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First principle simulations of a bias-dependent electrochemical cell[1] LUANA PEDROZA, Univ Federal do ABC, Brazil, PEDRO BRANDIMARTE, CFM CSIC-UPV/EHU and DIPC, Spain, MARIVI FERNANDEZ-SERRA, Stony Brook University, USA, ALEXANDRE R. ROCHA, IFT-UNESP, Brazil — Understanding the local structure of water molecules at the interfaces of metallic electrodes is a key problem in many electrochemical problems. Notably the system is under an external potential bias, which makes the task of simulating this setup difficult. To correctly compute the effect of an external bias potential applied to electrodes, we combine density functional theory and non-equilibrium Green's functions methods, with and without van der Waals interactions. In this work, we apply this methodology to study the electronic properties and forces of water molecules at the interface of different metallic electrodes. We find that the water molecule is sensitive to the sign and magnitude of the applied bias. We also show that it changes the position and orientation 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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