Supplementary Information for

Effect of $MoSe_2$ nanoribbons with NW30 edge reconstructions on electronic and catalytic properties by strain engineering

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Table S1 Free energy (ΔG_{H^*}) of one hydrogen atom adsorbed on different sites of three systems with and without critical tensile strain.

		ZZSe-GB4-Se	ZZSe-Mo-NW30	NW30
without strain	site 1	0.339	0.280	−0.534
	site 2	−0.172	−0.497	−0.332
	site 3	0.216	−0.035	/
with strain	site 1	−0.019	0.151	-0.884
	site 2	−0.375	−0.576	-0.861
	site 3	−0.050	−0.061	/

Table S2 Free energy (ΔG_{H^*}) of second hydrogen atom adsorbed on different sites of three systems with and without critical tensile strain.

		ZZSe-GB4-Se	ZZSe-Mo-NW30	NW30
without strain	site 1	0.630	−0.489	−0.299
	site 2	0.545	−0.240	−0.823
with strain	site 1	0.232	−0.971	−0.569
	site 2	0.265	−0.277	−0.709

Table S3 The energy differences between initial and transition or final states for ZZSe-Mo-NW30, ZZSe-GB4-Se and ZZMo-NW30 $MoSe_2$ edges in Tafel and Heyrovsky reactions.

		ZZSe-Mo-NW30	ZZSe-GB4-Se	ZZMo-NW30
Tafel	ΔE_1	0.40	1.61	0.49
	ΔE_2	0.05	0.34	0.18
Heyrovsky	ΔE_1	−0.84	−0.41	−0.02
	ΔE_2	−1.40	−1.11	−0.67

