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Water adsorption on  $\alpha$ -V<sub>2</sub>O<sub>5</sub> surface and absorption in V<sub>2</sub>O<sub>5</sub>•nH<sub>2</sub>O xerogel: DFT study of electronic structure

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**Highlights**

- Adsorption on V site does not change the electronic structure of  $V_2O_5$  surface.
- Adsorption on O site locates one-electron states of water within the forbidden gap.
- Water molecule electronic levels reduce the forbidden gap in xerogel  $V_2O_5 \cdot nH_2O$ .

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