

Supplementary Materials

First-principles analysis of photocurrent in monolayer α -selenium p - n junctions optoelectronic device

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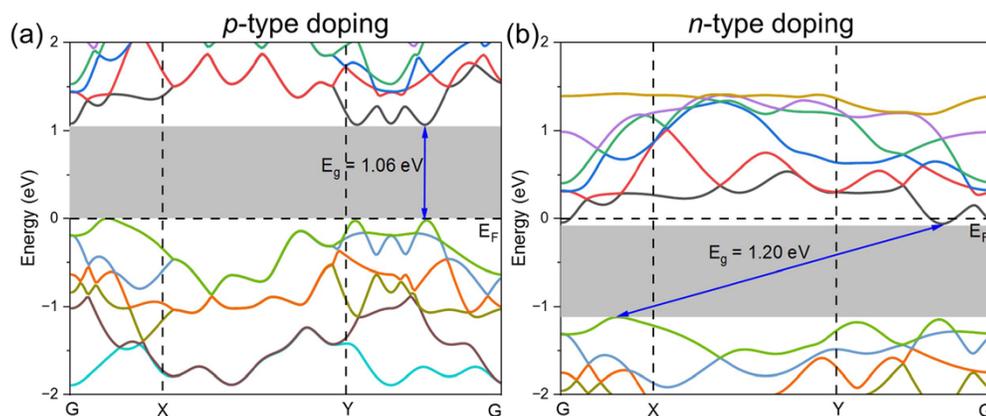


Fig. S1 Band structure of the monolayer (ML) α -selenium with (a) p - and (b) n -doping (doping concentration is $8.21 \times 10^{14} \text{ cm}^{-2}$).

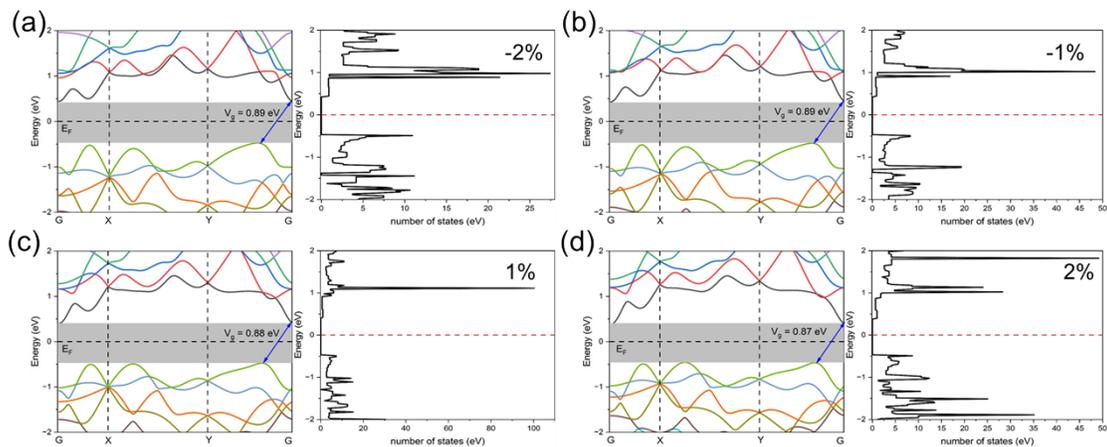
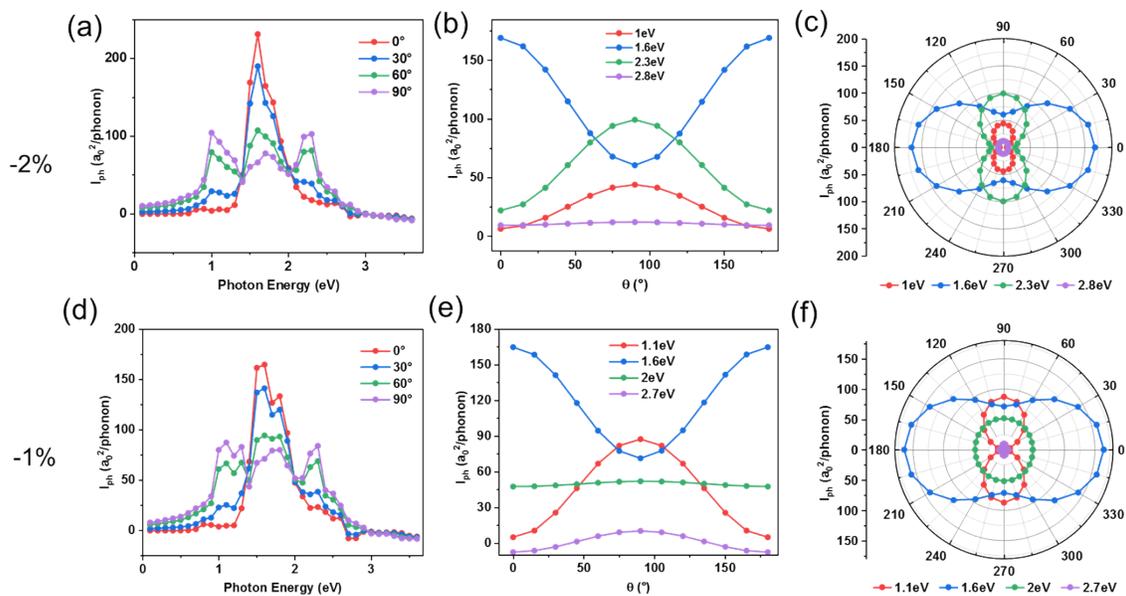


Fig. S2 Band structure and density of state of the ML α -selenium with different stress (a) -2%, (b) -1%, (c) 1%, and (d) 2%.



