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. 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 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. 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: