Tutorial on SHARC and excited state dynamics

Monday 3rd October (Währinger Strasse 17)	
9:00-9:30	**González**: Welcome and practical information
9:30-10:30	**González: Lecture 1.** Basic concepts in photochemistry • Motivation • Jablonski diagram • The time-dependent (TDSE) and time-independent (TISE) Schrödinger equations. • Solving the time-independent Schrödinger equation (TISE): Born-Oppenheimer approximation, non-adiabatic couplings • Adiabatic versus diabatic representations • Conical intersections and avoided crossings
10:30-11:00	Coffee Break
11:00-12:30	**González**: **Lecture 2.** Solving the electronic TISE. Methods overview for excited states • Single reference methods • Multi-reference methods • Advantages and disadvantages • Useful guide for excited state computations
12:30-14:00	Lunch Break at Königshofer
14:00-15:30	**Plasser: Lecture 3.** A closer look into electronic wavefunctions • Excited-State Phenomenology • Reduced Density Matrices • Transition / Difference Density Matrices • Analysis of Exciton Wavefunctions • Introduction to TheoDORE
15:30-16:00	Coffee Break
16:00-18:30	**Plasser: Hands On 1**. Potential energy curves and wavefunction analysis on NaI
19:00-	Dinner at Culinarium

Tuesday 4th October (Währinger Strasse 17)	
9:00-10:30	**Oppel**: **Lecture 4.** Introduction to quantum dynamics • Solving the nuclear TISE • Wavepackets • Solving the nuclear TDSE • Following wavepackets experimentally: Pump-probe
10:30-11:00	Coffee Break
11:00-13:00	**Marquetand: Hands On 2**. Wavepacket propagation on NaI
13:00-14:30	Lunch Break at Königshofer
14:30-16:00	**Marquetand: Lecture 5.** From quantum dynamics to classical and semiclassical dynamics • Quantum dynamical effects • Classical molecular dynamics • Ab initio molecular dynamics • Methods overview
16:00-16:30	Coffee Break
16:30-18:30	**Nogueira: Hands On 3**. Classical Molecular Dynamics on pyrrole • Choice of suitable force field parameters • Generation of an ensemble from classical molecular dynamics • Calculation of absorption spectrum
19:00-	Dinner at Bierheuriger zum Gangl

Wednesday 5th October (Währinger Strasse 17)	
9:00-10:30	**Mai: Lecture 6.** Introduction to surface hopping • Tully fewest switches method • Representations, potential vs. nonadiabatic couplings (revisited) • SHARC: State transformations
10:30-11:00	Coffee Break
11:00-12:30	**Mai: Lecture 7.** SHARC workflow • Initial conditions (Frequency calculation, Wigner, initial state) • Propagation (Loop over nuclear, electronic dynamics, ab initio calls)
12:30-14:00	Lunch Break at Königshofer

14:00-16:00	**Mai: Hands On 4**. Wigner distribution in pyrrole • Generation of initial conditions • Visualization of geometry distributions • Vertical spectrum vs. convoluted spectrum
16:00-16:30	Coffee Break
16:30-18:00	**Mai: Hands On 5**. SHARC Dynamics in pyrrole • Running trajectories • Monitoring trajectories
19:00-	Dinner at Pizza Angolo No. 22

Thursday 6th October (Währinger Strasse 17)	
9:00-10:30	**Mai: Hands On 6**. Analysis of the ensemble. Part I • Populations and transition numbers • Kinetics
10:30-11:00	Coffee Break
11:00-12:30	**Mai: Hands On 6**. Analysis of the ensemble. Part II • Monitoring changes in molecular structures • Essential dynamics analysis • Hopping geometries
12:30-14:00	Lunch Break at Königshofer
14:00-15:00	**Mai: Hands On 6**. Analysis of the ensemble. Part III • Proposing a mechanism
15:00-16:00	**Marquetand: Lecture 8.** Concluding remarks • Advantages and Pitfalls • Comparison with experiment
17:00-19:00	Haus des Meeres. Tour on SHARKs
20:30-	Dinner at 7STERN BRÄU

Friday 7th October (Sky Lounge, Oscar-Morgenstern-Platz 1)	
9:00-11:00	**Graham Worth.** Complete Quantum Dynamics: From Grid-based to Direct Methods via MCTDH • Chemical Dynamics: why a full quantum solution is needed • Solving the TDSE using a grid representation • Larger System: The MCTDH Method • Solving the potential problem: Direct Dynamics and DD-vMCG
11:00-11:30	Coffee Break
11:30-13:00	**Basile Curchod.** Ab initio multiple spawning • Nonadiabatic dynamics with Gaussian basis functions • Full Multiple Spawning • Approximations towards Ab Initio Multiple Spawning • On-the-fly Ab Initio Multiple Spawning • Extensions of Ab Initio Multiple Spawning • Selected applications
13:00-14:30	Lunch Break
14:30-16:00	**Gerrit Groenhoff.** Watching excited state dynamics in the lab • Molecular movies • Multi-scale simulations • Time-resolved spectroscopy • Time-resolved serial femtosecond x-ray diffraction (TR-SFX) • Time-resolved x-ray scattering (TR-WAXS/SAXS) • Communicating with experimentalists
16:00-16:30	Coffee Break
16:30-18:00	**Marquetand.** Group discussions • Big challenges in chemical dynamics theoretical developments • Future application areas • Better interplay between experiment and theory • Visions
18:00-18:15	**Closing and evaluation**
19:30-	Banquet dinner at Fuhrgassl-Huber