# Exercise 04

# Equations of motion

**Deadline:** Please hand in your protocol in pdf format by Thursday, the 24th of May 2018, 10 am to jan.joswig@fu-berlin.de. The protocol should contain analytical solutions, short discussions, Python-code and plots.

## 4.1 Integration of the equation of motion (100 points)

In this task you should solve the equation of motion for a harmonic diatomic vibration analytically and numerically. Write a commented python script for the numeric solution. Both ways should be compared. The harmonic potential is given as:

$$U(q) = \frac{k}{2}(q - q_0)^2 \tag{1}$$

Assume a reduced mass of $\mu = 6.00\,\mathrm{u}$, a force constant of $k = 6.15 \times 10^5\,\mathrm{kJ\,mol^{-1}\,nm^{-2}}$ and an equilibrium bond distance of $q_0 = 0.134\,\mathrm{nm}$ (corresponding to a C=C bond). Use molecular units throughout your calculations (compare script p. 190).

1. Calculate the angular frequency $\omega$, the frequency $f$ and the period length $T$. Give the equation of motion for the harmonic oscillation and derive the analytical solution $q(t)$.
2. Let the bond distance at time $t = 0$ be $q(0) = 0.187\,\mathrm{nm}$ and the velocity $v(0) = \dot{q}(0) = 0\,\mathrm{nm\,ps^{-1}}$. Draw a curve for the analytical solutions to $q(t)$ and $\dot{q}(t)$.
3. What would be an appropriate time step $\tau$ for the numerical solution?
4. Calculate $q(t + \tau)$ and $\dot{q}(t + \tau)$ starting from $t = 0$, $q(0) = 0.187\,\mathrm{nm}$ and $v(0) = 0\,\mathrm{nm\,ps^{-1}}$.
5. Write a script that solves the equation of motion by a) an Euler algorithm and b) an Verlet algorithm. The result should be visualised graphically.
6. Let the program run for an appropriate number of timesteps (at least 100 fs) and variate $\tau$ (at constant simulation lengths), so that the difference between the two algorithms and between (nearly) exact and completely wrong behaviour becomes obvious.
7. Discuss shortly the difference between analytical and numerical solution.