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

Fundamental insights of electronic structures on zigzag MoS_2 nanoribbons

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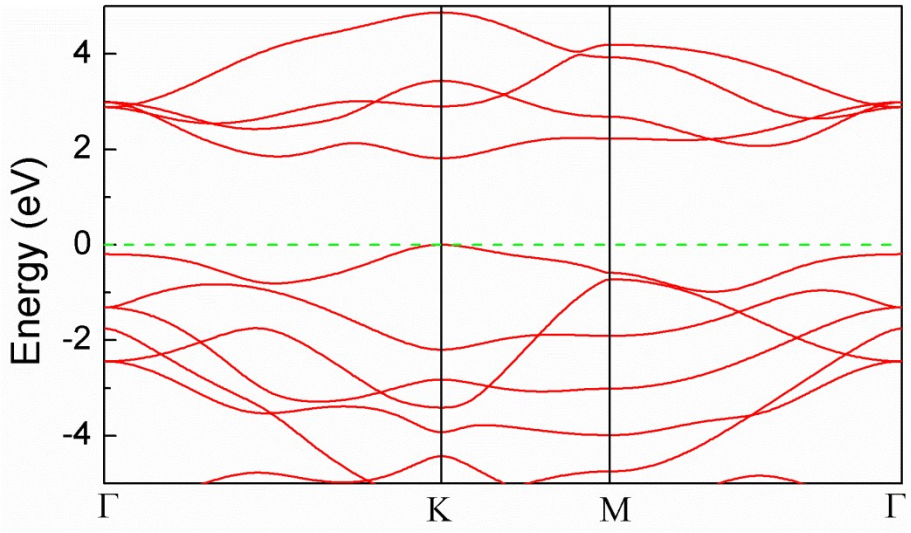
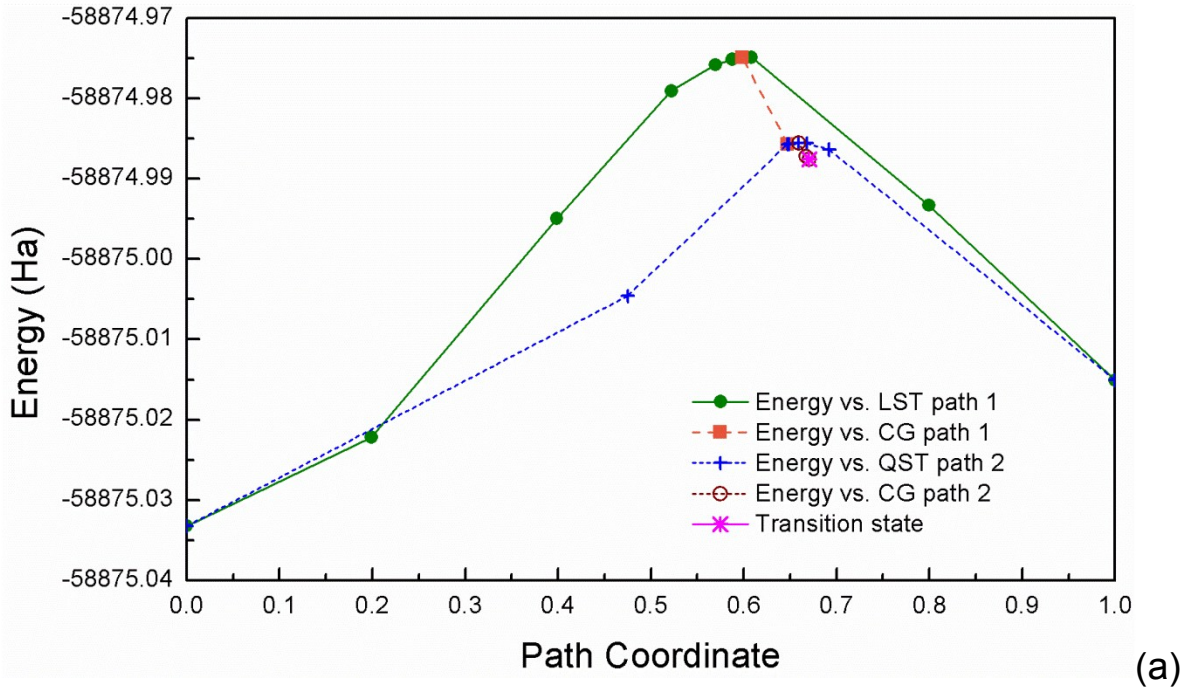


Fig. S1. Calculated band structure of MoS_2 monolayer is exhibited, which has a direct gap of 1.811 eV at K point. The Fermi level is set as 0 eV.



