Study of the modes of adsorption and electronic structure of hydrogen peroxide and ethanol over TiO2 rutile (110) surface within the context of water splitting.

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Highlights

- Geometric and electronic structure of H_2O_2 adsorbed on TiO_2(110) are studied computationally.
- Its adsorption energy (fully dissociated) of 0.95 eV is comparable to that of ethanol.
- The (-) changes in the workfunction are highest for molecular adsorption and lowest for the fully dissociated mode.
- DOS indicated that the H_2O_2 HOMO level is not overlapping with O_{3c} atoms of TiO_2 surface.