Supplementary Information (SI) for RSC Advances.

Supplementary material

Atomic-scale description of the 2D Janus MoSO and MoSeO formation: oxidation patterns and band gap engineering

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1 O_2 adsorption on the S/Se vacancies of MoS_2 and $MoSe_2$.

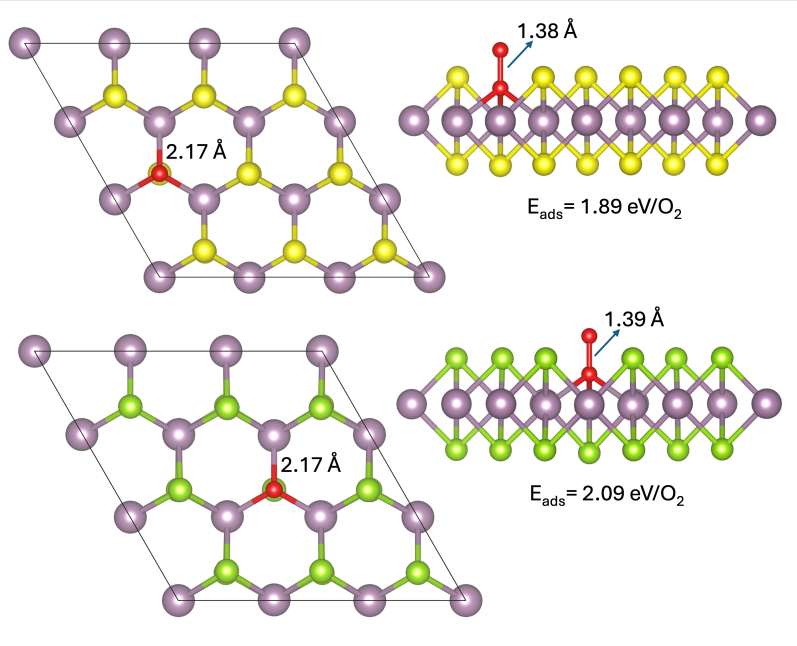

Figure 1: O_2 adsorption on the S/Se vacancy of MoS_2/$MoSe_2$ monolayers.

2 Effective band structures

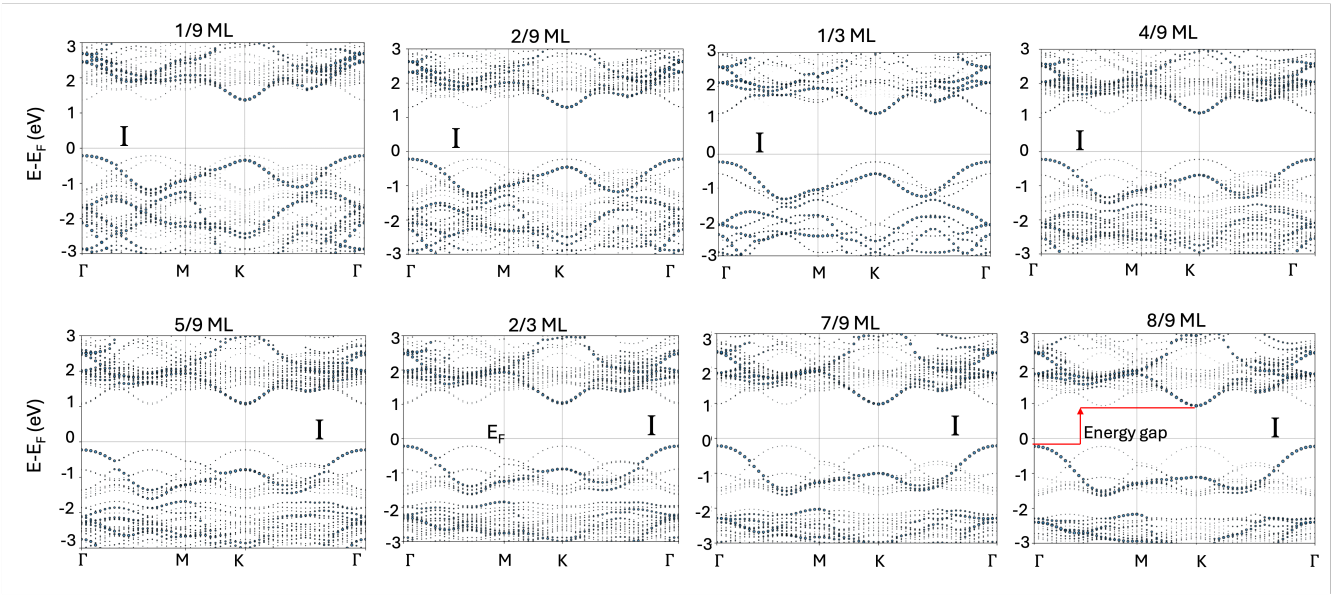

Figure 2: Effective band structures for different oxygen coverages in MoS_2. Red arrow is to identify the band gap visually. I stands for indirect transition.