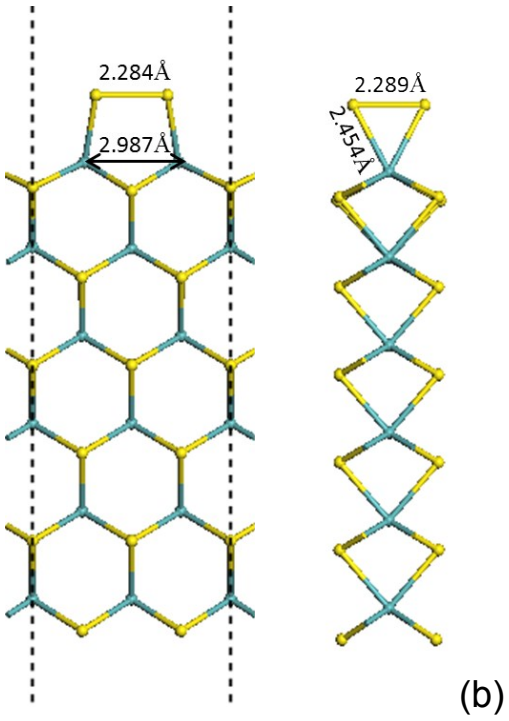


Fig. S2. (a) The plots of transition state search from NR-2 (path coordinate: 0.0) to NR-2' (path coordinate: 1.0) are exhibited. The energy of reaction is 11.393 kcal/mol, and energy of barrier is 28.632 kcal/mol. (b) The geometric structure of transition state is shown.

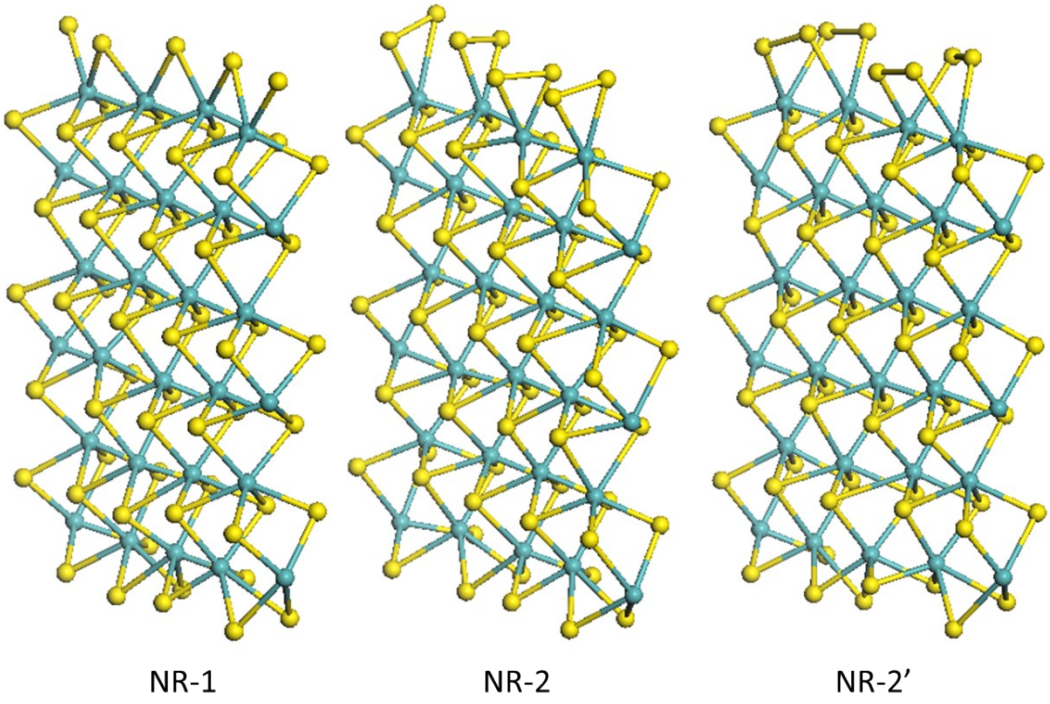


Fig. S3. Snapshots of NR-1, NR-2 and NR-2’ system after a 10ps molecular dynamics simulation at 1000K are shown.

