Übersicht über den Vorlesungsinhalt der "Special lecture in physical chemistry: Computational modelling in python"

Dr. Inga Ulusoy

1. Introduction to Computer Modelling
   - basic python scripts (Problem1)
   - linear regression (Problem2)
2. Interpolation
   - linear interpolation and cubic splines (Problem3)
   - functions and classes in python; the "programming paradigm" (Problem4)
3. Python fundamentals
   - lists, tuples, arrays, loops, case selection (Problem5)
   - 2D and 3D plotting (Problem6)
4. Integration
   - magic functions (magic functions)
   - numerical integration methods (Problem7)
5. Differentiation
   - numerical differentiation (Problem8)
   - ordinary differential equations, classical harmonic oscillator (Problem9)
6. Particle in a box
   - quantum mechanics on a computer
   - solutions to eigensystems (Problem10)
7. Particle in a box II and quantum harmonic oscillator
   - quantum dynamics on a computer and superposition states (Problem11)
   - eigenstates of the quantum harmonic and anharmonic oscillator (Problem12)
8. Quantum harmonic oscillator II
   - quantum dynamics (Problem13)
   - connection to spectroscopy, Fourier transforms and filtering methods (Problem14)
9. Presentation of the programs developed through weeks 6-8 (Problems 10-14)
   - Students will present their programs either in a recorded movie or in a live lecture on heiconf (preferred)
10. Quantum chemistry
    - using libraries for electronic structure calculations (Problem15)
11. Machine learning
    - fundamentals
    - Pandas and TensorFlow (Problem16, Problem17)
12. Machine learning: Keras/TensorFlow
    - regression (Problem18)
13. Machine learning: Keras/TensorFlow
    - classification (Problem19)

The topics in the weeks marked in blue are combined and the task for these weeks encompasses several lectures, as you will write a program containing the different examples. This is an optional task and will not be graded, but is highly recommended.