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First principles molecular dynamics of metal/water interfaces under bias potential[1] LUANA PEDROZA, State Univ of NY- Stony Brook, PEDRO BRANDIMARTE, Univ of Sao Paulo - Sao Paulo, Brazil, ALEXANDRE ROCHA, IFT-UNESP, Sao Paulo, Brazil, MARIVI FERNANDEZ-SERRA, State Univ of NY- Stony Brook — Understanding the interaction of the water-metal system at an atomic level is extremely important in electrocatalysts for fuel cells, photocatalysis among other systems. The question of the interface energetics involves a detailed study of the nature of the interactions between water-water and water-substrate. A first principles description of all components of the system is the most appropriate methodology in order to advance understanding of electrochemically processes. In this work we describe, using first principles molecular dynamics simulations, the dynamics of a combined surface(Au and Pd)/water system both in the presence and absence of an external bias potential applied to the electrodes, as one would come across in electrochemistry. This is accomplished using a combination of density functional theory (DFT) and non-equilibrium Green's functions methods (NEGF), thus accounting for the fact that one is dealing with an out-of-equilibrium open system, with and without van der Waals interactions.

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