

Local order of liquid water at the electrochemical interface

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Understanding the aqueous electrochemical interface in an atomic level is of fundamental importance in many areas, such as catalysis and materials science.

In this work we analyze in detail the structural, dynamic and energetic properties of liquid-water interacting with (111) Pd and Au surfaces at ambient temperature, using first principles molecular dynamics, with and without van der Waals interactions. We show that, contrary to what was found when studying ice-like water layers, van der Waals interactions play a critical role in modeling the aqueous/electrode interface.

We observe the formation of domains of preferred orientations of the water molecules at the metal surface, which is strongly dependent on the charge transfer that occurs at the interface.