Water adsorption on ZnO($10\bar{1}0$): From single molecules to partially dissociated monolayers*

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Abstract

Static and dynamic density functional calculations have been used to study the structure and energetics of water adsorbed on the main cleavage plane of ZnO. In the single molecule limit we find that molecular adsorption is strongly preferred. The water binding energy increases for higher coverages due to an almost isotropic attractive water–water interaction which leads to clustering and formation of monolayer islands in the low water coverage regime. A thermodynamic analysis further shows that the full water monolayer is clearly the most stable phase until water starts to desorb. The water monolayer is even more stabilized by a partial dissociation of the water molecules, yielding as most stable configuration a (2×1) superstructure where every second water molecule is cleaved. The dissociation barrier for this process is very small which allows for an auto–dissociation of the water molecules even at low temperatures as observed experimentally. Finally we find that the energy cost involved to form [$1\bar{2}10$]–oriented domain boundaries between (2×1) patches with different orientation is almost negligible which explains the abundance of such domain boundaries in STM images.