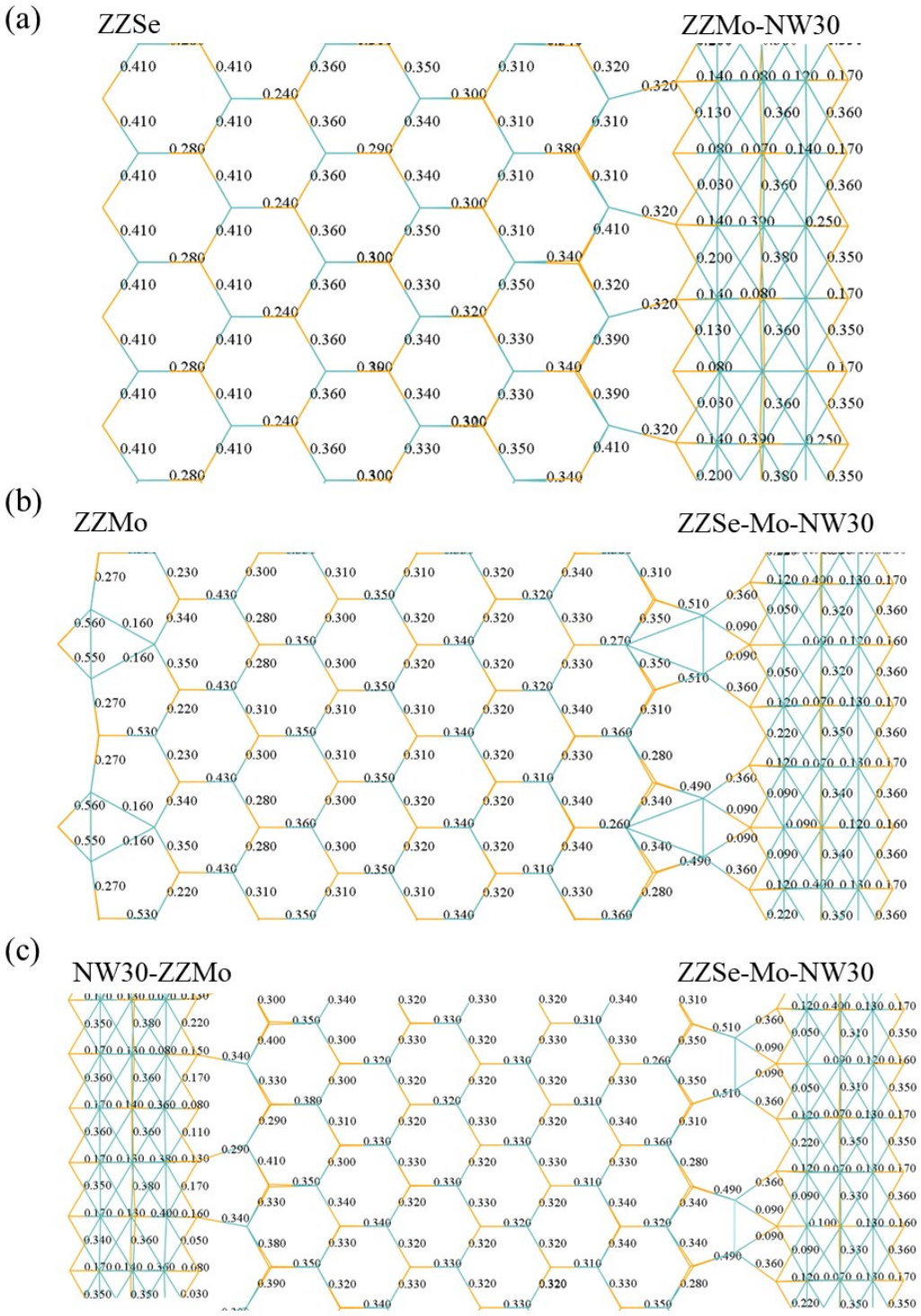

Fig. S1 Mulliken bond population analysis of three different $MoSe_2$ nanoribbons. The values of bond population are labeled by black. In pristine $MoSe_2$ monolayer, the bond population is about 0.32.

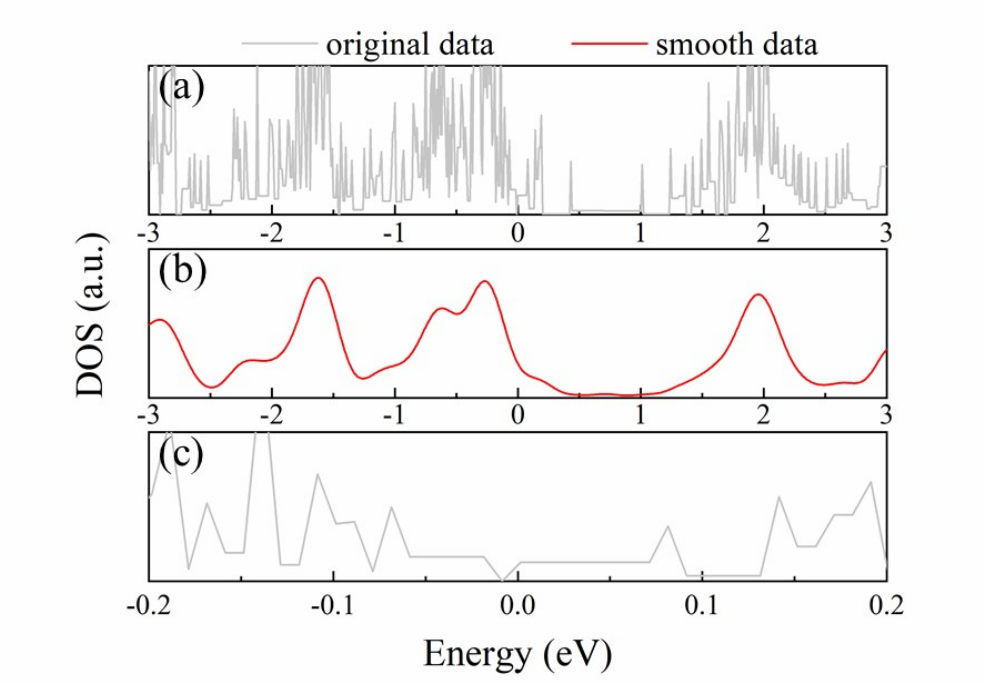

Fig. S2 The PDOS of NW30 nanowire with ε = 7% (a) original data (b) smooth data with the energy range from −3 eV to 3 eV. (c) original data with the narrowed energy range from −0.2 eV to 0.2 eV.

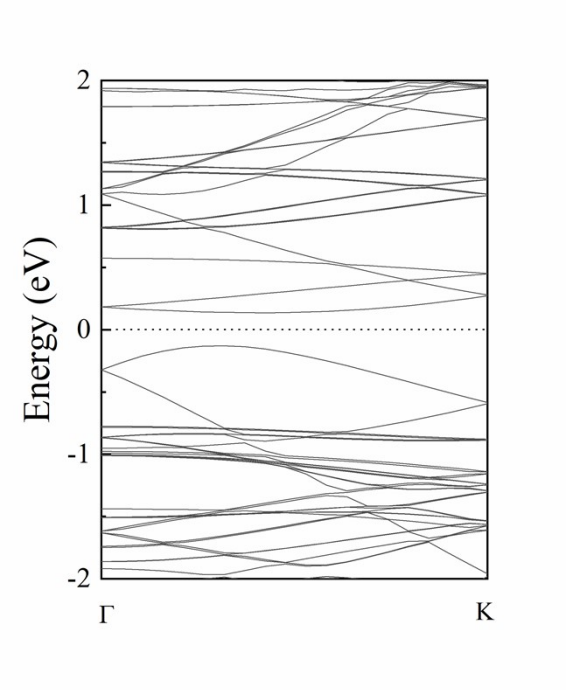

Fig. S3 The electronic band structure of perfect NW30 nanowire with the energy range from −2 eV to 2 eV using HSE06 hybrid functional and open the band gap of 0.27 eV.

