

Questaal Workshop on Many-Body Perturbation Theory

Agenda: 11-14 March 2024

		<i>Monday March 11</i>	<i>Tuesday March 12</i>	<i>Wednesday March 13</i>	<i>Thursday March 14</i>
Time [MST]	<i>8:15</i>	<i>Shuttle from Hotel and Security Check-In</i>	<i>Shuttle from Hotel</i>	<i>Shuttle from Hotel</i>	<i>Shuttle from Hotel</i>
	<i>08:45-09:00</i>	<i>Introductions (Attendees)</i>			
	<i>09:00-10:00</i>	Introduction to Questaal (MvS/JJ)	Ayush Asthana , "Quantum chemistry in the era of quantum computing - opportunities and challenges."	Lucia Reining , "Improved effective interactions for many-body perturbation theory: excitons in metals, and other frontiers"	Vojtech Vlcek , "Overcoming Conceptual and Computational Hurdles of MBPT"
	<i>10:00-10:20</i>	<i>Break</i>	<i>Break/Group Photo</i>	<i>Break</i>	<i>Break</i>
	<i>10:20-11:20</i>	Felipe Jornada , "Capturing large exciton interactions and nonlinearities in 2D materials from first principles"	Many Body Perturbation Theory (MvS)	QSGW and BSE Optics QSGW I (SA)	Spin susceptibility, real space representation of excitons (JJ, DP)
	<i>11:20-12:30</i>	Introduction to Questaal (cont'd.) (JJ)	Quasiparticle Self-Consistent GW (MvS)	QSGW and BSE Optics QSGW II (SA)	Dynamical self-energy, zone unfolding, other functions (DP, MvS)
	<i>12:30-13:30</i>	<i>Working Lunch/Posters Remote Attendee Break</i>	<i>Working Lunch Remote Attendee Break</i>	<i>Working Lunch/Posters Remote Attendee Break</i>	<i>Working Lunch Remote Attendee Break</i>
	<i>13:30-14:30</i>	Tutorial: DFT with Questaal	Tutorial: QSGW with Questaal	Tutorial: BSE Optics	Tutorials: Spin susceptibility, Dynamical Self-energy, Spectral functions
	<i>14:30-15:00</i>	<i>Break</i>	<i>Break</i>	<i>Break</i>	<i>Break</i>
	<i>15:00-18:00</i>	Hands-on: DFT with Questaal	Hands-on: QSGW with Questaal	Hands-on: Optics with Questaal	Hands-on: Special Functions (attendee's choice)
	<i>18:00</i>	<i>Shuttle to Hotel</i>	<i>Shuttle to Hotel</i>	<i>Shuttle to Hotel</i>	<i>Shuttle to Hotel</i>
<i>19:00-21:30</i>			<i>Informal dinner - TBD (not included)</i>		