Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

Tuning Dirac points by strain in MoX_2 nanoribbons (X = S, Se, Te) with 1T' structure

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1. The edge states in MoX_2 nanoribbons

For H-passivated MoX_2 nanoribbons (Fig. S1), the gapless edge states are formed for both the nanoribbons with the zigzag- and armchair-like edges. In MoX_2-ANRs, the coupling between the two edge states can be prevented for ribbon widths larger than 9 nm. However, the edge states near the Γ point are somewhat extended into the bulk region, as illustrated in the planer-averaged charge density (Fig. S3). Since the PBE band gaps are too small for MoX_2-ANRs (Table 1), the edge states are not completely separated from the bulk states. We confirmed that the mixture of the edge states with the bulk states also occurs for the larger ribbon with of 11.2 nm. For $MoTe_2$-ANR, the edge states lie in the conduction band and hybridize with the bulk states. On the other hand, for MoS_2-ZNR, the edge states are well localized near the edge region (Fig. S4).

Table S1. The bond distances of the Mo-S and Mo-Mo bonds ($l_{Mo\text{-}S}$ and $l_{Mo\text{-}Mo}$ in units of Å), and the bond angles formed by three adjacent Mo atoms (α in units of degree), and the positions of the Dirac points (E_{DP} in units of meV) with respect to the Fermi level in the middle and edge regions of bare and H-passivated MoS_2-ZNRs.

	In the middle region			Near the edge region			E_{DP}
	$l_{Mo\text{-}S}$	$l_{Mo\text{-}Mo}$	α	$l_{Mo\text{-}S}$	$l_{Mo\text{-}Mo}$	α	
Bare MoS_2-ZNR	2.479	2.777	69.80	2.388	2.798	69.25	–52
H-passivated MoS_2-ZNR	2.479	2.779	69.85	2.491	2.751	70.62	–62

