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 (H2O) up to water tetramer ((H2O)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.