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Significant enhancement of piezoelectricity induced by oxygen adsorption in monolayer and multilayer MoS_2

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I. The structural and electronic properties of O@MoS_2 under different O concentration.

Fig. S1 (a) – (d) display the energetically favorable structures of MoS_2 with O adsorption concentration of 16.667%, 33.333%, 66.667% and 83.333%, corresponding to two, four, eight, and ten S atoms adsorbed by O atoms in 2×3 supercell respectively.

As the concentration increases, the lattice parameters of armchair and zigzag direction are increased gradually as shown in Fig. S3 (a). Nevertheless, the band gap is decreased with the increment of concentration as displayed in Fig. S3 (b).

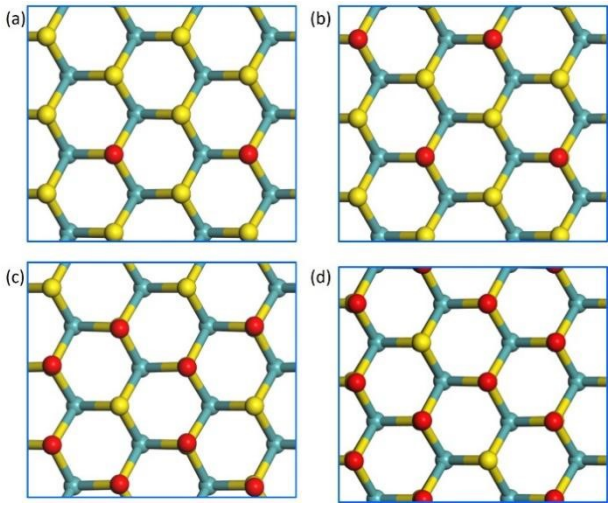

Fig. S1 (a)-(d) The energetically favorable structures of MoS_2 with O adsorption concentration of 16.667% (2O), 33.333% (4O), 66.667% (8O) and 83.333% (10O).

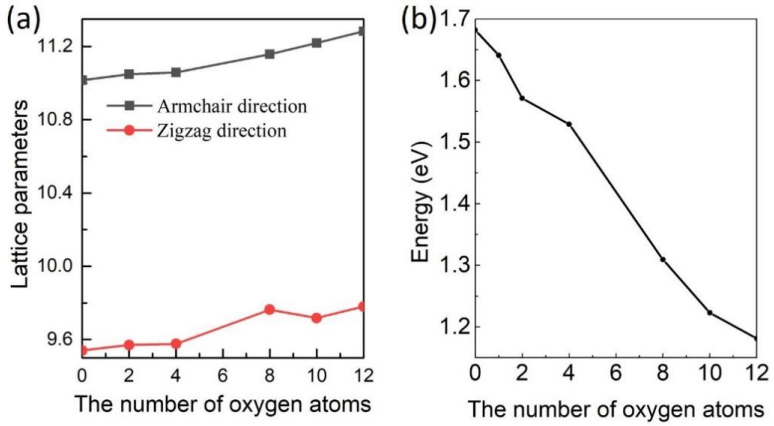

Fig. S2 (a) The lattice parameters of O@MoS_2 as functions of O adsorption concentration; (b) The band gap variation of O@MoS_2 as a function of O adsorption concentration.

