Water adsorption on α-V_2O_5 surface and absorption in $V_2O_5 \bullet nH_2O$ xerogel: DFT study of electronic structure

Vitaly V. Porsev , Andrei V. Bandura , Robert A. Evarestov

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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 $V_2O_5 \cdot nH_2O$.