Title: **Addressing electrified water-metal interfaces at the atomic level with TranSIESTA**

Author: **Pablo Ordejón** - Catalan Institute of Nanoscience and Nanotechnology - ICN2 (CSIC-BIST), Barcelona, Spain

Abstract:
SIESTA [1,2] is one of the flagship codes of the MaX CoE. The TranSIESTA method and code [3,4] were developed within the SIESTA project to study problems involving steady-state non-equilibrium problems in nanoscale costrictions, where an external electric bias is applied between the two sides of the constriction, establishing a steady electric current. Non-equilibrium Green's Functions are used there to solve the problem, as they can deal with open, non periodic systems (leads plus nanoconstriction) driven out of equilibrum (external applied bias). This machinery can be also used to study electrified solid/liquid interfaces [5], where an external bias is applied to the solid electrode. Here, one is not concerned with the quantum electronic transport, but with the effect of the external bias on the properties and the chemical reactions induced at the metal/liquid interface. I will show examples of application of this idea, as a proof of concept for future realistic, atomistic first-principles simulations of electrochemical processes. I will also discuss issues of efficiency of the code in HPC environments.

References:

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