# DENSITY-FUNCTIONAL THEORY (DFT) CALCULATIONS FOR WATER CLUSTERS AND THE ADSORPTION OF WATER AT METAL SURFACES

The participants will use the pseudo-potential plane wave code PWSCF and perform DFT calculations on water clusters and the adsorption of water at a typical metal surface.

The experiment consists of two parts:

• Determination of the optimized geometries of simple water clusters including the water monomer ($H_2O$) up to water tetramer ($(H_2O)_4$). The binding energies of these water clusters will be evaluated, plotted and discussed, and the hydrogen bond patterns will be analyzed.

• A slab model of the copper (111) surface will be constructed. For this purpose first the copper lattice constant needs to be determined. Then, a single water molecule will be placed at the surface and its adsorption geometry and energy will be investigated. The role of van der Waals interactions will be discussed.