

The problem of dispersion interaction in the DFT is reviewed, followed by a systematic study of the behaviour, in particular the transferability, of the LAP method. Dispersion is a kind of van der Waals forces, dominant in important molecular systems such as biomolecules or adsorption systems. The DFT is an ever increasingly used method for modelling chemical systems. However, dispersion is rendered rather poorly in the DFT. We give an illustration of the problem and present some known correction methods. One of them is the local atomic potential (LAP) approach which we develop further from its original formulation, and this enables us to exactly match the benchmark interaction curves. We apply this development on systems consisting of benzene and a noble gas. We construct the LAPs for noble gas atoms and for carbon. It is shown that the LAP approach is poorly transferable based on our calculations. The investigation reported in this bachelor's thesis represents the first attempt for a detailed study of the behaviour of the LAP method.