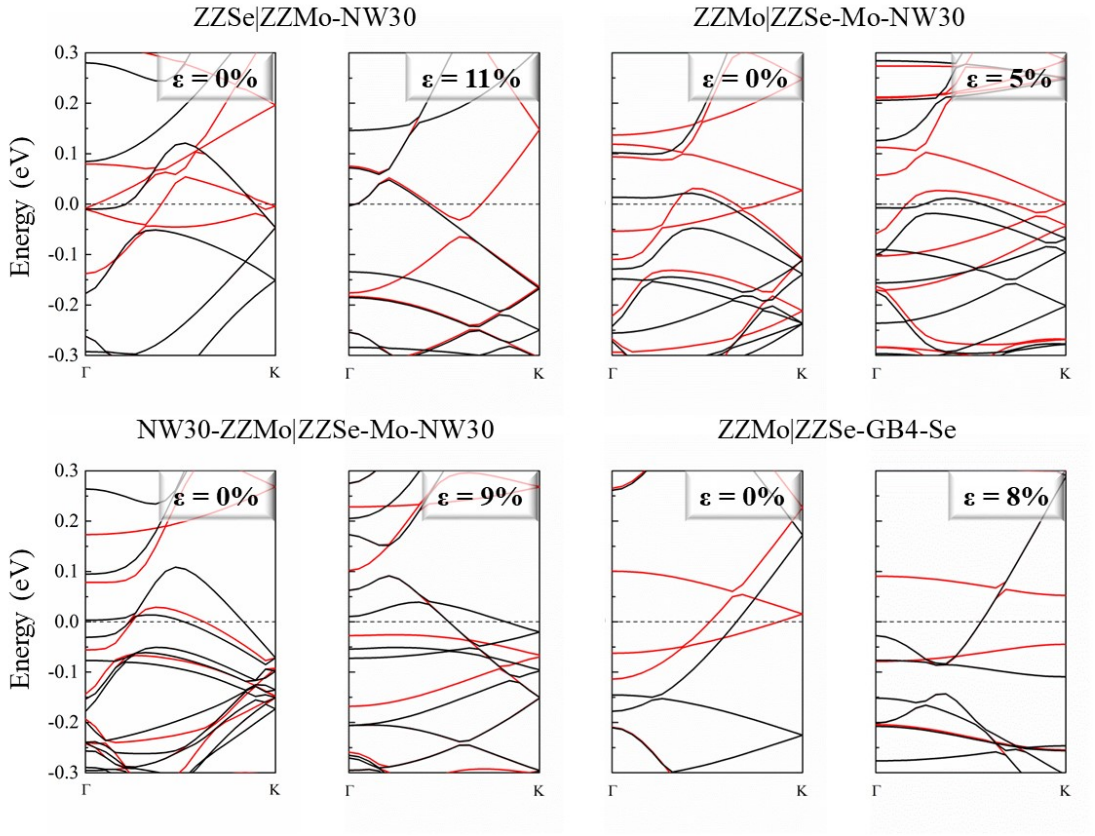

Fig. S4 Electronic band structure of four different $MoSe_2$ nanoribbons with and without critical tensile strain and the energy range from −0.3 eV to 0.3 eV. The spin-up and spin-down states are shown in red and black, respectively. The Fermi energy is shifted to zero.

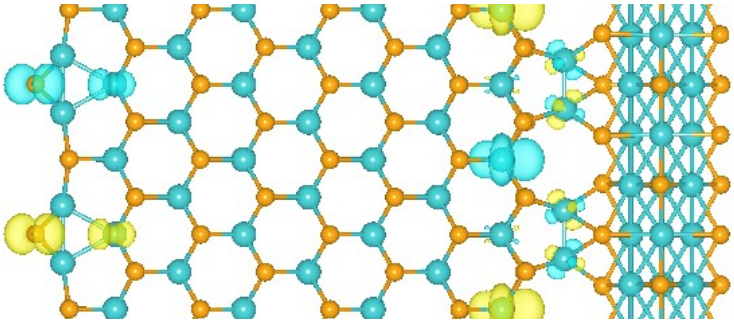

Fig. S5 Spin densities of ZZMo|ZZSe-Mo-NW30 nanoribbon with antiferromagnetic (AFM) state. The yellow and cyan surfaces represent charge densities of spin-up and spin-down states, respectively, with isosurface of 0.002 e/Å^3. The AFM is non-stable and the energy of AFM state is higher than Ferromagnetic (FM) state about 0.03 eV.