Supplementary Figures

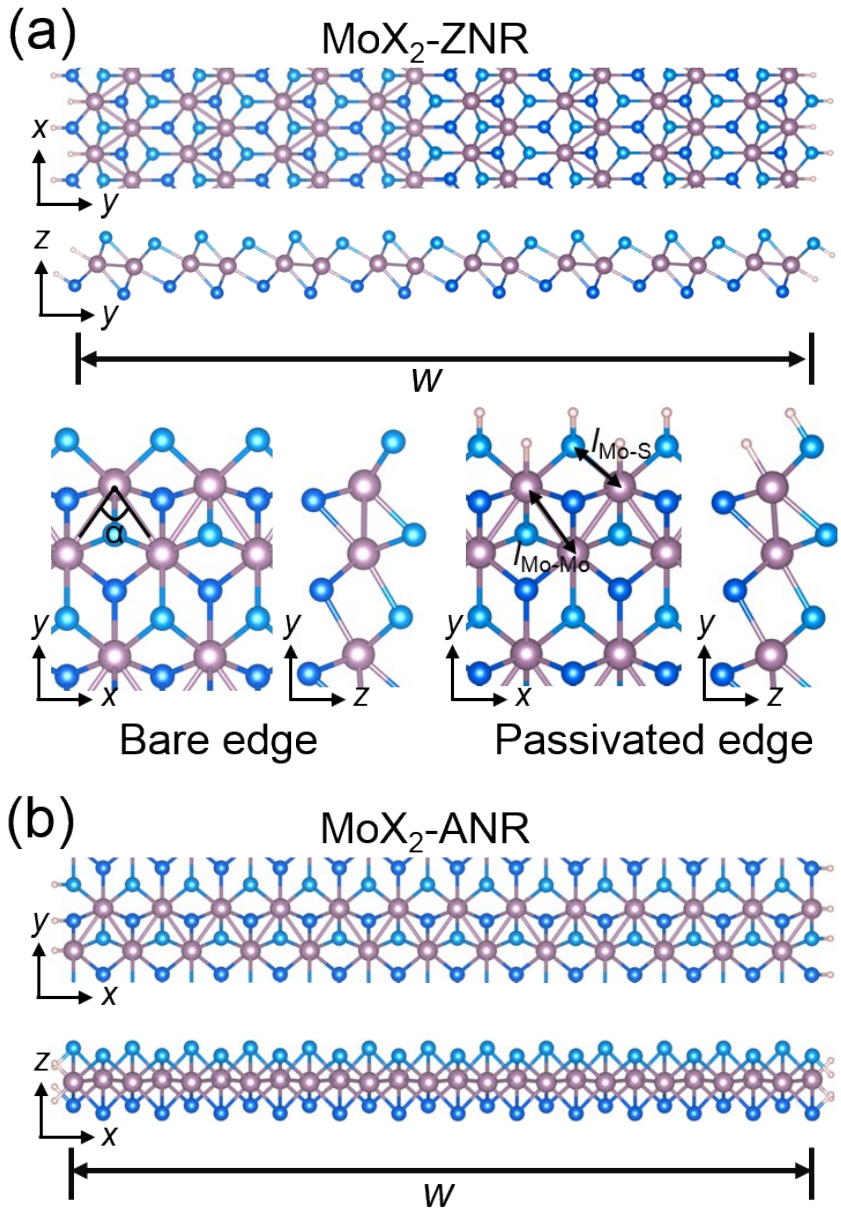

Fig. S1. (a) Top and side views of the atomic structures of bare and H-passivated MoX_2-ZNRs. (b) Top and side views of the atomic structure of H-passivated MoX_2-ANR. *w* represents the width of nanoribbons. Small white balls represent the H atoms which passivate the edge atoms, whereas blue and purple balls stand for the Mo and X atoms, respectively.