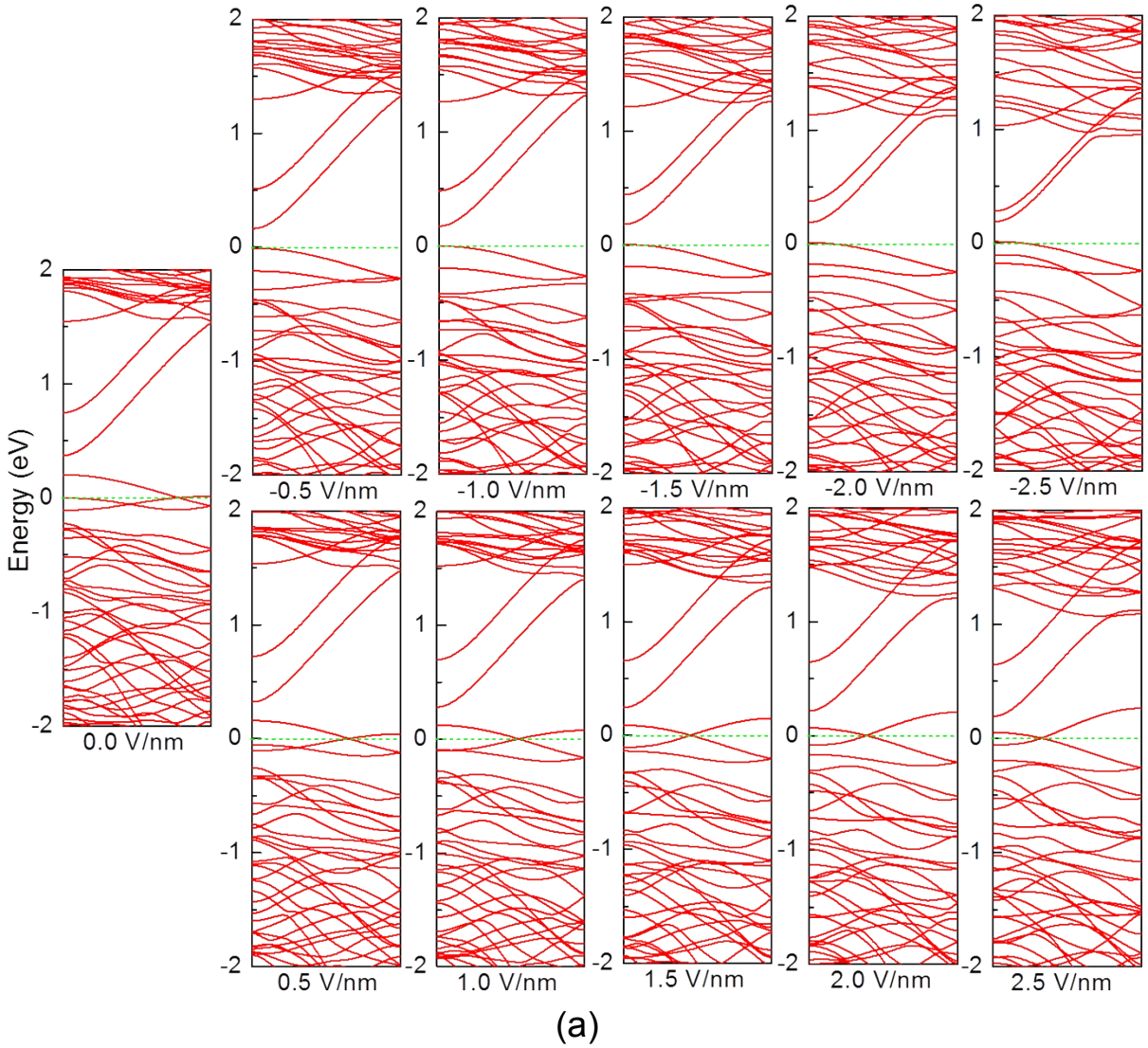


Fig. S4a. The calculated band structures of NR-1 as a function of a static external electric field. The Fermi level is set as 0 eV.