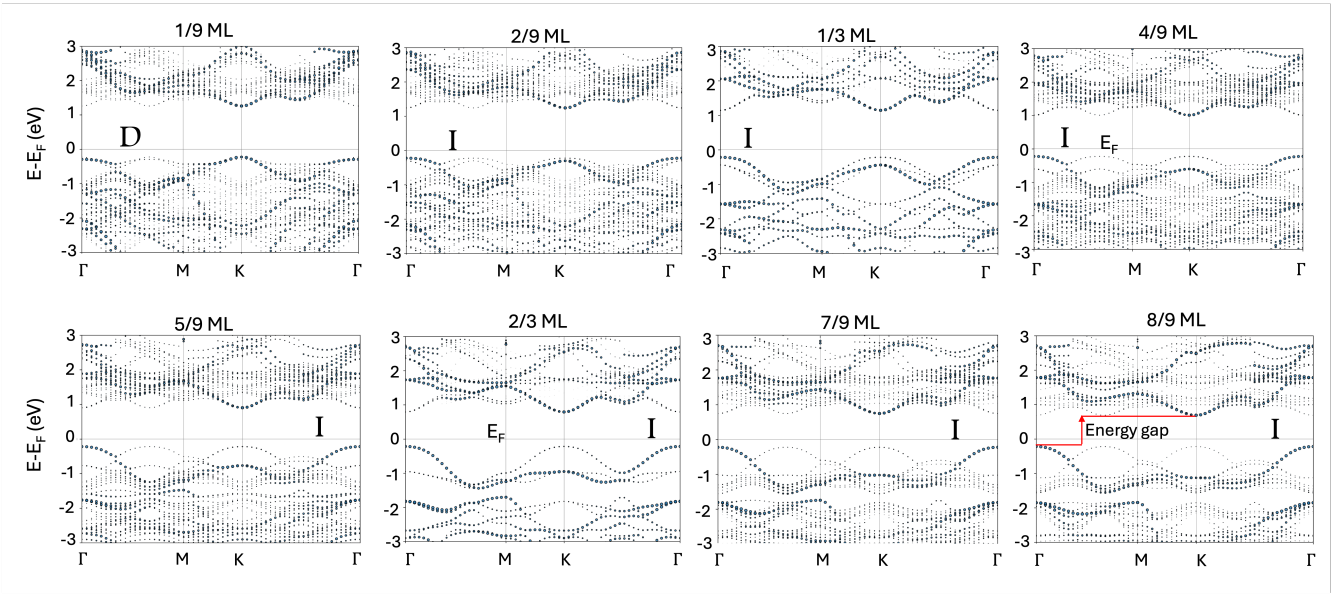

Figure 3: Effective band structures for different oxygen coverages in $MoSe_2$. Red arrow is to identify the band gap visually. D, and I stand for direct and indirect transitions, respectively.

3 Projected density of states

The PDOS helps us describe the atoms' contributions to the density of states and confirm the semiconductor character of the monolayers in each oxidation step. In our case, the PDOS helps us determine which type of orbitals contribute to the Fermi level. We calculated the PDOS for both monolayers at each oxidation stage. As the oxygen concentration increases in one plane of the systems, the sulfur and selenium atoms contribute less with energy states close to the Fermi level, while the oxygen atoms start to contribute more with electronic states close to the Fermi level. Furthermore, in both monolayers, notice that the orbitals that contribute more to the valence band are the d-orbitals of molybdenum and the p-orbitals of oxygen (MoS O and MoS eO). Here, there is an interesting change due to the oxygen substitution by S and Se p-orbitals, which do not contribute close to the Fermi energy, while in the pristine layers, these orbitals were the ones with the largest contributions. This fact is directly related to the difference in electronegativity between O and S or Se, potentially conducting to a large reactivity in the oxidized side of the monolayers.

