# Introduction into DFTB

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## 1 Geometry optimization

- **1Waterdimer**:
  Optimize the structures of the three water dimers wat1.gen, wat2.gen and wat3.gen.
  - Use cgr for that (option 4) and view the result with molden. What is the energy difference and what is the dimer binding energy?
  - Use steepest descent for that (option 3)
- Do the same for the strongly H-bonded systems in **2Stronghbonds**: what are the binding energies compared to the water dimer?
- **3Watercluster**:
  Optimize the waterclusters and calculate the binding energy of every one: Plot the binding energy vs. cluster size. Use the shell script 'R' to achieve this.
- Simple peptides: **4peptides**
  - Use the script from 3Watercluster to convert the peptide structures to xyz-format: view them with molden.
  - Optimize all structures with the script and look at the relative energies. Are all conformers stable?

## 2 Dispersion

- Dispersion: do the examples in **5DISPERSION-example**

- **6DNAbasepairs**:
  Optimize the structures with and without dispersion. What do you find?

- **7benzene:** optimize with and without dispersion.

- **8peptides:** Only do single point energies with Dispersion for the structures and for those of 4peptides. Get a feeling, at which size dispersion starts to matter.

# 3 Vibrational frequencies

- Calculate the vibrational frequencies of water in **10vib/h2o**.

# 4 MD

Look at the inputfile doh.dyn in **11MD**. After running, move all out.gen*v to another place, and then run Rcollect to get the trajectory XMO.