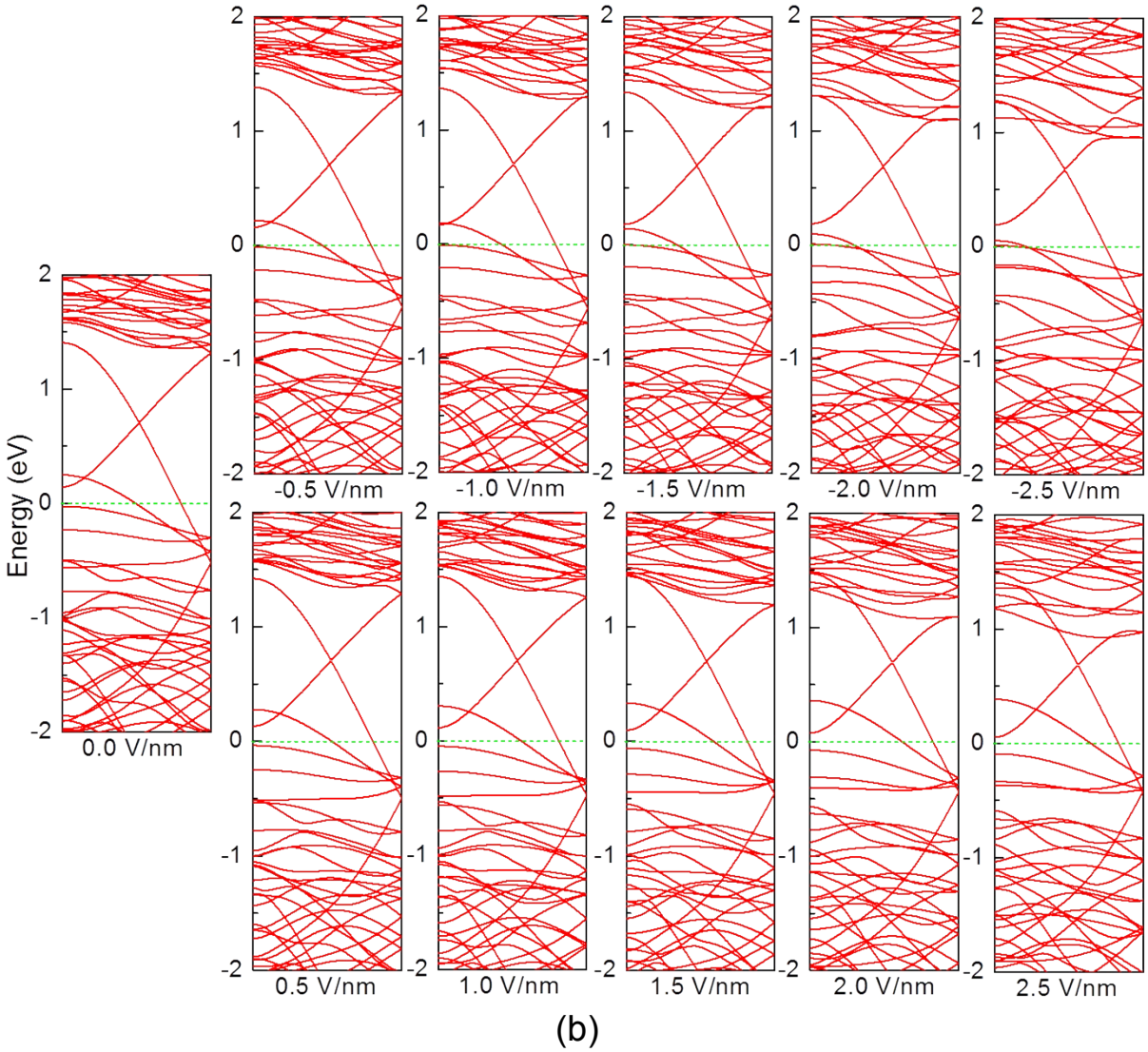


Fig. S4b. The calculated band structures of NR-2 as a function of a static external electric field. The Fermi level is set as 0 eV.

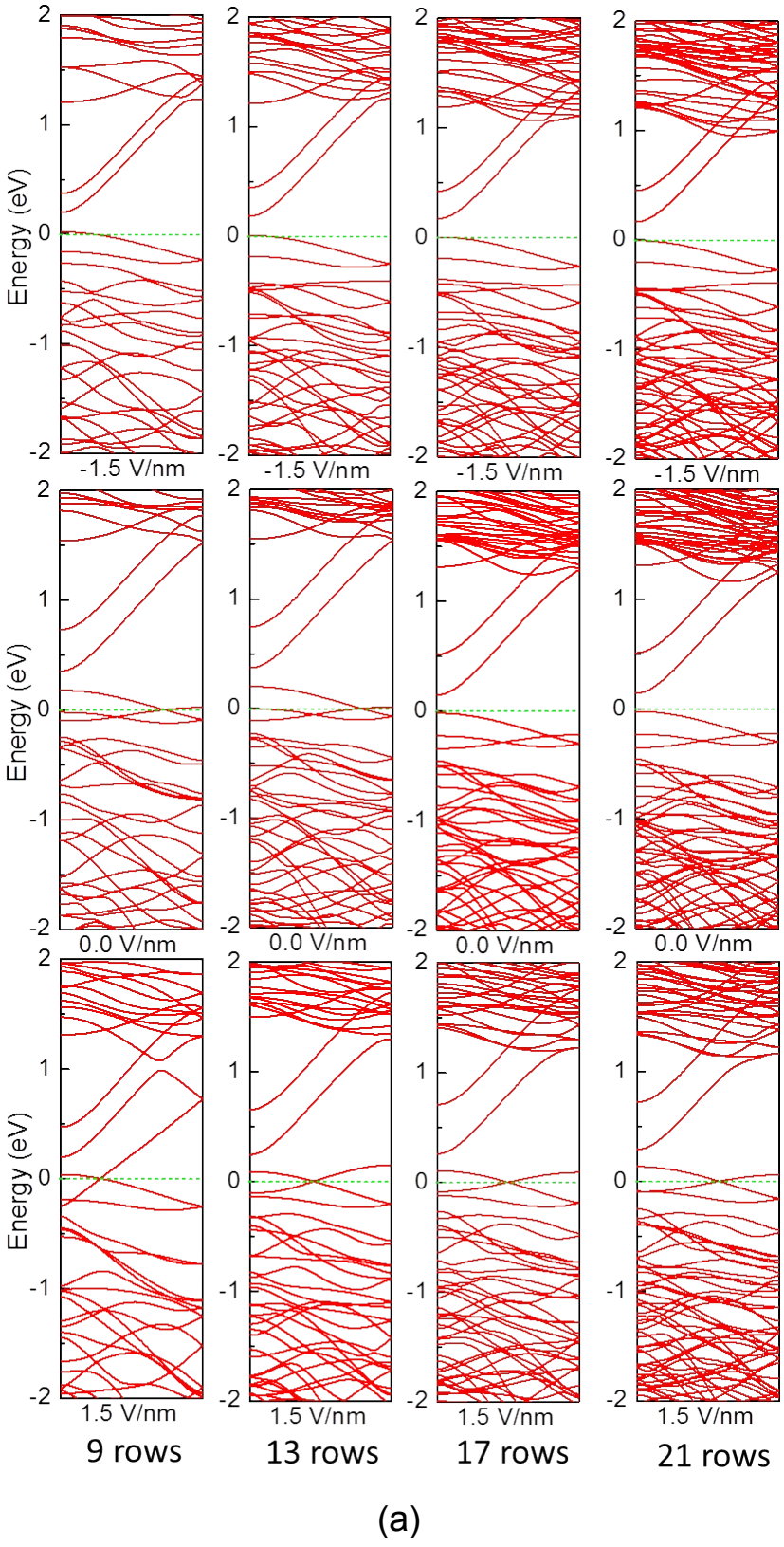


Fig. S5a. The calculated band structures of NR-1 as a function of width under a static external electric field. The Fermi level is set as 0 eV.

