On the electronic structure of 2H-MoS_2: Correlating observations made by in-situ mechanical bending on TEM

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SUPPLEMENTAL MATERIALS

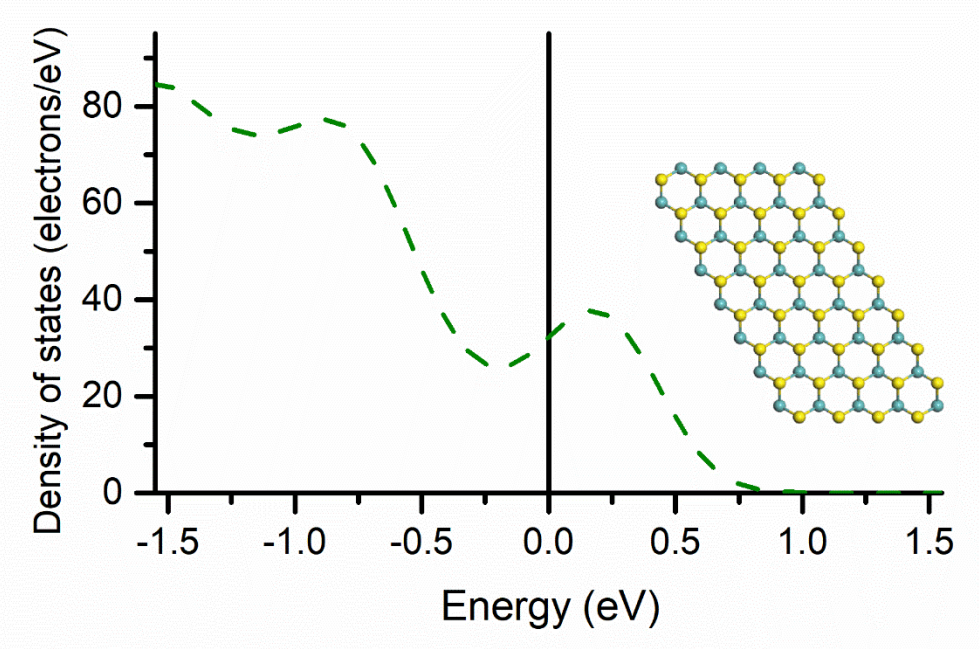

Figure S1. Total density of states of the 2H-MoS_2 molecular layer with no bending. Cyan balls represent the position of molybdenum and yellow balls represent sulfur.

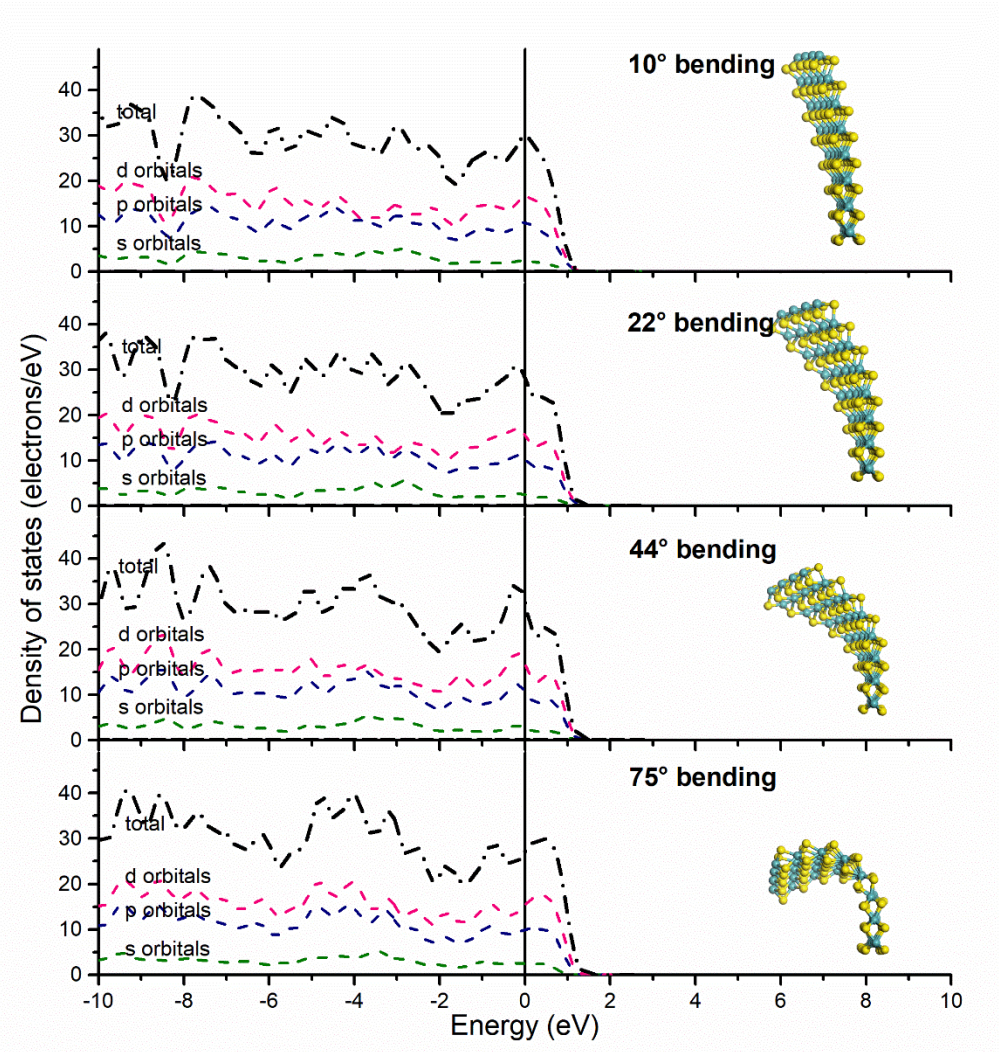

Figure S2. Total and partial density of states computed for the MoS_2 molecular model at 10°, 22°, 44° and 75° of mechanical bending from -10 eV to 10 eV. The observations made by in-situ HRTEM technique, showing the induced bending curvature for 2H-MoS_2 layers, were used to extract the molecular models used for the calculations. Cyan balls represent the position of molybdenum and yellow balls represent sulfur.