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

Supporting Information

First-Principles Studies of Energetics of MoS_2 Nanosheets: Size Effects and Odd-Even Effects

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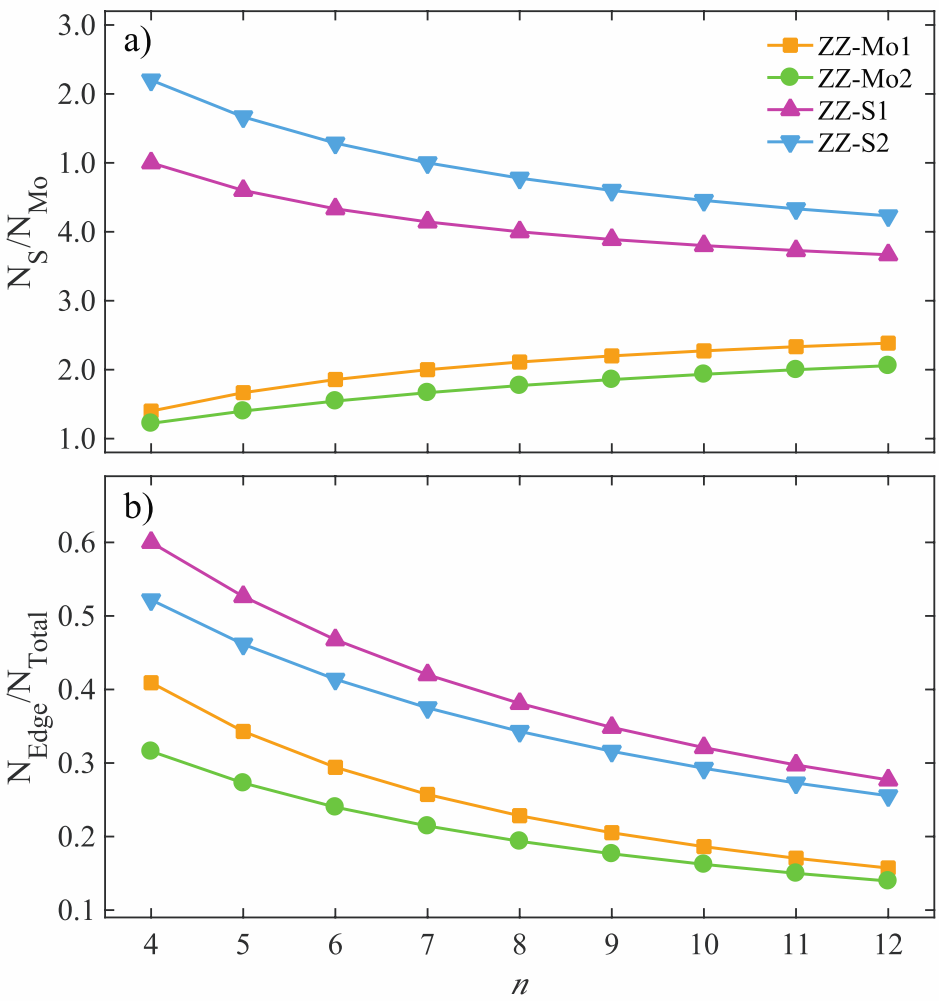

Figure S1: Atomic ratio **a)** between the number of S and Mo atoms (N_S/N_{Mo}) and **b)** between the number of atoms on the edge and total atoms (N_{Edge}/N_{Total}) as a function of the size of the MoS_2 nanosheets, *n*.

