Atomistic simulations of water/metal interfaces

Luana S. Pedroza[1]*
[1]*Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, Santo André, Brasil*

*email: l.pedroza@ufabc.edu.br

The interest in renewable sources of energy has demanded a deeper understanding of the electrochemical process since it is one of the pillars of green energy sources. Therefore, first principles computer simulations, notably Density Functional Theory (DFT) ones, have provided crucial insights into the molecular and electronic structure of water-metal interfaces, dealing with charge and energy transfer reactions, adsorption, and heterogeneous catalysis. Despite these recent developments, the atomistic description of the structural and vibrational properties of the water-metal interface under an applied bias potential is still a challenge. In this work we show how we can obtain these properties using DFT coupled to Non-Equilibrium Green's Functions, and analyze the results for Gold and Palladium water interfaces. We also discuss how we can increase the system size and simulation time, still at the DFT-level, using Neural Network force fields.