

Strained Hydrogen Bonded Networks on Metal Surfaces

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The metal-water interface is important for various research areas. Naturally, most of the published research work focuses on the direct interactions between the metal and the water adjacent to it.

The model of the virtual surface allows us to shift the focus from the metal-water to the water-water interactions. A virtual surface is a mesh of auxiliary geometrical points, which is used to mimic the bonding geometry of the interface in quantum chemical calculations independently of the precise electronic structure of the metal surface. Hence small water clusters on a hexagonal virtual metal surface are used to analyze the growth mechanism and the properties of the water layer at the interface.

Calculations for the water trimer on a hexagonal virtual surface predict correctly the experimentally observed transition between a two dimensional growth mechanism preferring direct water-metal bonds and a three dimensional one preferring the formation of water islands via water-water interactions.

The water hexamer can be used to analyse the structure of the water bilayer itself. In agreement with UHV results (ultra high vacuum) our calculations predict the water molecules to rest parallel to the metal surface on metals with large values for the surface lattice constant d_1 , while ring puckering in the water hexamer can be observed on metals with small values for d_1 .

The smallest water cluster observed in UHV experiments so far seems to be the nonamer. Calculations using the virtual surface can be used to explain the enhanced stability of individual nonamers in comparison with isolated hexamers or large water islands.

All our calculations show clearly, that the hydrogen bonded network within the water layers is of a great importance for the metal-water interface and that most properties of the interface depend much stronger on the geometrical strain acting on this network than on the metal-water interactions.