Supporting information

NO₂ physical-to-chemical adsorption transition on Janus WSSe monolayers realized by defect introduction

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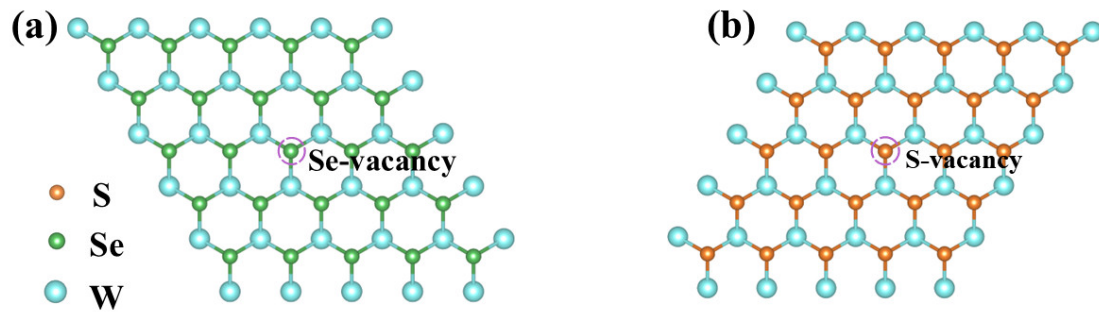
Figure S1. The location of Se (a) and S vacancy defects (b) considered in our study, which is circled by purple dashed line.
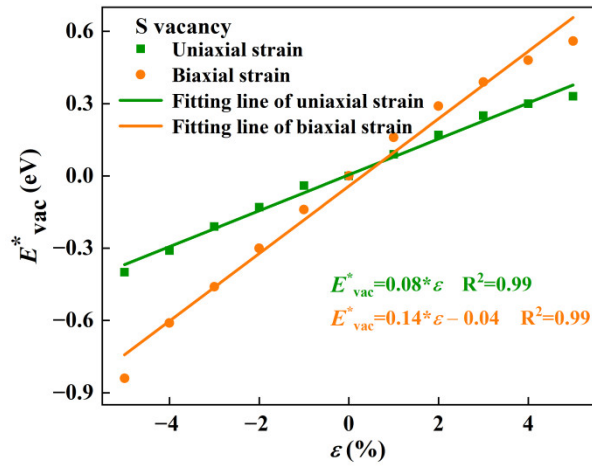

Figure S2. The relative E^*_{vac} of S vacancy under the different uniaxial (blue) and biaxial strains (orange). The value of E^*_{vac} under no strain is selected as a reference value.

Table S1. The adsorption energy of NO_2 gas molecules on pristine and defective Janus WSSe monolayer.

WSSe	Adsorption energy
Pristine	-0.56 eV
Defective	-3.53 eV

Table S2. The calculated charge of one Se atom from Janus WSSe monolayer under -10% , 0 and 10% strain.

Strain	Charge
-10%	6.41 e
0	6.44 e
10%	6.46 e