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Excess proton at water/hydrophobic interfaces: An ab initio Molecular Dynamics study

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Recently, both experimental and computational studies suggest that protons are preferably located on water/hydrophobic surfaces [1, 2]. The reasons are still unclear, although this is shown to be linked with the electronic structure of hydronium ions [3]. Therefore, a fully understanding of this phenomenon is highly desirable and will impact significantly on how we look at biological interfaces, such as presented in protein folding, protein/protein interaction and lipid membrane.

We investigate here the structure and the energetics of an excess proton at the water/hydrophobic surface with ab initio molecular dynamics for a system size about 1800 atoms. The free energy profile of the proton to the surface, constructed by using the metadynamics method [4, 5], gives the state of the art answer to this fundamental question.

References

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