Spontaneous structure deformation of MoS$_2$ nanoribbons in Au(111)/ MoS$_2$/Au(111) heterojunctions

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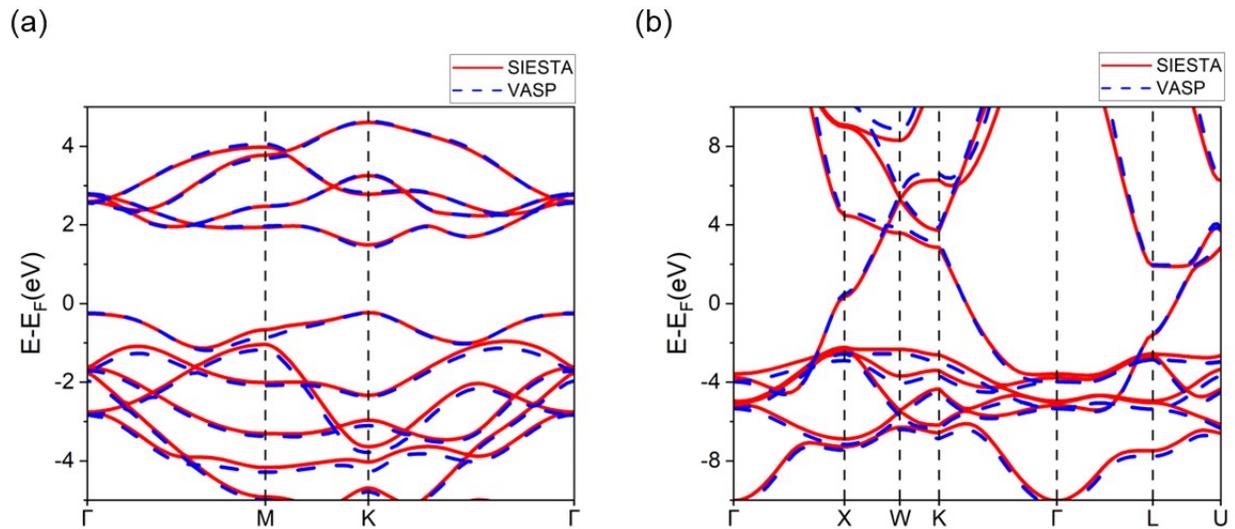
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FIG. S1. Band structures of (a) Monolayer MoS_2 and (b) Bulk Au, computed using SIESTA (red solid lines) and VASP (blue dashed lines). Both are plotted in the first Brillouin zone with the Fermi level set to 0.0 eV.
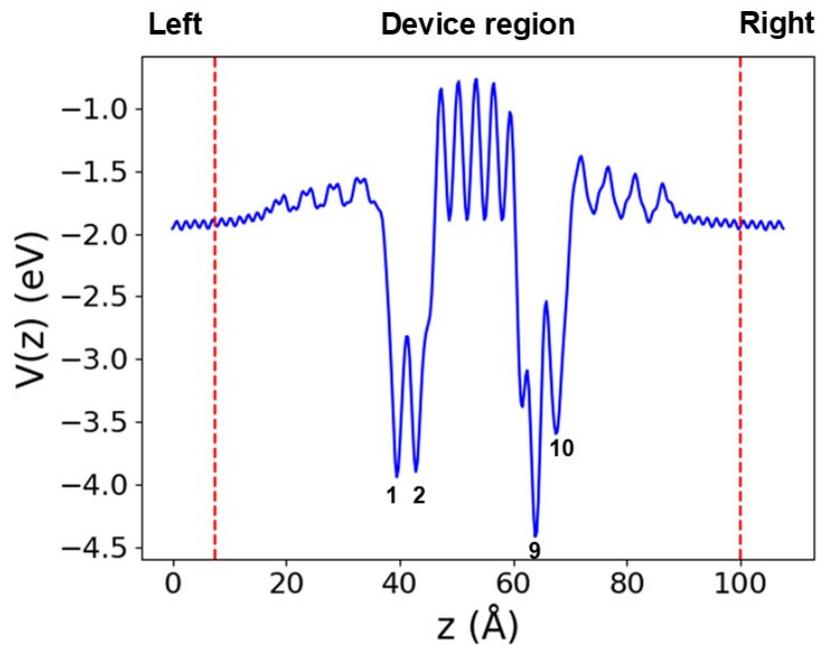

FIG. S2. Planar-averaged electrostatic potential V(z) along the transport direction for the deformed MoS_2 nanoribbon device. Locations of 4 Mo layers (1,2,9 and 10) are labelled in the figure. The boundaries between the left electrode, device region, and right electrode are marked by two red dashed lines.

Table S1. Effective curvature, curvature radius, stretching, and deformation-induced bandgap drop of MoS₂ nanoribbons with different widths (N).