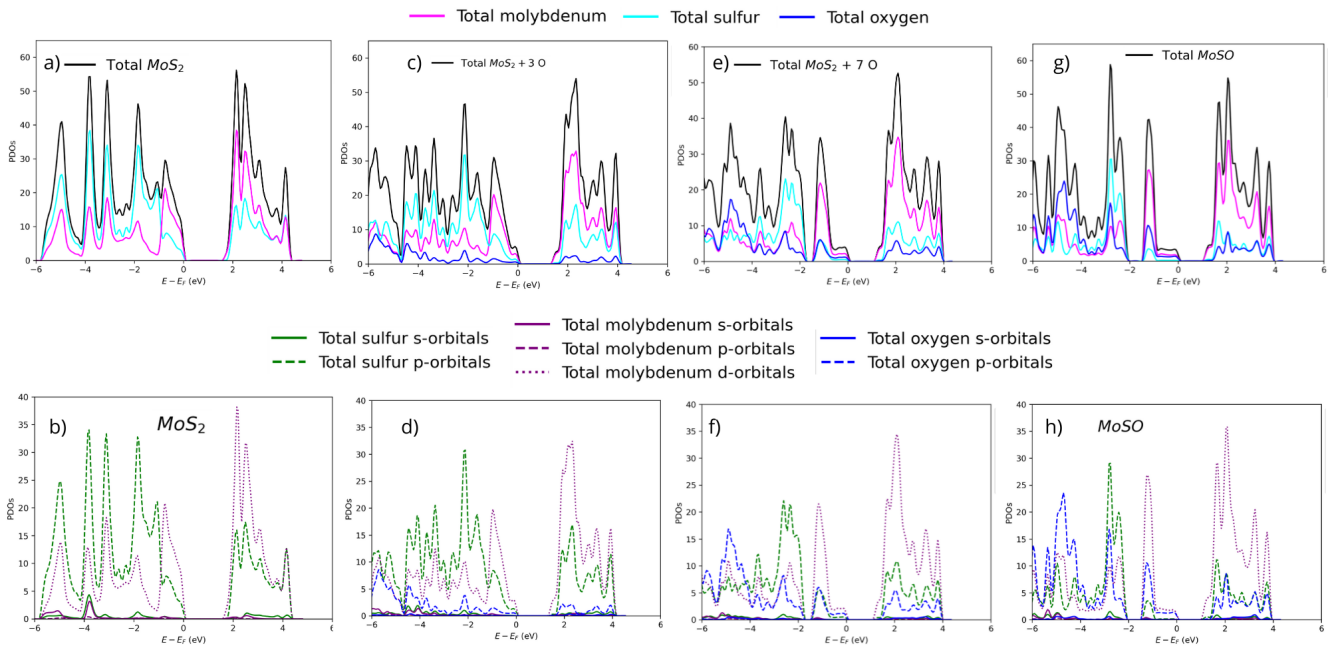

Figure 4: Projected density of states (PDOs) are separated per atom and per orbital. The labels a and b correspond to the pristine monolayer (MoS_2), b and c correspond to the monolayer with three oxygen atoms, e and f correspond to the monolayer with seven oxygen atoms, and g and h correspond to the Janus monolayer $MoSO$.

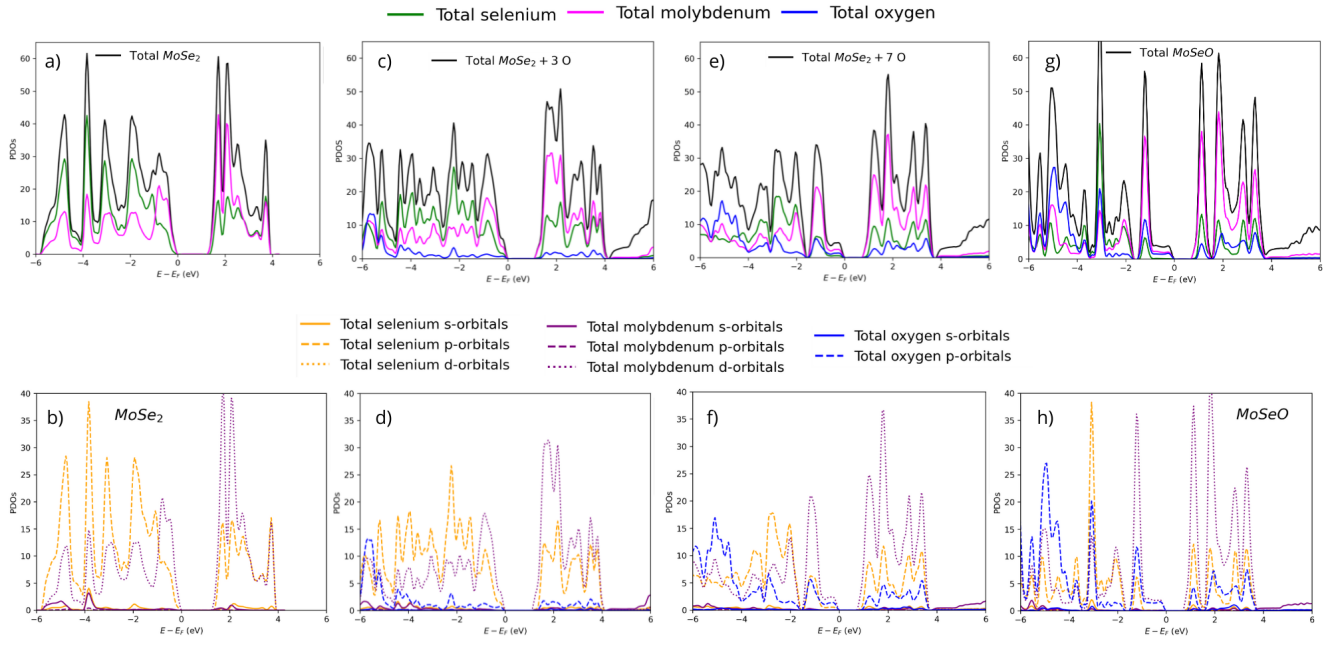

Figure 5: Projected density of states (PDOs) are separated per atom and per orbital. The labels a and b correspond to the pristine monolayer ($MoSe_2$), b and c correspond to the monolayer with three oxygen atoms, e, and f correspond to the monolayer with seven oxygen atoms, and g and h correspond to the Janus monolayer $MoSeO$.