Selected Topics

1. Ab initio modelling of biological systems
2. Earth and planetary materials

NO Chemistry: Interaction with water clusters

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NO clusters play an important role in both atmospheric and biological chemistry, however their interaction with water is insufficiently understood. It has been shown previously that the water dimer plays an important role as a greenhouse gas, but its contribution to the IR absorption spectra is still under debate. Of additional atmospheric importance is the solvation and interaction of atmospheric pollutants, such as NO and CO, with small water clusters $(H_2O)_N$, (N=1,3), which is still to be understood.

Here we present an *ab initio* computational study, based on DFT and TD-DFT, on the water dimer, $(H_2O)_2$, and the (H_2O-NO) complex. After characterisation of the ground state properties, we focus our attention on the calculation of their spectroscopic profile.