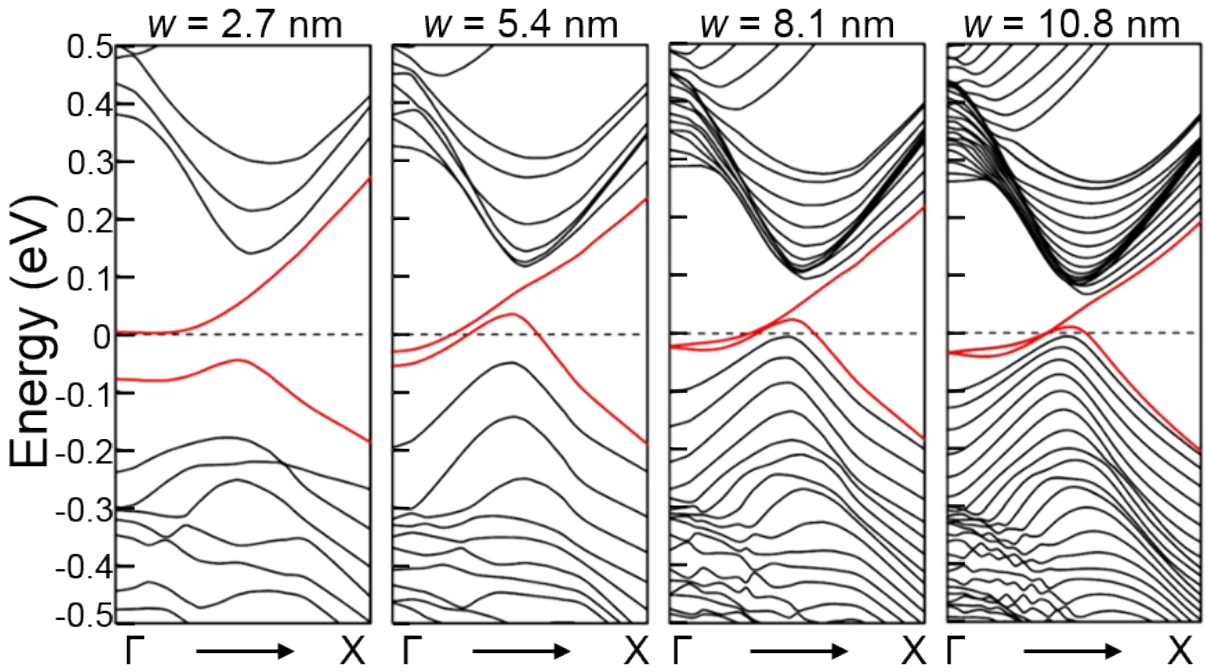

Fig. S2. The PBE band structures of MoS_2-ZNRs with the different ribbon widths of 2.7, 5.4, 8.1, and 10.8 nm. Red lines indicate the edge states.

