QDMS SCHEDULE 2025

	7/14	7/15	7/16	7/17	7/18
	MONDAY	**TUESDAY**	**WEDNESDAY**	**THURSDAY**	**FRIDAY**
9:00 AM	**Talk: Welcome to QDMS** Speaker: Francesco Paesani	**Talk: Building MB-nrg models for Small-Molecules** Speaker: Ethan Bull-Vulpe	**Talk: Vibrational Spectroscopy & PIMD Approaches** Speaker: Richa Rashmi	**Talk: Basics of DFT** Speaker: Bhaskar Rana	**Talk: MD, DFT and QM/MM on GPUs** Speaker: Andreas Götz
9:30 AM		**Tutorial II: Many-Body Model Build-Along**	**Tutorial IV: PIMD Simulations & Spectra Calculation**	**Tutorial VI: QEpy hands-on**	
10:00 AM	**Technology Setup**				**Talk: GPU Accelerated QUICK and Robust Charges** Speaker: Vikrant Tripathy
10:20 AM	Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break
10:40 AM	**Talk: Fundamentals** Speaker: Etienne	**Tutorial II (cont.): Many-Body Model Build-Along**	**Tutorial IV (cont.): PIMD Simulations & Spectra Calculation**	**Talk: Implicit solvation with ENVIRON** Speaker: Dr. Andresussi	**Tutorial IX: Hands on QUICK**
11:30 AM	**Tutorial I: Many-Body Simulations with LAMMPS & MBX**				
12:00 PM	Lunch	Lunch	Lunch	Lunch	
12:30 PM					**Closing Remarks**
1:00 PM					END OF DAY
1:30 PM	**Tutorial I (cont.): Many-Body Simulations with LAMMPS & MBX**	**SDSC Data Center Tour**	**Tutorial V: Hybrid Force-Field / Many-Body Simulations**	**Tutorial VII: ENVIRON Simulations**	
2:00 PM		**Challenge II: BYOMBM, Part 2: PIP Generation, Physical Parameterization, Energy Calculations**			
2:30 PM				**Tutorial VIII: sDFT and QM/MM**	
3:00 PM	**Challenge I: From Scratch to Simulation**				
3:30 PM	Coffee Break	Coffee Break	Coffee Break	Coffee Break	
3:50 PM	**Challenge I (cont.): From Scratch to Simulation**	**Talk: MB-nrg PEFs for Biomolecular Simulations** Speaker: Ruihan Zhou	**Tutorial V (cont.): Hybrid Force-Field / Many-Body Simulations**	**Tutorial VIII (cont.): sDFT and QM/MM**	
4:30 PM	**Challenge II: BYOMBM, Part 1: Training Set Construction**	**Tutorial III: Polypeptide Simulation with MBX+LAMMPS**	**Challenge II: BYOMBM, Part 3: PIP Parameterization**	**Challenge II: BYOMBM, Part 4: C++ Implementation**	
5:00 PM	END OF DAY	END OF DAY	END OF DAY	END OF DAY	
5:30 PM					
6:00 PM	***Reception & Dinner***				
6:30p					
7:00p					