

Supporting Information

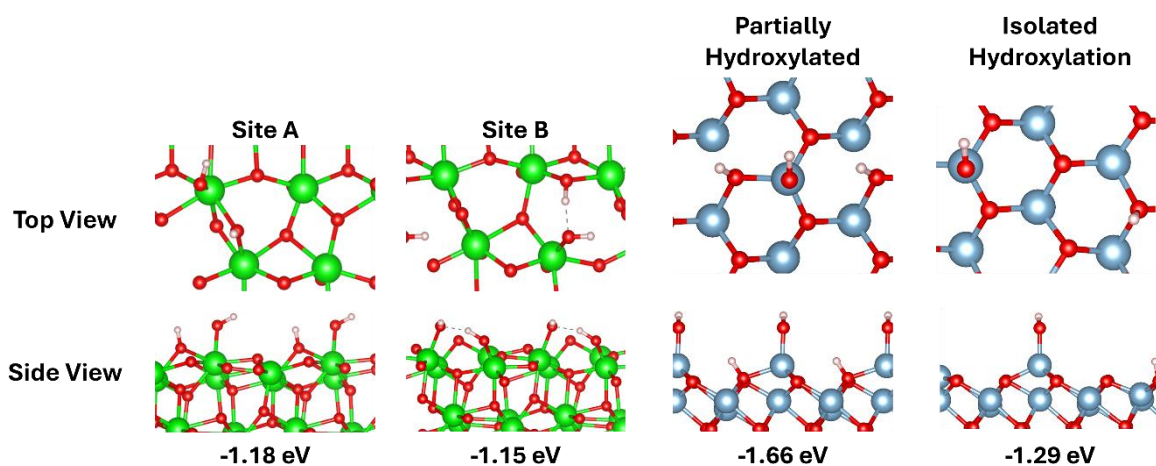


Figure 1: Top and side view of different hydroxyl surface sites on zirconia (left) and alumina (right). Single water adsorption energy informed at the bottom.

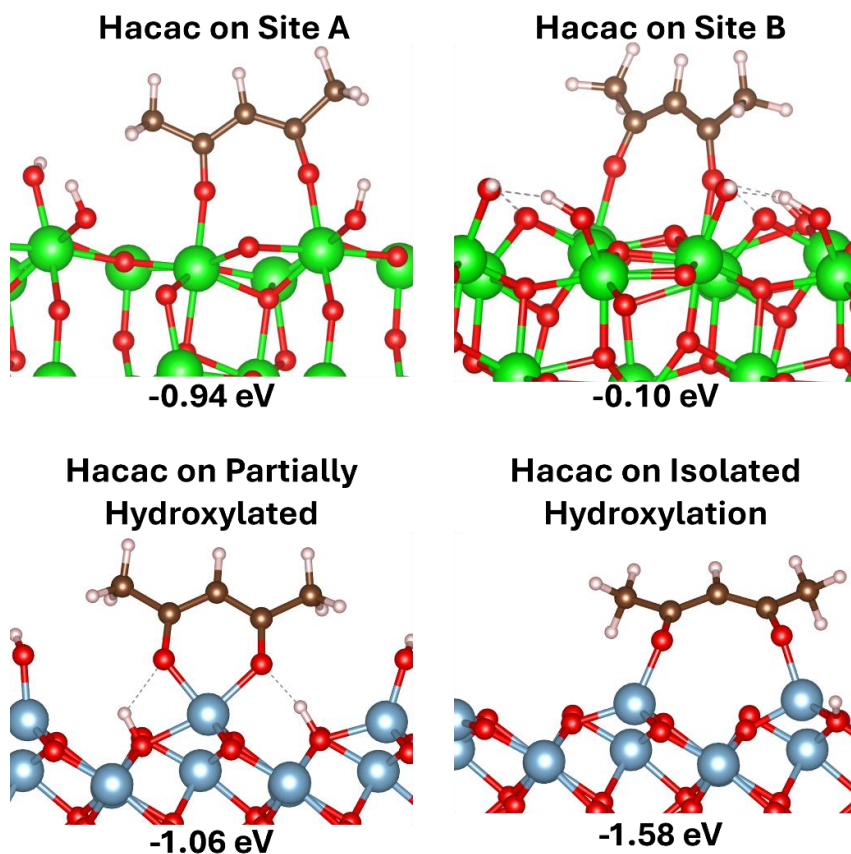


Figure 2: Side views of Hacac inhibitor adsorbed on different sites of zirconia (up) and alumina (bottom).