



MLQC4Dyn - Week 2

September 12

10:00 - 10:30	Onsite registration - coffee
10:30 - 10:50	Presentation of the Pascal Institute by the Director Denis Ullmo
10:50 - 11:00	Introduction by the organizers Chair: Dario Rocca
11:00 - 12:00	Markus Meuwly - University of Basel <i>Classical and Quantum Dynamics on Machine-Learned Potential Energy Surfaces</i>
12:00 - 13:40	Lunch break Chair: Tomas Bucko
13:40 - 14:40	Bingqing Cheng (R) - Institute of Science and Technology (IST) Austria <i>Predicting material properties with the help of machine learning</i>
14:40 - 15:40	Julia Westermayr - University of Warwick <i>Machine learning for excited-state molecular dynamics</i>
15:40 - 16:00	Coffee break
16:00 - 17:00	Max Pinheiro Jr - Aix-Marseille University <i>Unraveling patterns in nonadiabatic molecular dynamics data with machine learning</i>

September 13

	Chair: Jan Hermann
08:45 - 09:45	Igor Poltavskiy (R) - University of Luxembourg <i>On Electrons and Machine Learning Force Fields</i>
09:45 - 10:00	Coffee break

10:00 - 11:00	Basile Herzog - Université de Lorraine <i>Solving the Schrödinger Equation in the Configuration Space with Generative Machine Learning</i>
11:00 - 12:00	Nicolas Sisourat - LCPMR Sorbonne Université <i>Speeding-up quantum chemistry, and thus quantum molecular dynamics, with machine learning</i>
12:00 - 14:00	Lunch break Chair: Max Pinheiro Jr
14:00 - 15:00	Jan Hermann - Freie Universität Berlin <i>Neural-network wave functions for quantum chemistry</i>
15:00 - 15:15	Coffee break
15:15 - 16:15	Anatole von Lilienfeld (R) - University of Toronto <i>Quantum Machine Learning in Chemical Compound Space</i>
16:15 - 18:00	Group discussions / Round tables
19:30 - 21:30	Social dinner

September 14

	Chair: Jérôme Rey
08:45 - 09:45	Volker Deringer - University of Oxford <i>Machine-learning-driven molecular dynamics for inorganic materials chemistry</i>
09:45 - 10:00	Coffee break
10:00 - 11:00	Tomas Bucko - Comenius University in Bratislava <i>MLPT – an effective method for determining free energies at multiple electronic structure levels</i>
11:00 - 12:00	Julien Lam (R) - CEMES CNRS Toulouse <i>Observing the birth of crystals using machine-learning assisted simulations</i>
12:00 - 14:00	Lunch break

	Chair: Julia Westermayr
14:00 - 15:00	Reinhard Maurer - University of Warwick <i>Machine learning of electronic structure for dynamics at surfaces</i>
15:00 - 15:15	Coffee break
15:15 - 16:15	Mario Barbatti (R) - Aix-Marseille University <i>Nonadiabatic dynamics in the long timescale: the next challenge in computational photochemistry</i>
16:15 - 18:00	Group discussions / Round tables

September 15

	Chair: TBA
08:45 - 09:45	Pavlo Dral (R) - Xiamen University <i>Accelerating and improving quantum chemistry and dynamics with machine learning</i>
09:45 - 10:00	Coffee break
10:00 - 11:00	Daniel Pelaez Ruiz - Université Paris-Saclay <i>Analytical low-rank representation of high-dimensional tensors: Application to Tucker and Canonical Polyadic forms</i>
11:00 - 12:00	Nada Doslic - Ruđer Bošković Institute <i>Progress and Challenges in Modelling Photoinduced Processes</i>
12:00 - 14:00	Lunch break
	Chair: Mario Barbatti
14:00 - 15:00	Michele Ceriotti - EPFL <i>Full quantum (thermo)dynamics with integrated machine learning models</i>
15:00 - 15:15	Coffee break
15:15 - 16:15	Jean-Philip Piquemal - LCT Sorbonne Université <i>Machine Learning and molecular simulations: from many-bodydispersion to free energies</i>
16:15 - 19:00	Happy hour

September 16

	Chair: Michael Badawi
08:45 - 09:45	Milica Todorovic (R) - University of Turku <i>Computational materials engineering with active learning</i>
09:45 - 10:00	Coffee break
10:00 - 11:00	Bastien Casier - Université d'Artois <i>FCInet: An iterative machine learning classification neural network for a smartly selective CI</i>
11:00 - 12:00	Andrea Grisafi - ENS Paris <i>Predicting electronic structure properties with equivariant and long-range machine-learning methods</i>
12:00 - 12:15	Concluding remarks
12:15 - 14:00	Lunch break
14:00	Departure

(R) denotes remote speakers