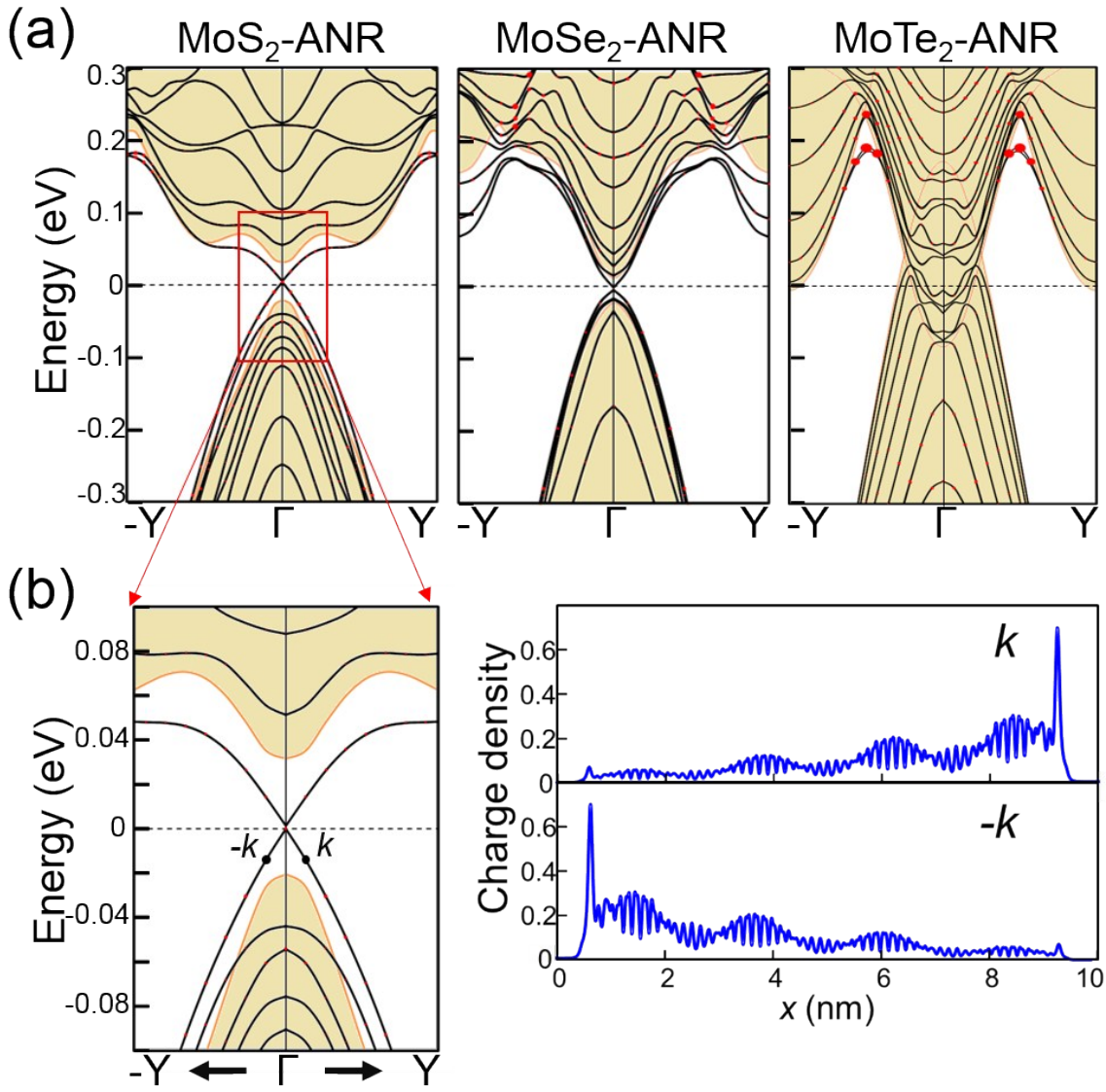

Fig. S3. (a) The PBE band structures of MoX_2 nanoribbons with the armchair-like edges. (b) The enlarged view of the edge states near the Γ point (left panel) and the planer-averaged charge density in units of $10^{-2}e/\text{Å}$ plotted along the ribbon width at the two representative *k* points (right panel) for MoS_2-ANR.

