature zone CVD system using 2.5-inch quartz tubes in a 30-inch horizontal furnace, as shown in Figure 1(a).We used a P-type 100 crystalline silicon substrate with SiO_2 thickness of 275 microns.After the silicon substrate is cut into small pieces, it is shaken with 99.7% anhydrous ethanol and distilled water, and then blow-dried with argon gas.The selenium, sulfur, molybdenum trioxide precursors and Si tablets loaded by ceramic vessels were placed upstream (350, 250℃) and downstream (850℃) of the furnace area respectively.When S source position is 0, the relative positions of Se substrate, MoO_3 substrate and Si substrate are 25cm, 47cm and 70cm respectively.In the experiment, the Si substrate was placed directly above the MoO_3 vessel and the third temperature zone of the tubular furnace.We use different shades of red for different temperatures.At the beginning of the experiment, the furnace body was heated to 650℃ at a speed of 10℃/min, 200 sccm 9 torr, and selenium was heated to 350℃ and sulfur to 250℃ respectively through heating belt.When the furnace temperature reaches 850℃, the imported gas argon brings the vaporized selenium, sulfur and molybdenum trioxide to the substrate during the deposition process.After growing, the furnace is cooled to room temperature. In the experiment, the cooling process of the tubular furnace is shown in Fig. SI. 1.At the beginning of the cooling, the cooling rate is faster, because of the larger temperature difference between the room temperature and the furnace.As the furnace temperature decreases, the temperature difference decreases and the cooling rate slows down until the room temperature.

XPS characterization The XPS diagram of S 2p and Se3d orbitals changing with doping concentration as shown in the Fig. SI. 2. The binding energy of both S 2p orbital and Se 3d orbital increases with doping concentration, which is in accordance with the law that the band gap energy value increases from MoS_2 to $MoSe_2$. The 3D Se layer is full of shells and does not participate in electron hybridization.However, with the increase of Se doping concentration, the interaction between Se atoms is enhanced, and the nucleus has a stronger binding ability to 3d electrons.As the S 3p orbital increases with the doping concentration, the contribution to the conduction band and valence band decreases (as can be seen from Figure 5). The electrons involved in the interaction are confined around the atom, so the binding energy is enhanced.

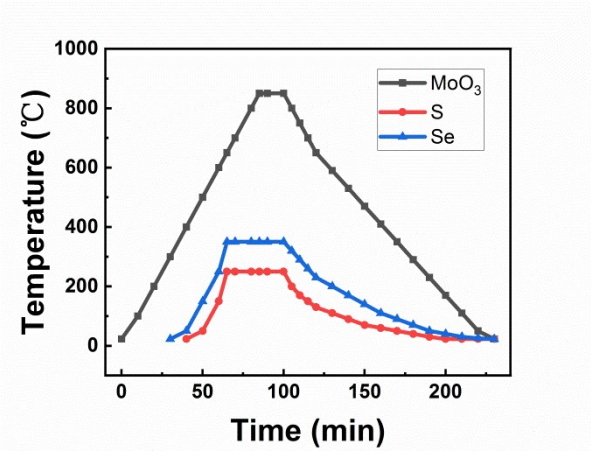

Fig. SI. 1 Cooling rate diagram of the tube furnace during experiment

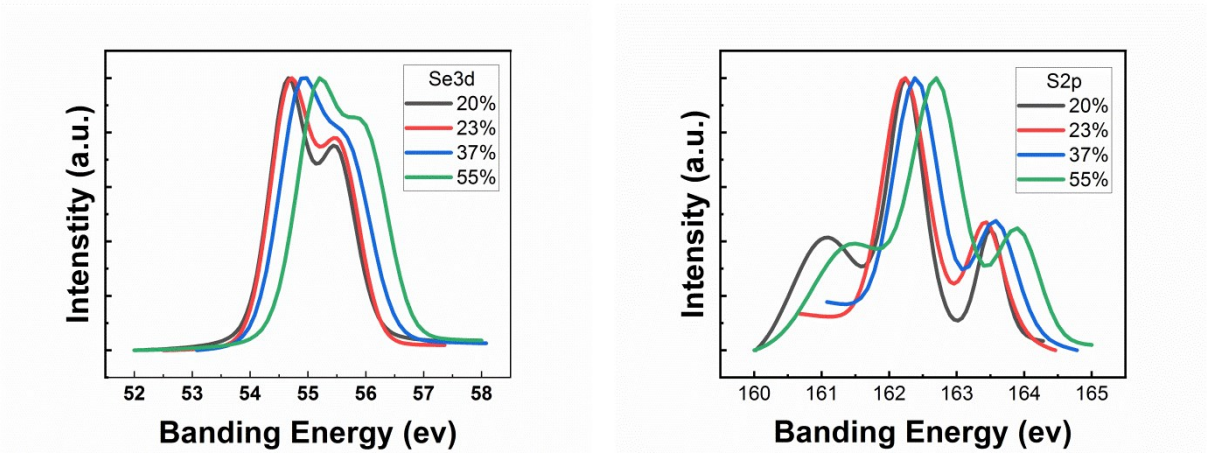

Fig. SI. 2 Energy diagram of Se 3d and S 2p orbitals with different doping densities