WATER ADSORPTION ON O(2X2)/Ru(0001)

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We present a combined theoretical and experimental study of water adsorption on Ru(0001) pre-covered with 0.25 monolayers (ML) of oxygen forming a (2x2) structure. Several structures were obtained by means of Density Functional Theory calculations for which STM simulations were performed and compared with experimental data.[1] Up to 0.25 monolayers the molecules bind to the exposed Ru atoms of the 2x2 unit cell via the lone pair orbitals. The molecular plane is almost parallel to the surface with its H atoms pointing towards the O atoms of the 2x2 unit cell with which they form H-bonds. The adsorption energy of this configuration is approximately 616 meV, which is 220 meV more stable than on the clean surface in a similar configuration.[2,3] This is due to the additional H-bonds with the O atoms of the unit cell. The energy shows only a weak dependence on water coverage, with a shallow minimum for a row structure at 0.125 ML. This is consistent with the STM experiments that show a tendency of the molecules to form rows at intermediate coverage. Our calculations also suggest the possible formation of water dimers near 0.25 ML.

References:

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