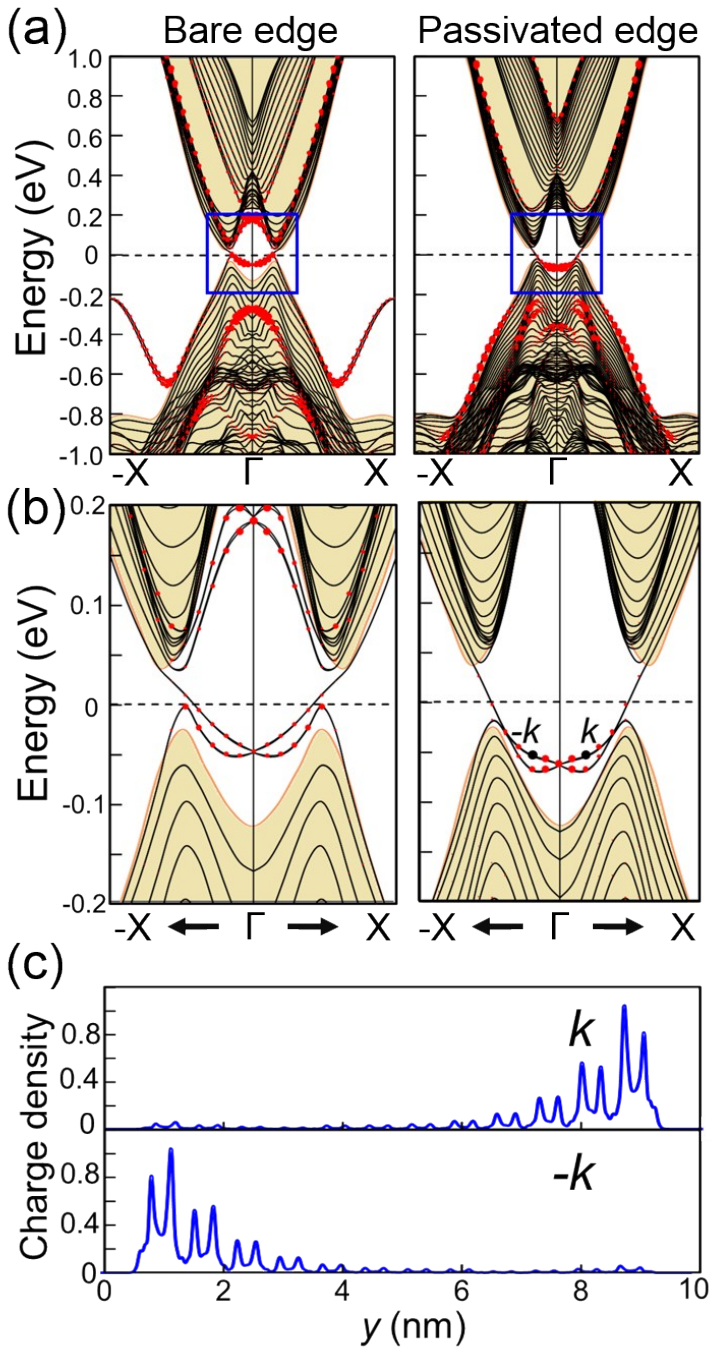

Fig. S4. (a) The PBE band structures of bare and H-passivated MoS_2-ZNRs. (b) The enlarged view of the edge states near the Fermi level. (c) The planer-averaged charge density in units of $10^{-2}e/\text{Å}$ plotted along the ribbon width at the two representative *k* points in (b).

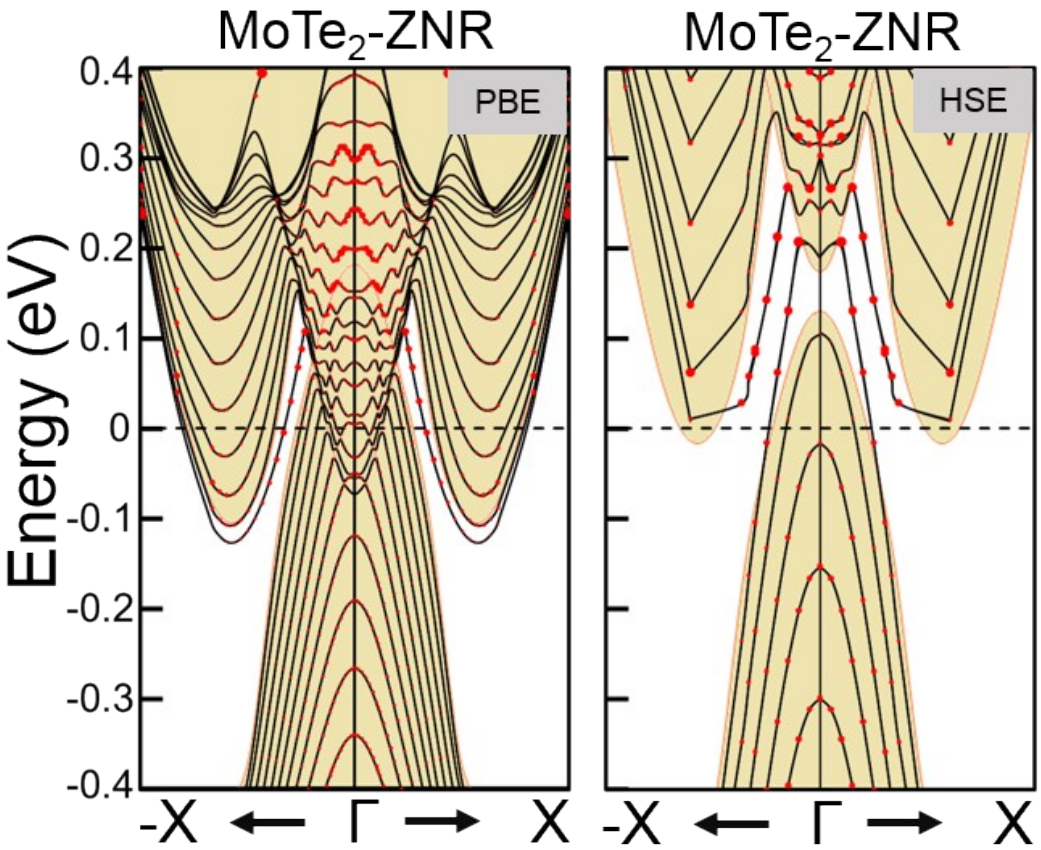

Fig. S5. The (a) PBE and (b) HSE band structures of strain-free $MoTe_2$-ZNR with the edge atoms passivated with hydrogen.