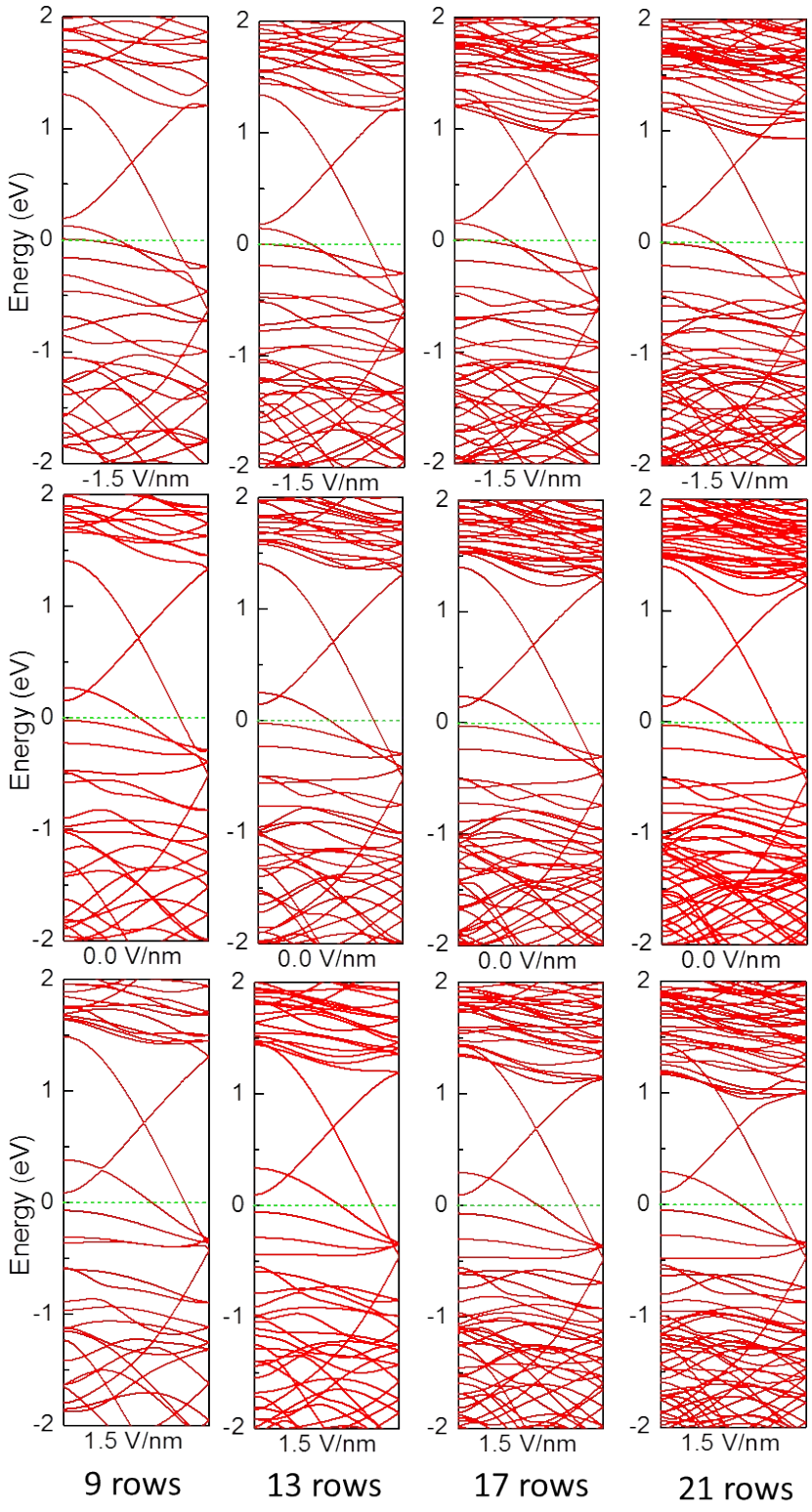


Fig. S5b. The calculated band structures of NR-2 as a function of width under a static external electric field. The Fermi level is set as 0 eV.