II. The possible stacking sequences of O@MoS_2/MoS_2.

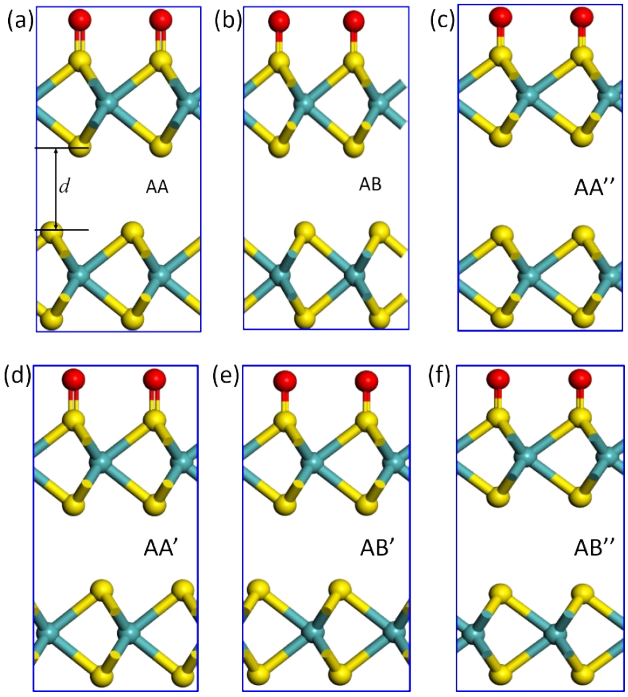

Fig. S3 (a)-(f) The stacking sequences of O@MoS_2/MoS_2.

III. The interlayer distances of AA and AB stackings under different O concentration.

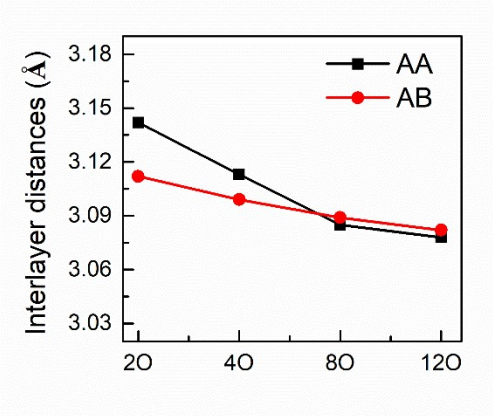

Fig. S4 The interlayer distances of AA and AB stackings under different O concentration.

IV. The AAA stacking of trilayer MoS_2 and the charge transfer of AA''.

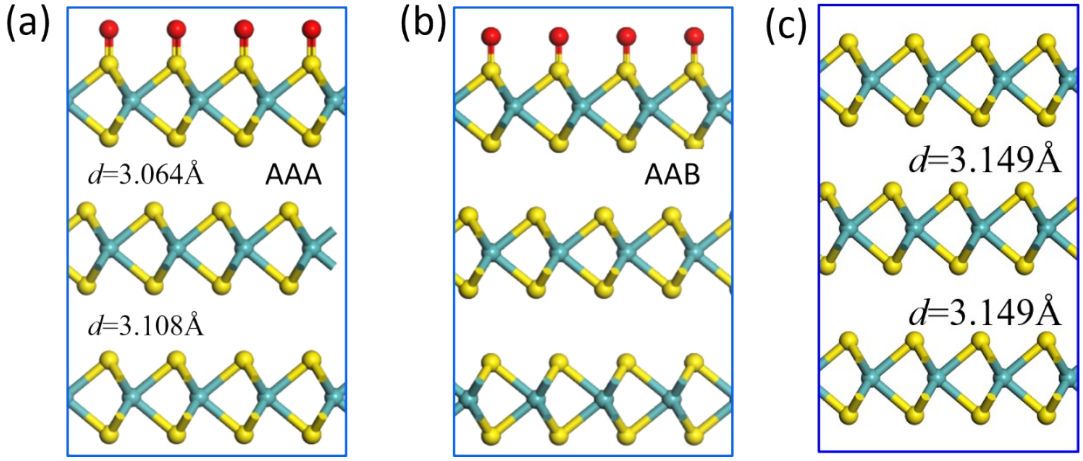

Fig. S5 (a) The structure of AAA stacking, the interlayer distances are shown in (a); (b) the structure of AAB stacking; (c) the structure of AAA stacking for pure MoS_2.

