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Structure and dynamics of the liquid water-ZnO($10\bar{1}0$) interface from first principles GABRIELE TOCCI, ANGELOS MICHAELIDES, London Centre for Nanotechnology & University College London, Department of Chemistry — Liquid water-metal oxide interfaces are of fundamental and technological interest. In this context, the water-ZnO($10\bar{1}0$) interface is an extensively studied system, which is also relevant for instance to the field of heterogeneous catalysis and photocatalysis. Yet, whether or not water dissociates at this surface at coverages exceeding one monolayer is still a matter of debate. Likewise questions about proton transfer to the surface, water diffusion and rearrangement within the hydrogen-bonded network remain unanswered. Here we report the first density functional theory (DFT) molecular dynamics study of a liquid water film on ZnO($10\bar{1}0$) and of water at monolayer coverages. The water structure obtained for the first layer in the liquid simulation differs quite significantly from that at monolayer coverage. Hydrogen bonding between the first layer and the water overlayer plays a crucial role in the stabilisation of the new adsorption structure. Rapid proton transfer and rattling within the hydrogen bonding network at the interface is observed and analysed in detail. On the whole, this study provides considerable new insight into water structure and dynamics and proton transfer at ZnO($10\bar{1}0$) and in the field of liquid water-metal oxides interfaces in general.

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