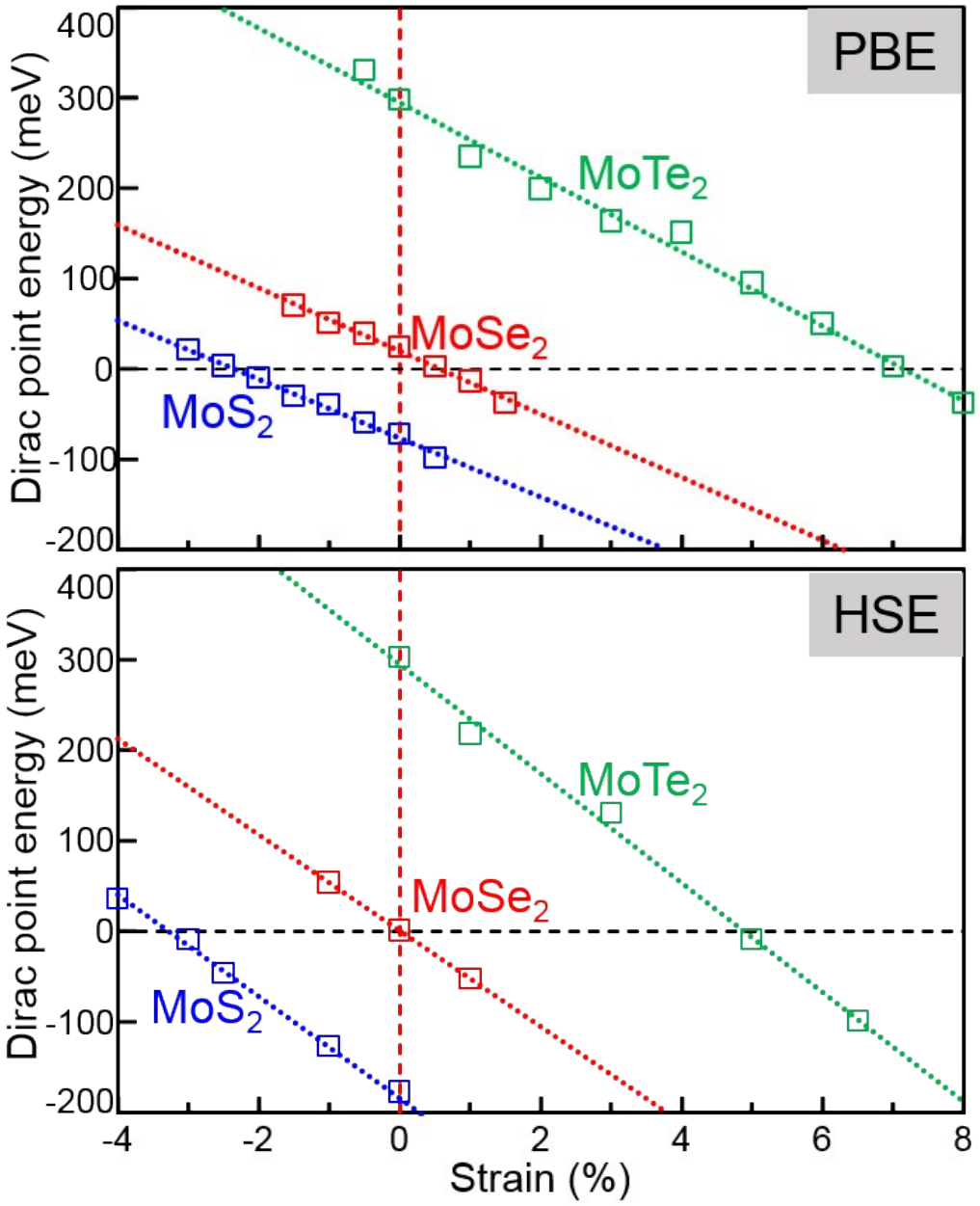

Fig. S6. The energy of the Dirac point with respect to the Fermi level is plotted as a function of uniaxial strain for MoX_2-ZNRs, based on the PBE and HSE calculations.