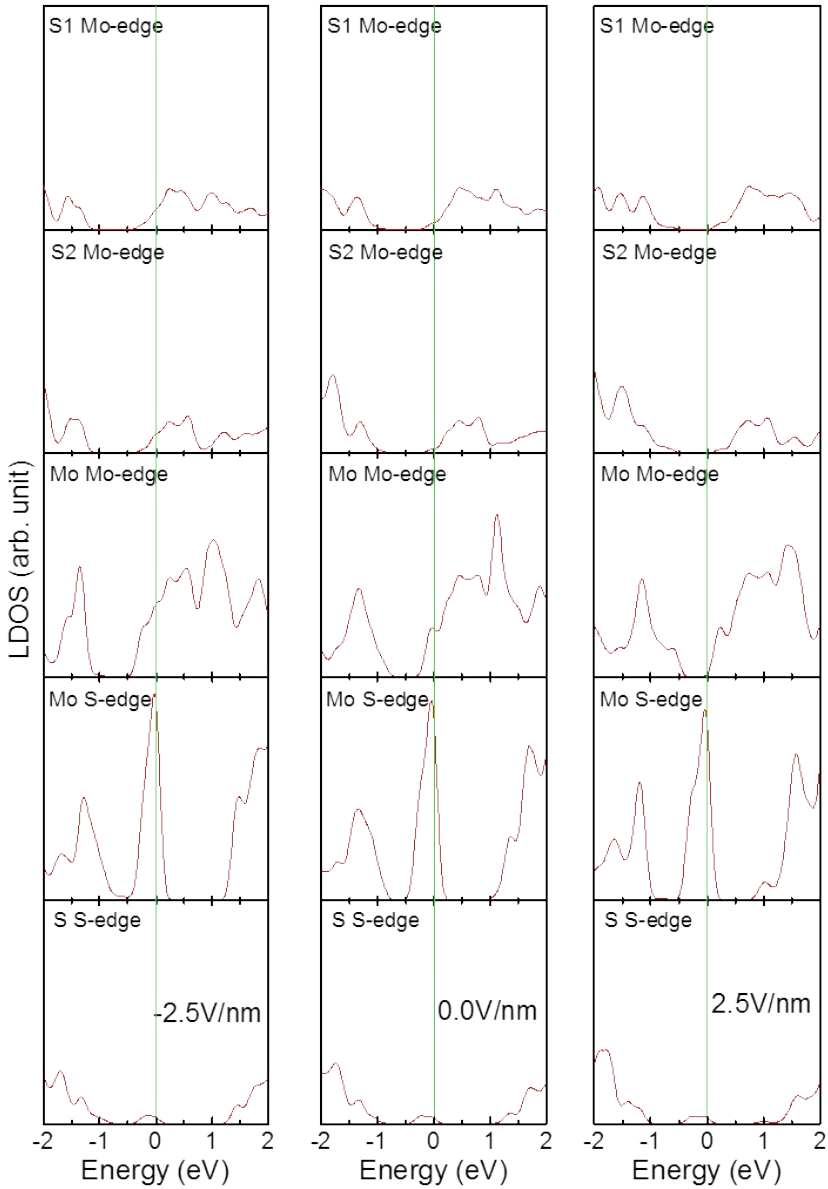


Fig. S6. LDOS of hydrogen passivated NR-1 ($Mo_{(100\%H)}$-$S_{(100\%H)}$) under E_{ext}=-2.5 V/nm, 0.0 V/nm and 0.25 V/nm are compared.

