Time	Monday	Tuesday	Wednesday	Thursday	Friday
08:30 – 09:00		Coffee/tea	Coffee/tea	Coffee/tea	Coffee/tea
09:00 – 09:30		J. Neugebauer **Subsystem-based TDDFT**	*J. Westermayr* **Deep learning for excited states**	*R. Baer* **Stochastic Vector Techniques**	*L. Visscher* **Novel methods for theoretical spectroscopy**
09:30 – 10:00	**Welcome by Lorentz Center**	*C. Manio*	*F. Buda*	*E. Coccia*	*R. van den Berg* **AI4Science at Microsoft Research**
10:00 – 10:30	**Introduction to the Workshop**	***Discussions*** *Challenges for Theoretical Spectroscopy* **+** ***Coffee Break***	***Discussions*** *Machine Learning in Theoretical Spectroscopy* **+** ***Coffee Break***	***Discussions*** *Technical Implementations* **+** ***Coffee Break***	
10:30 – 11:00	Fundamentals 1 *R. Baer* **DFT/TDDFT**				***Discussions*** *Future Developments and Frontiers* **+** ***Coffee Break***
11:00 – 11:30		*M. Barbatti* **Nonadiabatic dynamics in the long timescale**	*M. Rupp* **Predicting Spectra with atomistic ML**	*D. Golze* **Core & valence excitations: GW in large systems**	
11:30 – 12:00		*M. Brütting*		*A. Förster*	**Closing**
12:00 – 12:30					**Lunch**
12:30 – 13:00	**Lunch & Informal Discussions**	**Lunch & Informal Discussions**	**Lunch & Informal Discussions**	**Lunch & Informal Discussions**	
13:00 -13:30					
13:30 – 14:00					
14:00 – 14:30	Fundamentals 2 *P. Rinke* **GW/BSE**	*J. Martirez* **Capped density functional embedding**	*I. Duchemin* **All-electron GW and BSE in complex systems**	*M. Del Ben* **Portability Strategies for Next Gen Exascale**	
14:30 – 15:00		*H. Bahmann* **Flexible hybrid density functionals**	*J. Wilhelm* **Low-scaling GW calculations**	*M. Rohlfing* **LDA+GdW for layered materials**	
15:00 – 15:30					
15:30 – 16:00	Coffee Break	Coffee Break	**Exploring Leiden**	***Discussions*** *Embedding Methods* **+** ***Coffee Break***	
16:00 – 16:30	Fundamentals 3 *C. Filippi* **QMC**	*C. Filippi* **QMC for excited states**			
16:30 – 17:00					
17:00 – 17:30		**Poster Session**		*P. Rinke* **Frontiers in MBPT**	
17:30 – 18:00	**Poster Pitches**			*C. Guido*	
18:00 – 18:30			**Dinner**		
18:30 –	**Wine & Cheese**				

Monday, March 20	
09:30 – 10:00	**Welcome by the Lorentz Center**
10:00 – 10:30	Björn Baumeier, Linn Leppert, Stephan Kümmel, Sandra Luber **Introduction to the Workshop**
10:30 – 12:00	*Roi Baer* **Density Functional Theory and Time-Dependent Density Functional Theory**
12:00 – 14:00	Lunch
14:00 – 15:30	*Patrick Rinke* **GW+Bethe-Salpeter Equation Approaches**
15:30 – 16:00	Break
16:00 – 17:30	*Claudia Filippi* **Quantum Monte Carlo**
17:30 – 18:15	**Poster Pitches**
18:15 –	**Wine & Cheese**

Tuesday, March 21	
09:00 – 09:45	*Johannes Neugebauer* **Subsystem-based TDDFT: Exact Approaches, Efficient Approximations, and Extensions towards Higher Accuracy**
09:45 – 10:05	*Carlo Manio* **Excited State Machine-Learning for Chromophores in Complex Environments**
10:05 – 10:55	**Discussions + Coffee Break** *Topic: Challenges for Theoretical Spectroscopy*
10:55 – 11:40	*Mario Barbatti* **Nonadiabatic dynamics in the long timescale: The next challenge in computational photochemistry**
11:40 – 12:00	*Moritz Brütting* **Using and developing range-separated hybrid functionals: Natural light harvesting and local range separation**
12:00 – 14:00	Lunch
14:00 – 14:45	*John Mark P. Martirez* **Capped density functional embedding theory for excited-state simulations of covalent compounds**
14:45 – 15:30	*Heike Bahmann* **Flexible hybrid density functionals for the electronic structure at interfaces**
15:30 – 16:00	Coffee Break
16:00 – 16:40	*Claudia Filippi* **Quantum Monte Carlo for excited-state calculations**

16:45 – 18:00	**Poster Session**

Wednesday, March 22	
09:00 – 09:45	*Julia Westermayr* **Deep learning for excited states**
09:45 – 10:05	*Francesco Buda* **Microscopic origin of the efficient exciton transport in chlorosomes**
10:05 – 11:15	**Discussions + Coffee Break** *Topic: Machine Learning in Theoretical Spectroscopy* Discussion leaders: Julia Westermayr, Matthias Rupp
11:15 – 12:00	*Matthias Rupp* **Predicting Spectra with Atomistic Machine-Learning Models**
12:00 – 14:00	Lunch
14:00 – 14:45	*Ivan Duchemin* **Toward all-electron GW and Bethe-Salpeter calculations on complex systems**
14:45 – 15:30	*Jan Wilhelm* **Low-scaling GW calculations for complex 2D semiconductors**
15:30 – 18:00	**Exploring Leiden**
18:00 –	**Workshop Dinner**

Thursday, March 23	
09:00 – 09:45	*Roi Baer* **Stochastic Vector Techniques for Strongly Coupled Coulomb Systems**
09:45 – 10:05	*Emanuele Coccia* **Multiscale modelling of plasmon-assisted hot-carrier injection in molecules**
10:05 – 10:55	**Discussions + Coffee Break** *Topic: Technical implementations* Discussion leader: Arno Förster
10:55 – 11:40	*Dorothea Golze* **Accurate prediction of core and valence excitations with GW for large systems**
11:40 – 12:00	*Arno Förster* **Large scale GW-BSE calculations with explicit treatment of spin-orbit effects**
12:00 – 14:00	Lunch
14:00 – 14:45	*Mauro Del Ben*

	Portability Strategies for Next Generation Exascale Architectures: The BerkeleyGW Case Study
14:45 – 15:30	*Michael Rohlfing* **LDA+GdW calculations for layered materials using atom-resolved model dielectric functions**
15:30 – 17:00	**Discussions + Coffee Break** *Topic: Embedding Methods* Discussion leaders: J. Mark Martirez, Björn Baumeier
17:00 – 17:45	*Patrick Rinke* **Frontiers in many-body perturbation theory: strong correlation and machine learning**
17:45 – 18:05	*Ciro A. Guido* **Non-equilibrium dynamical effects on excited states within polarizable environment: perspectives from an open quantum system approach**

Friday, March 24	
09:00 – 09:45	*Lucas Visscher* **Novel methods for theoretical spectroscopy: embedding techniques, inclusion of relativity, and quantum algorithms**
09:45 – 10:30	*Rianne van den Berg* **AI4Science at Microsoft Research**
10:30 – 11:30	**Discussions + Coffee Break** *Topic: Future Developments and Frontiers* Discussion leader: Francesco Buda
11:30 – 12:00	**Closing**
12:00	Lunch