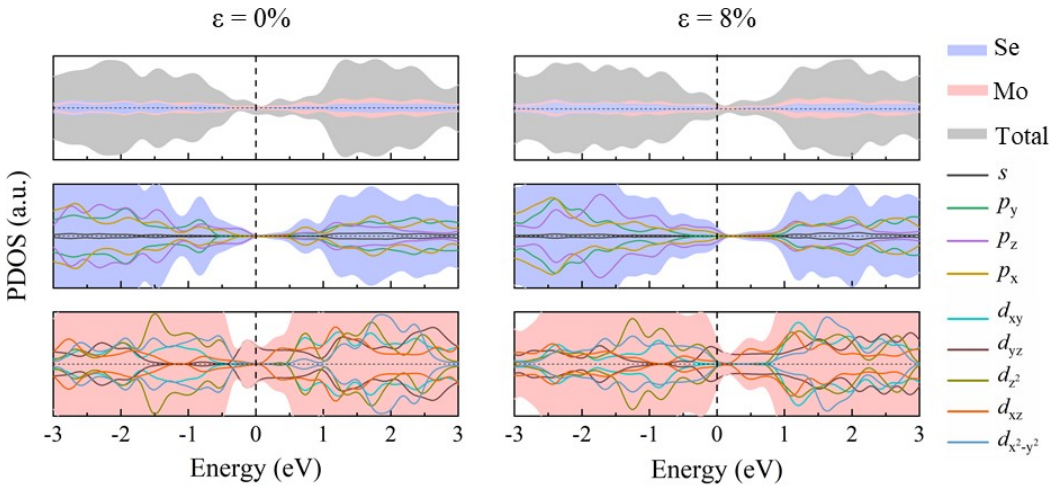

Fig. S6 Partial densities of states of ZZMo|ZZSe-GB4-Se nanoribbon with ε = 0% and 8% critical tensile strain. Blue, red and gray regions represent for the projected Se, Mo atoms and total system, respectively. The Fermi level is set as zero and shown as a dashed line.

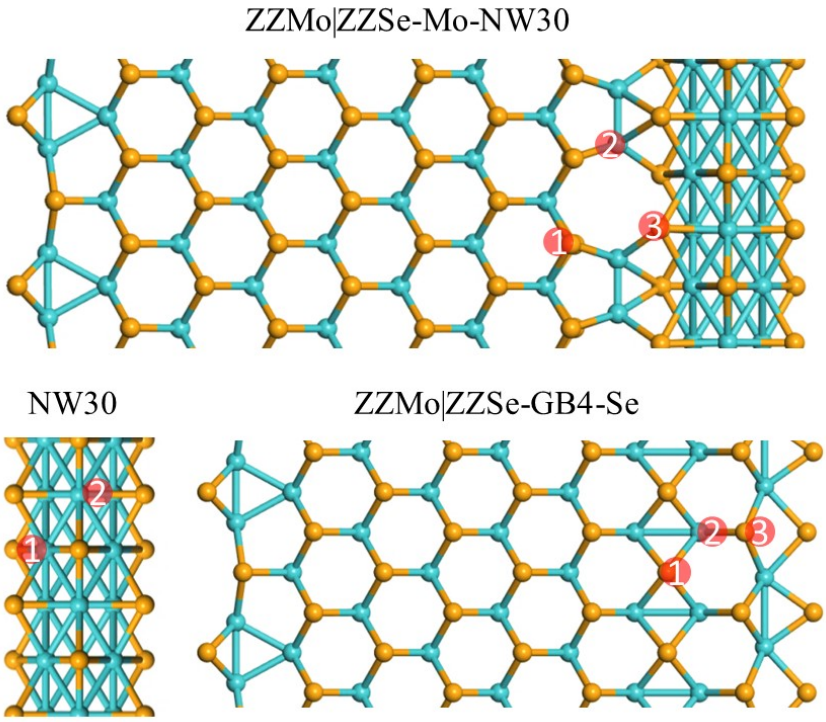

Fig. S7 The different sites of first hydrogen atom absorbed on three representative systems. The adsorption sites are highlighted in red circles.