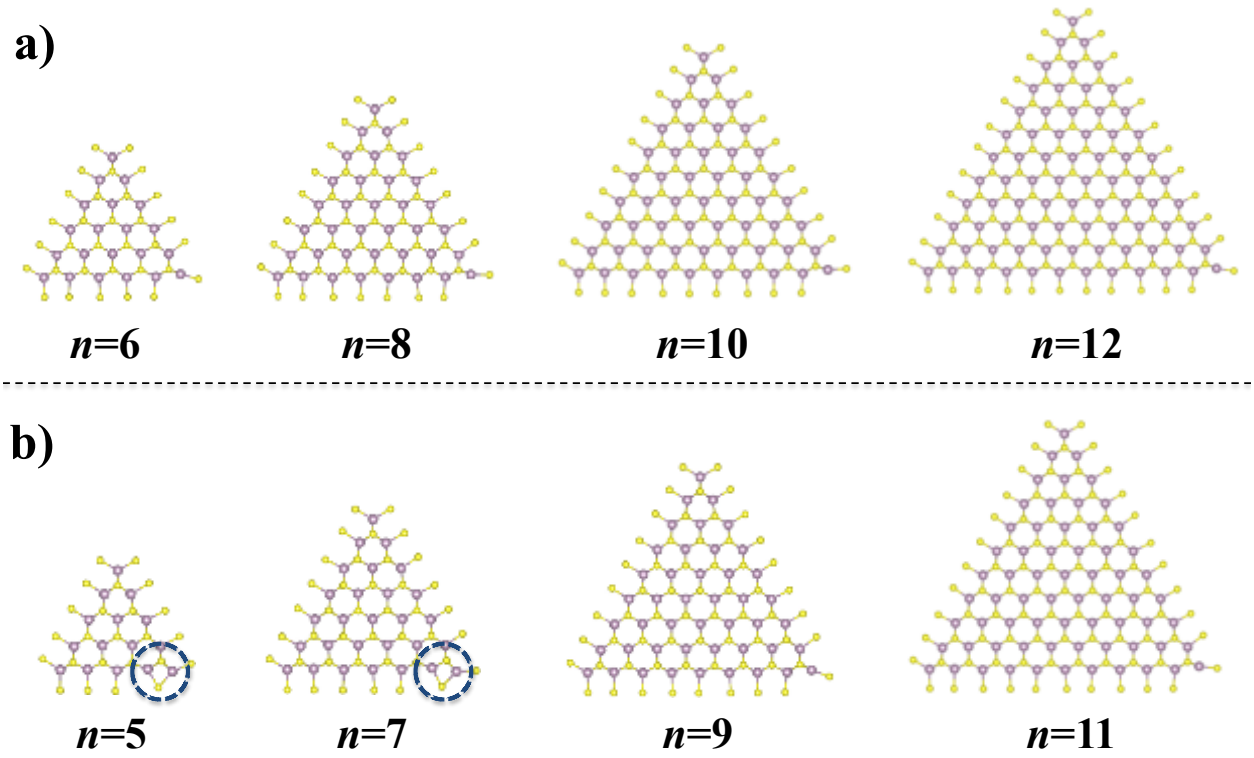

Figure S2: Geometrical structures of the relaxed MoS_2 nanosheets with sulfur vacancy at the corner of the edge (V_S@Cnr) for **a)** even-number size (n = 6, 8, 10, and 12) and **b)** odd-number size (n = 5, 7, 9, and 11). The new formed S-Mo bonds between the coordinatively unsaturated sites (Mo atoms with dangling bonds) and its adjacent S dimer are highlighted by the blue circle.

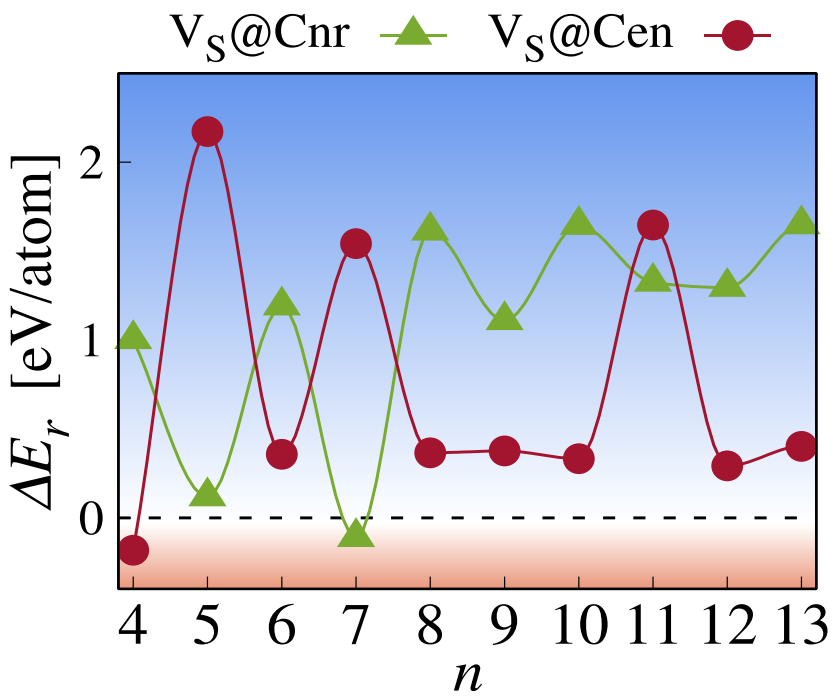

Figure S3: Calculated HDS reaction energy (ΔE_r) on the ZZ-S2 type MoS_2 nanosheet as a function of the size (n) of the nanosheets. The dash line indicates the ΔE_r at zero. Note that calculated final ΔE_r shares the same magnitude under S-rich and S-poor conditions, and is independent of sulfur chemical potential.