

Abstract Submitted
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Bias-dependent local structure of water molecules at an electrochemical interface¹ LUANA PEDROZA, ICTP-SAIFR - Brazil, PEDRO BRANDIMARTE, University of Sao Paulo - Brazil, ALEXANDRE R. ROCHA, IFT-UNESP, Brazil, MARIVI FERNANDEZ-SERRA, Stony Brook University — Following the need for new - and renewable - sources of energy worldwide, fuel cells using electrocatalysts can be thought of as a viable option. Understanding the local structure of water molecules at the interfaces of the metallic electrodes is a key problem. Notably the system is under an external potential bias, which makes the task of simulating this setup difficult. A first principle description of all components of the system is the most appropriate methodology in order to advance understanding of electrochemical processes. There, the metal is usually charged. To correctly compute the effect of an external bias potential applied to electrodes, we combine density functional theory (DFT) and non-equilibrium Green's functions methods (NEGF), with and without van der Waals interactions. In this work, we apply this methodology to study the electronic properties and forces of one water molecule and water monolayer at the interface of gold electrodes. We find that the water molecule has a different torque direction depending on the sign of the bias applied. We also show that it changes the position of the most stable configuration indicating that the external bias plays an important role in the structural properties of the interface.

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