V. The piezoelectric coefficients e_{11} and d_{11} of pristine multilayer MoS_2.

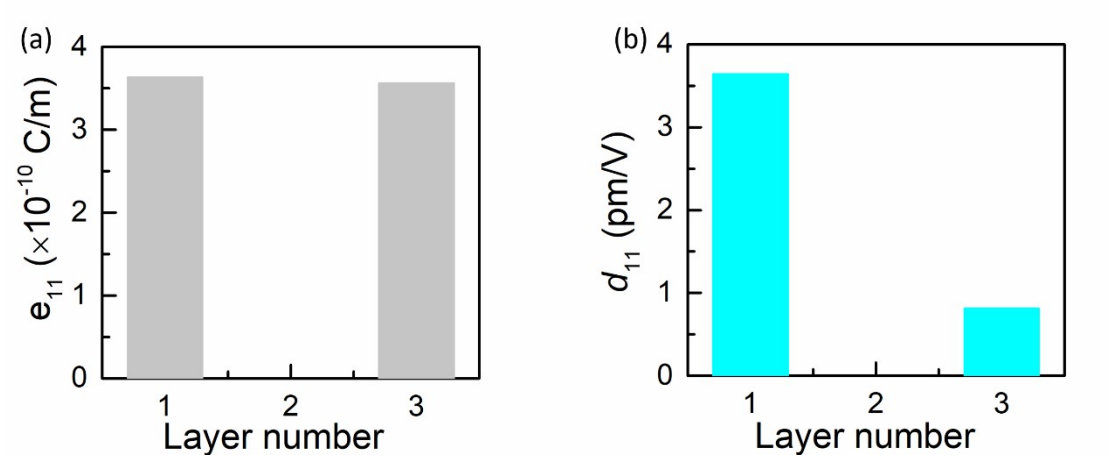

Fig. S6 The piezoelectric coefficients e_{11} (a) and d_{11} (b) of pristine multilayer MoS_2.

VI. The AA'' stacking and the charge transfer in AA''.

Fig. S7 shows the charge transfer in bilayer AA''. The overall trend is same with AA and AA', but there 0.005e has been transferred from Mo_1 to O_1, obviously larger than that in AA and AA'. The d_{33} is obtained as 20.409 pm/V, which is ten times as great as that of AA.

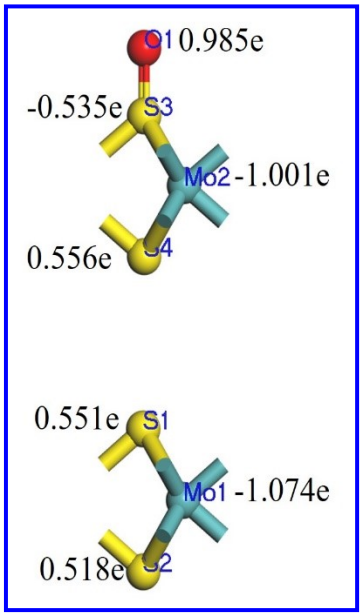

Fig. S7 the charge transfer of AA'' stacking.

VII. The structure of trilayer MoS_2 with the top layer full oxygen adsorption and the middle layer partial oxygen adsorption.

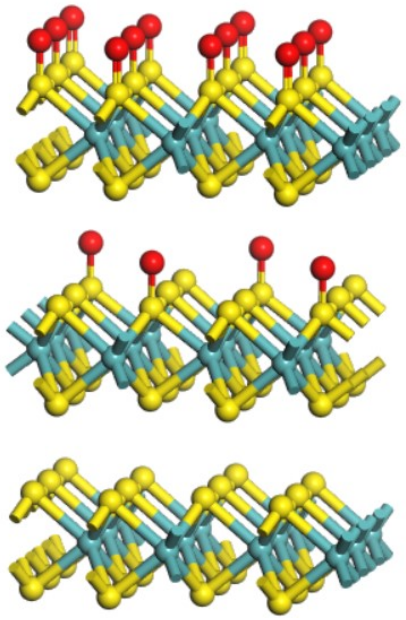

Fig. S8 The structure of trilayer MoS_2 with the top layer full O adsorption and the middle layer partial O adsorption.