Exercise 03

Equations of motion (short)

Deadline: Please hand in your protocol in pdf format by Thursday, the 17th of May 2018, 10 am to jan.joswig@fu-berlin.de. The protocol should contain analytical solutions, short discussions, Python-code and plots.

3.1 Harmonic oscillator (100 points)

Build a harmonic oscillator model for the following stretching vibrations:

1. C–H: Wavenumber $\tilde{\nu} = \frac{\omega}{2\pi c} = 3000\,\mathrm{cm}^{-1}$
2. C–D: $\tilde{\nu} = 2100\,\mathrm{cm}^{-1}$
3. C–C: $\tilde{\nu} = 1000\,\mathrm{cm}^{-1}$
4. C=C: $\tilde{\nu} = 1700\,\mathrm{cm}^{-1}$
5. C≡H: $\tilde{\nu} = 2200\,\mathrm{cm}^{-1}$

A harmonic potential is given by:

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

1. Look up the definition of *wavenumber* and convert the values above to frequencies f and vibration periods T.
2. Calculate reduced mass μ and force constant k for the examples above.
3. Discuss the influence of μ and chemical bond strength on the vibrational frequencies for the given examples.