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Study of the modes of adsorption and electronic structure of hydrogen peroxide and ethanol over TiO<sub>2</sub> rutile (110) surface within the context of water splitting.

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**Highlights**

- Geometric and electronic structure of  $\text{H}_2\text{O}_2$  adsorbed on  $\text{TiO}_2(110)$  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  $\text{H}_2\text{O}_2$  HOMO level is not overlapping with  $\text{O}_{3c}$  atoms of  $\text{TiO}_2$  surface.

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