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H2O adsorption on PtSb₂(100) surface

We performed water adsorptions on the PtSb₂ (100) surface, where H₂O was adsorbed through oxygen on top of the surface Pt and Sb atoms. The (100) surface was explored by increasing the number of H₂O on the surface. The (100) surface was explored by increasing the number of H₂O on the surface. Lastly, the full-surface coverage (16/16 H₂O/Sb, Pt) was investigated where all Pt and Sb were adsorbed with H₂O. We observed that the H₂O molecules assemble at an angle on the surface and lie horizontal in particular for multi adsorptions. we found that in all cases the water molecule/s gave larger bond length between Pt/Sb and water O atoms (Pt–OH₂ and Sb–OH₂). As such, it indicated no bond formation between the surface and water molecules. The H₂O bond angle was slightly larger than the isolated H₂O molecule. Interestingly, for H₂O on Sb atom, we observed a bond formation between the top first surface layer Sb and the fourth surface layer Sb of Sb–Sb = 3.136 Å. This indicated that the top surface Sb relaxed deep into the surface. The calculated adsorption energy of –6.37 kJ/mol was obtained for Pt–OH₂ adsorptions, while the adsorption on Sb–OH₂ gave +10.34 kJ/mol. This showed that there was poor interaction of water on Sb atoms compared to the Pt atoms.

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