Summary of the online lecture Advanced Atomic and Molecular Physics (SoSe 2020)

1. Repetition atomic and molecular physics (script online)
    a. Einstein coefficients
    b. Laser concept
    c. Simple model systems: Particle in a box, harmonic oscillator, anharmonic oscillator
    d. Atomic orbitals, molecular orbitals (LCAO)
    e. Light matter interaction, selection rules, transitions
        i. Dipole approximation, Quadrupole approximation
        ii. Line shapes, pulse widths
    f. Born-Oppenheimer approximation
        i. Electronic and vibrational wavefunction
        ii. Limitations of BO-approximation: vibronic progression
2. Linear spectroscopic methods for molecules
    a. Visible spectroscopy
        i. Allowed transitions, symmetry
        ii. Gouterman model, mixing of states
        iii. Charge transfer transitions
        iv. Dichroism
    b. Fluorescence spectroscopy
        i. Lifetimes, rate constants, yields
        ii. Stokes shift
        iii. Mirror image law
    c. Dipole coupling spectroscopy
        i. FRET, Dexter and others
    d. Infrared spectroscopy
        i. IR-active vibrations, symmetry
        ii. Gas phase spectroscopy
            1. Lines, populations, isotopomers
            2. Rotational contributions, Vibrational-rot. contributions, R-,P-, Q-branch, transitions, selection rules
            3. Temperature sensitivity of lines and lasers
            4. FLIP-device, LiMAx-Test
        iii. FTIR spectroscopy
            1. Techniques, steady state, time-resolved
        iv. Couplings
            1. Davydov-coupling
            2. Fermi-resonance
            3. Overtones, combinational bands
    e. Raman spectroscopy
            1. Raman active vibrations, symmetry
            2. Energy relaxation and pseudo-temperature in molecules
    f. CD spectroscopy
        i. Transitions, helicity, secondary structure information
    g. X-ray diffraction
        i. From diffraction patterns to structures
3. Non-linear processes, light conversion processes
    a. SHG, SFG, DFG, OPG
    b. Self-phase modulation

c. Kerr-gating
d. Detection of ultrashort pulses
    i. Autocorrelator
    ii. FROG
    iii. Frequency resolved Kerr gating
e. Generation of ultrashort pulses
    i. OPA
    ii. NOPA

4. Non-linear and time-resolved spectroscopic methods for molecules
    a. Fluorescence spectroscopy
        i. Up-conversion, coherent oscillations
        ii. Anisotropy spectroscopy, rotation correlation
    b. Non-linear formalism, Feynman diagrams
        i. PFID
        ii. Pump-probe spectroscopy
        iii. Photon-echo spectroscopy
        iv. 2D-IR spectroscopy, signals during pulse overlap
    c. Pump-Probe spectroscopy
        i. VIS-pump VIS probe
            1. Reaction in “dyes”, photoisomerization, dissociation, polymerization
            2. Excited state electron transfer
            3. Excited state proton transfer
            4. Photodynamic therapy
        ii. VIS-pump IR probe
            1. Reaction in “dyes”, photoisomerization, dissociation, polymerization
            2. Excited state electron transfer
            3. Excited state proton transfer
            4. Hydrogen bond changes
        iii. IR-pump IR probe
            1. Reaction in “dyes”, Energy relaxation, hot ground states
            2. Dynamics of hydrogen bonds
            3. Dissociation reaction, ladder climbing
            4. Activation energy, thermal driven reactions
            5. Bimolecular reaction, alcoholysis reaction
    d. 2D – IR spectroscopy
    e. 2D – VIS spectroscopy