First principles study of the Ga(10\bar{1}0)/water interface

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Pure GaN is a water-splitting photocatalyst which works in UV light. A first-principles study shows monolayer of water molecules on the (10\bar{1}0) surface of wurtzite GaN have negligible barrier to be dissociated into OH\(^-\) which bind to Ga\(^+\) and H\(^+\) which bind to N\(^-\).

We present an ab initio molecule dynamics study of bulk water molecules on top of the (10\bar{1}0) surface of GaN. The dissociation of water molecules happens very fast within the first ps of simulation. We find that OH\(^-\) · · · OH\(^-\) Hydrogen bond are formed between two OH\(^-\) on the surface. We propose two different types of OH\(^-\) based on the different H-bond structure between them and the bulk water molecules. We also calculate the vibrational spectrum and the interface electronic structure of the semiconductor/aqueous system.

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