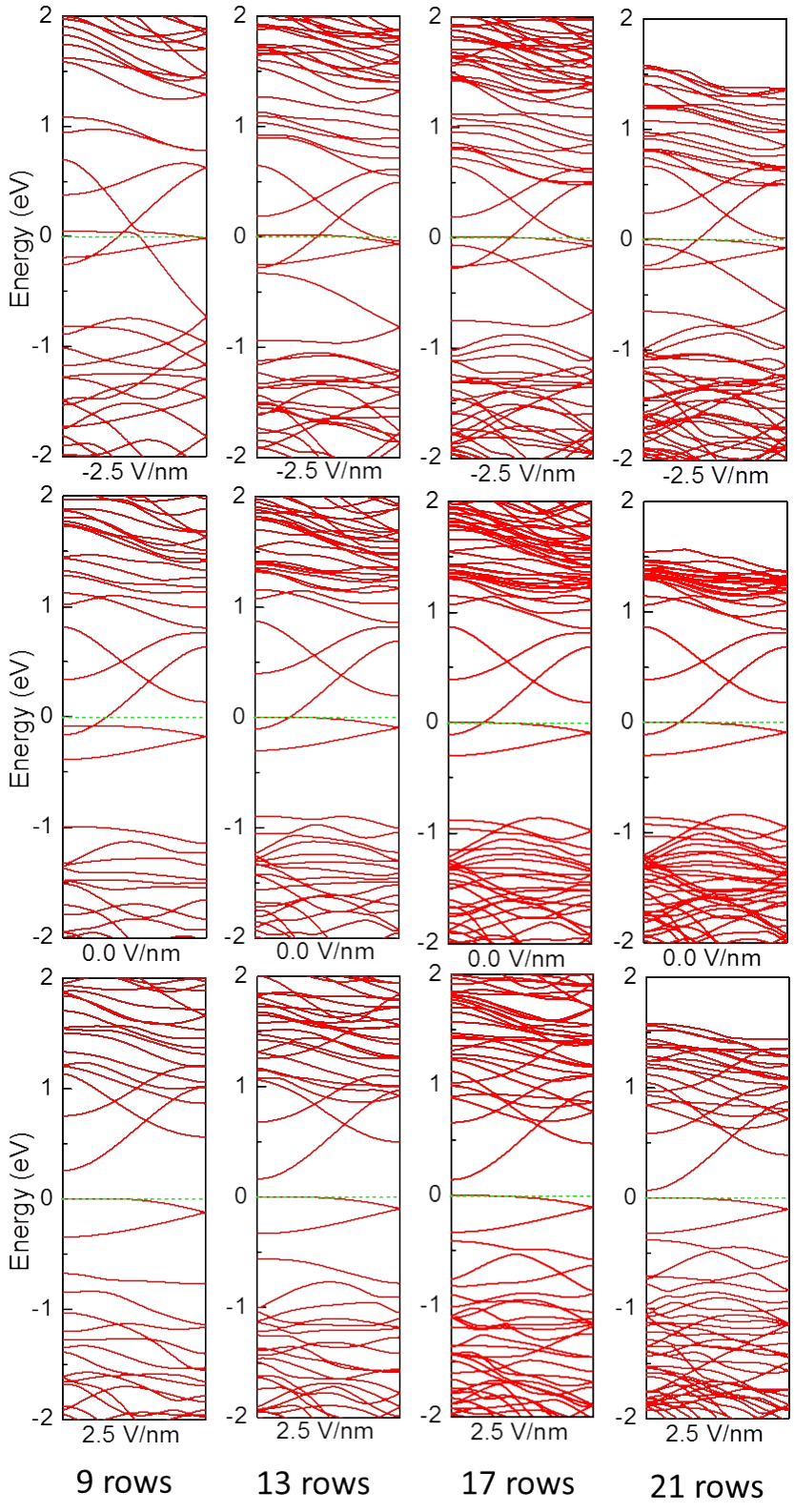


Fig. S7. The calculated band structures of hydrogen passivated NR-1 ($Mo_{(100\%H)}$-$S_{(100\%H)}$) as a function of width under a static external electric field are compared. The Fermi level is set as 0 eV.