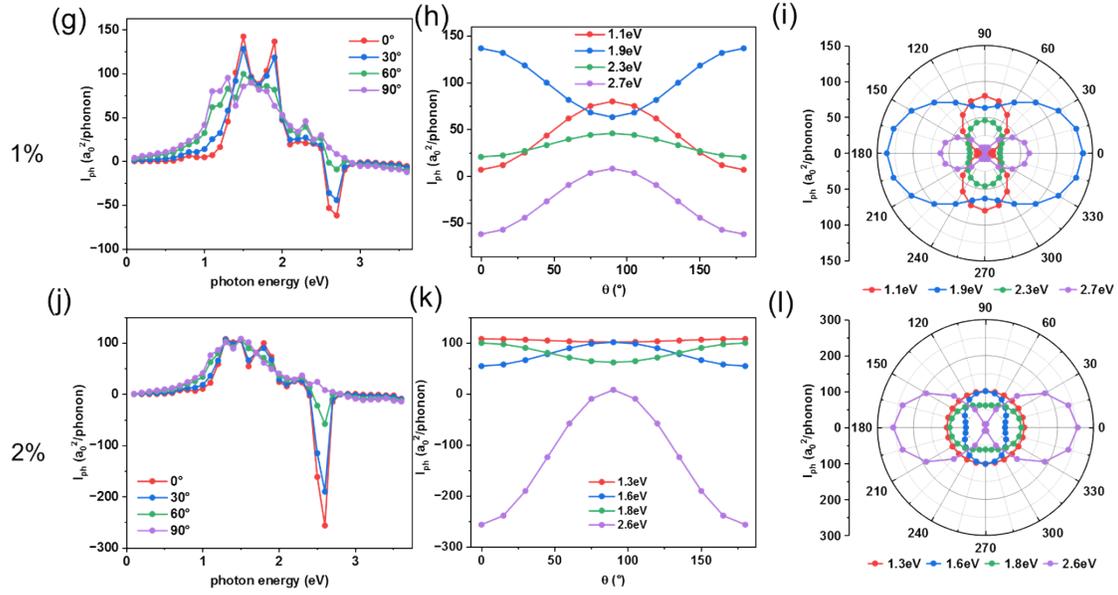


Fig. S3 Strain-dependent photoresponsivity of the ML α -selenium p - n junction optoelectronic device along ARM directions under different photon energies and linearly polarized direction (a) -2%, (g) -1%, (d) 1%, and (j) 2%. Strain-dependent photoresponsivity value of the ML α -selenium p - n junction optoelectronic device under different photon energy as a function of linearly polarized direction along the ARM direction direction (b)(c) -2%, (h)(i) -1%, (e)(f) 1%, and (k)(l) 2%.

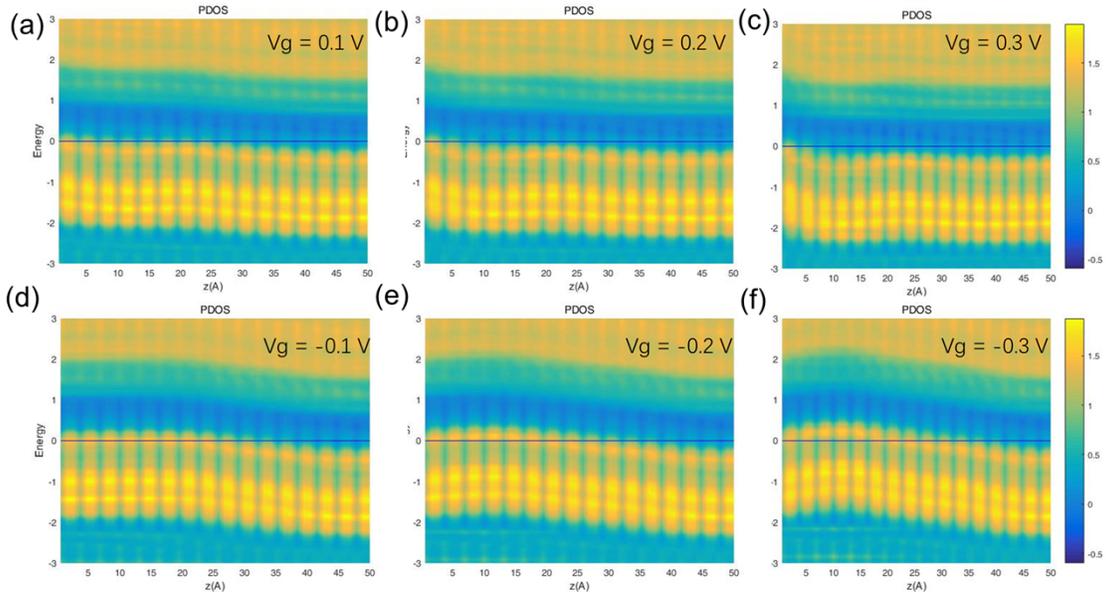


Fig. S4 Local device density of states (PDOS) of the ML selenium p - n junctions optoelectronic device under different gate voltage V_g .