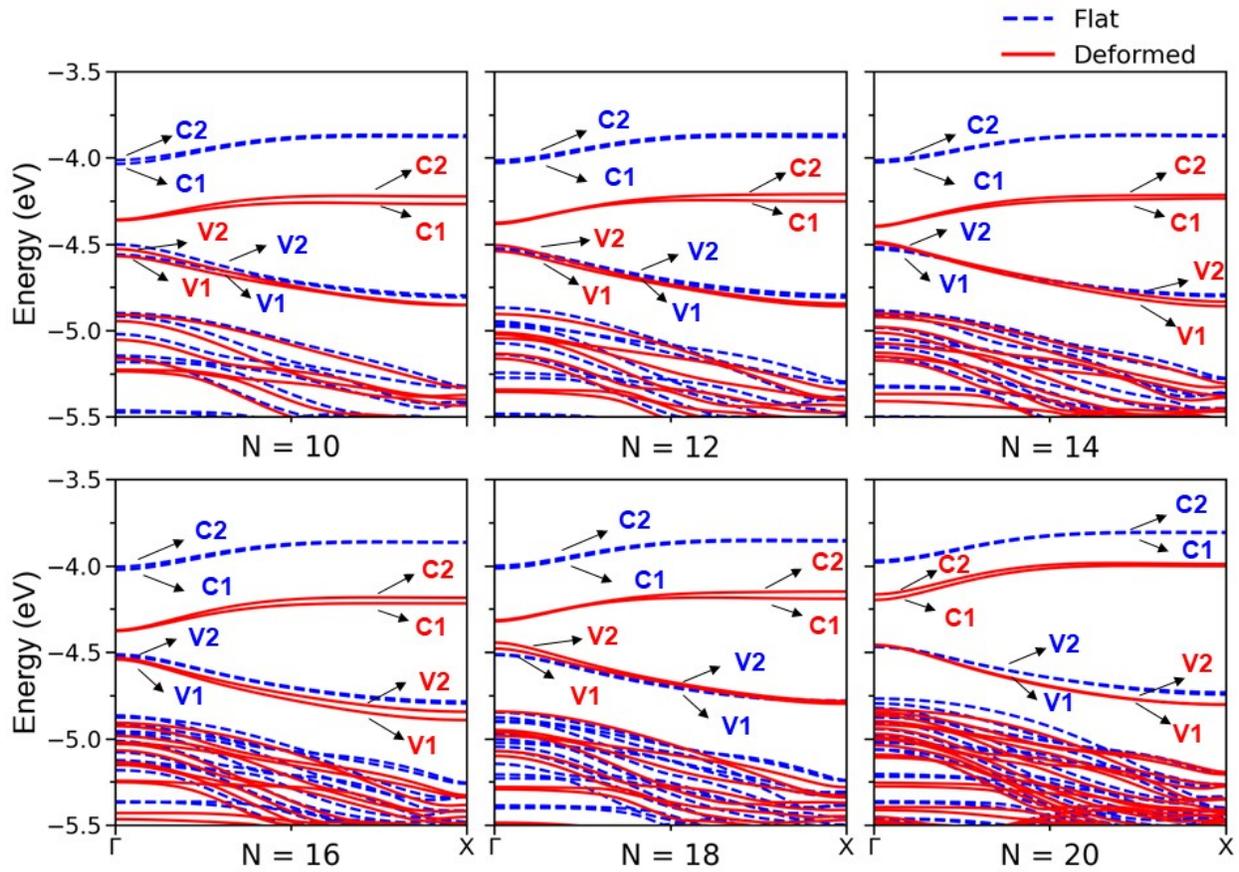| N	Curvature (Å⁻¹)	Radius (Å)	Stretching (Å)	Bandgap drop (eV)
10	0.031	32	0.122	0.30
12	0.018	55	0.074	0.37
14	0.014	70	0.074	0.41
16	0.017	59	0.171	0.33
18	0.014	71	0.168	0.27

FIG. S3. Band structures of isolated MoS₂ nanoribbons with different widths (N = 10, 12, 14, 16, 18, 20).
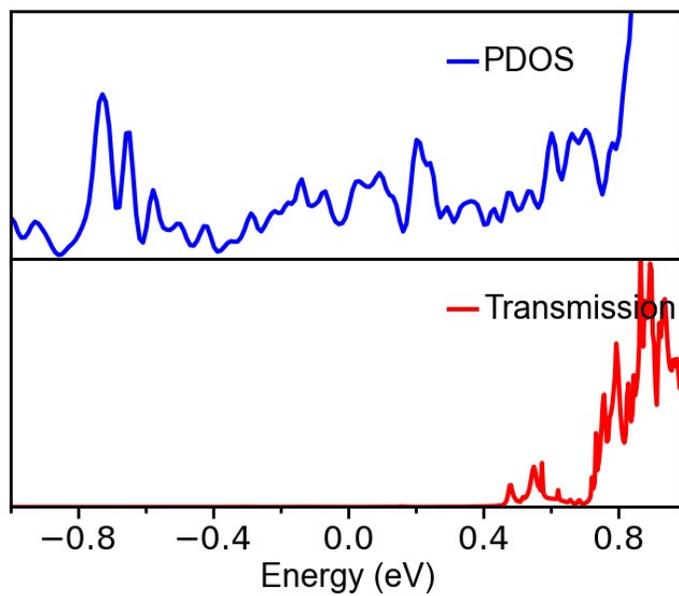
FIG. S4. PDOS and transmission spectrum for the deformed MoS_2 nanoribbon with N = 18.