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Local order of liquid water at the electrochemical interface[1]
MARIVI FERNANDEZ SERRA, LUANA PEDROZA, State Univ of NY- Stony Brook — 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 show the differences in the ordering of water at the interface for Pd and Au, and we explain the change in work functions of these two metals in aqueous solution.

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