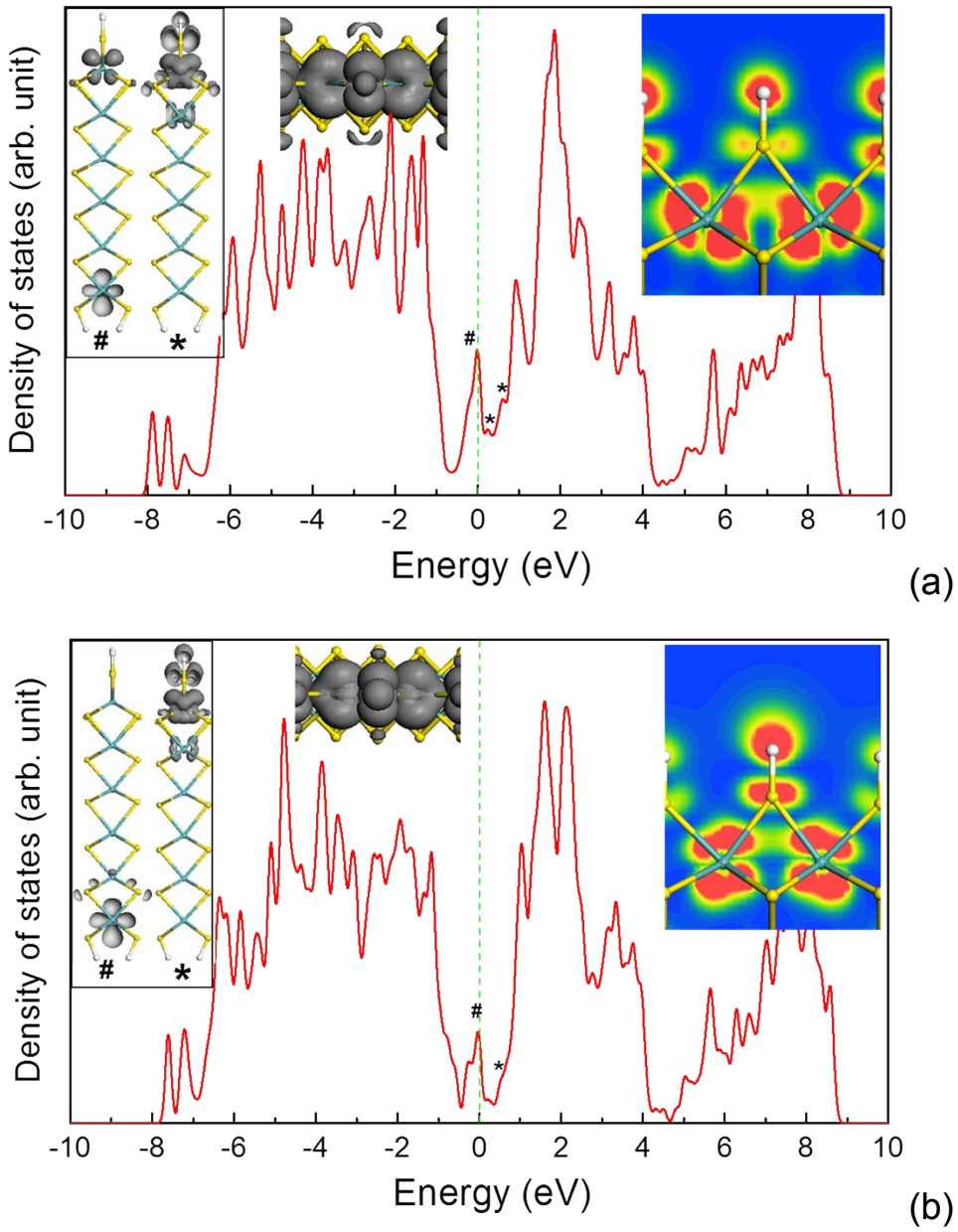


Fig. S8. TDOS of hydrogen passivated NR-1 ($Mo_{(100\%H)}$-$S_{(100\%H)}$) under (a) E_{ext}= -2.5 V/nm and (b) 2.5 V/nm are exhibited. Inset: the electronic states near the Fermi level. The Fermi level is set as zero. The isosurface value is 0.02 electrons/au^{-3}.

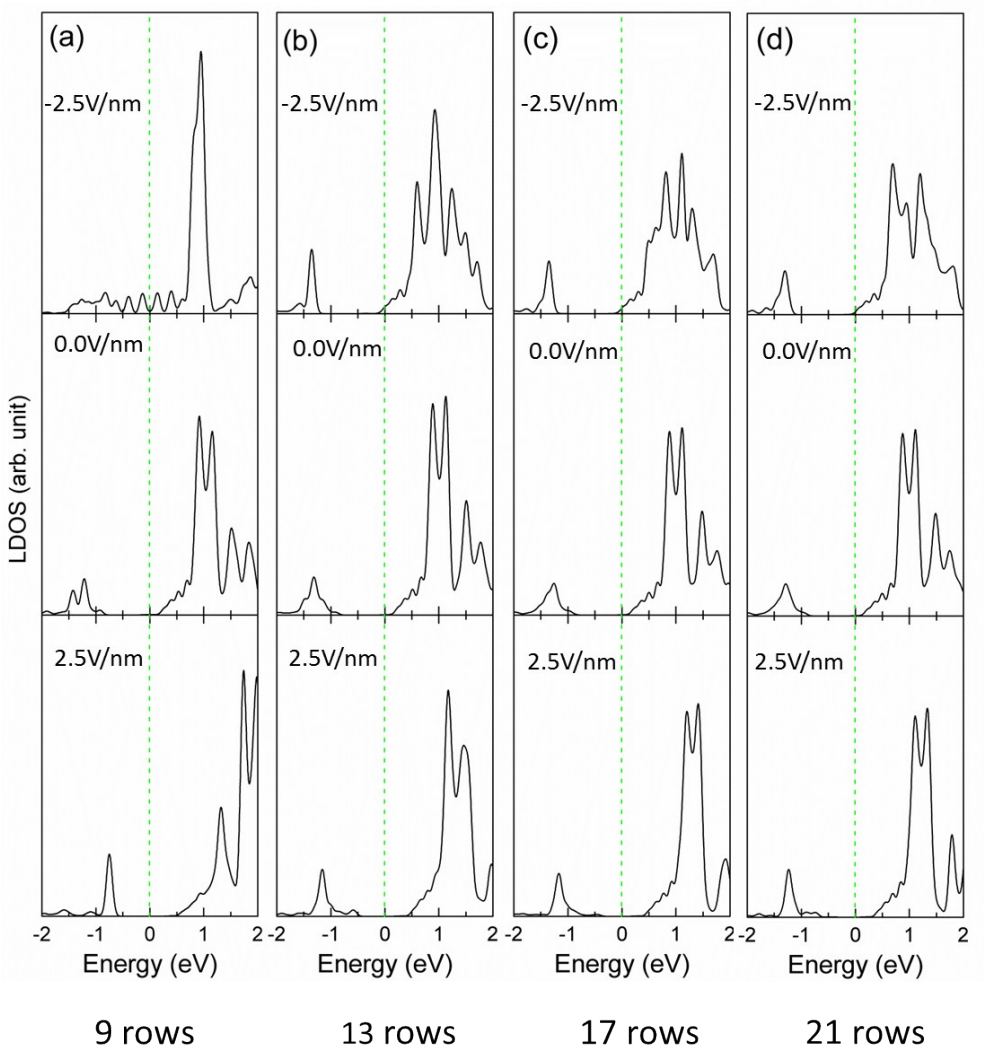


Fig. S9. LDOS of H atom at the Mo-edge as a function of width under E_{ext} are compared for hydrogen passivated NR-1 ($Mo_{(100\%H)}$-$S_{(100\%H)}$).