Chemisorption of CH3OH on Si(111)-7x7: Density-functional theory calculations

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CH_3OH is known to dissociate into CH_3O + H on the Si(111)-(7x7) surface. Despite many studies, however, the reactive site on the Si(111)-(7x7) surface towards CH_3OH molecules has not yet been identified. We investigate the chemisorption mechanism of CH_3OH on Si(111)-(7x7) using density-functional theory (DFT) calculations. The adatom site is found to be reactive towards CH_3OH, and the restatom site repulsive towards CH_3OH. CH_3OH molecules adsorbed on the adatom dissociate into CH_3O + H without a barrier, thus forming surface species CH_3O-Si (adatom) and H-Si (restatom). The present reaction picture of the higher adatom reactivity is consistent with a dissociation geometry reported by a scanning tunneling microscopy study[1], but differs from the prediction of photoemission spectroscopy studies[2,3] and a DFT study[4] that the restatom is more reactive than the adatom towards CH_3OH. The origin of the discrepancy between the present and the previous studies will be discussed.

References

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