

Band gap values of configuration 2 and configuration 4 of (a) the AlN/MoO_2 heterojunction (b) the AlN/WO_2 heterojunction.

Since the binding energies calculated for configuration 2 and configuration 4 are the same, we calculated the HSE06 band values for both configurations. The results showed that both configurations give the same result, so there is no difference between choosing configuration 2 or configuration 4.