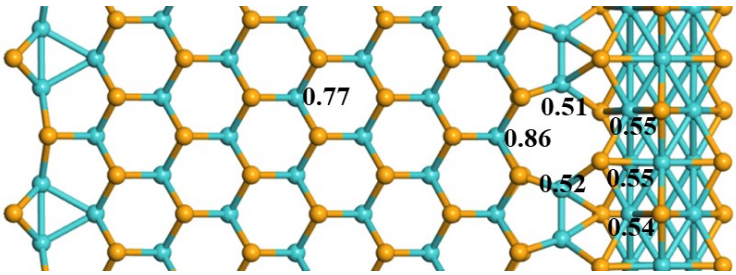

Fig. S8 Bader charge analysis of ZZMo|ZZSe-Mo-NW30 nanoribbon. The value of losing electrons of Mo atoms at defect edges and pristine $MoSe_2$ are labeled by black colors. For pristine $MoSe_2$, Mo atom approximately lost 0.77 electrons and Se atoms gain 0.38 electrons, respectively.

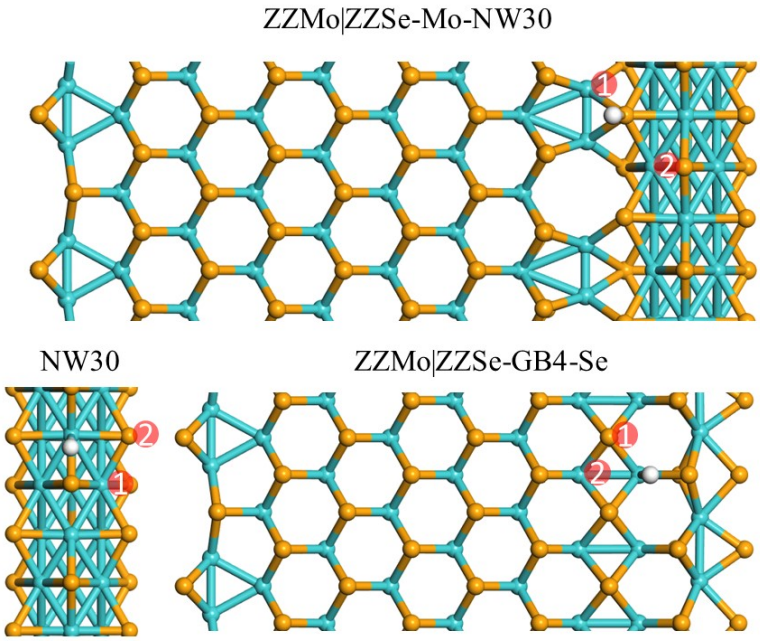

Fig. S9 The different sites of second hydrogen atom absorbed on three representative systems. The adsorption sites are highlighted in red circles.

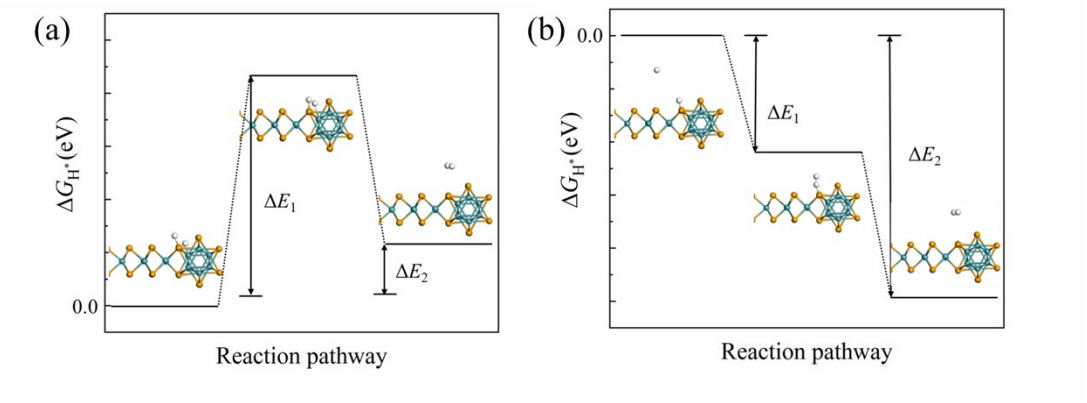

Fig. S10 Free energy diagrams of the (a) Tafel reaction and (b) Heyrovsky reaction for H_2 formation on the right edge of ZZMo|ZZSe-Mo-NW30 nanoribbon. The side views nanoribbons are shown for initial, transition and final states from the left to right. The energy of initial states is set to zero for reference and $\Delta E_1/\Delta E_2$ indicate the kinetic energy barriers compared to the initial states.