Workshop Schedule

Day	Package(s) and Instructor(s)
Day 1 Monday, 14 (11 am - 5 pm)	**First half of the day:** (11:00 am - 1:00 pm) Instructors: Alexey Akimov, Jeanette Sperhac, Sudhakar Pamidighantam Co-Instructors: Alexey Akimov ● Introductions ● Overview of **UB CCR** & **OnDemand**, **SEAGrid** ● Submitting jobs on UB CCR HPC and via SEAGrid *Break (1:00 pm - 2:00 pm)* **Second half of the day:** (2:00 pm - 5:00 pm) Instructors: Alexey Akimov ● Revision of Python and C++ programming and best practices ● Coding Molecular dynamics and Monte Carlo ● Introduction to **Libra** "methodology prototyping" package. Classical molecular dynamics, visualization, and convenience functions.
Day 2 Tuesday, 15 (11 am - 5 pm)	**First half of the day:** (11:00 am - 1:00 pm) Instructors: Ivan Infante, Felipe Zapata, Alexey Akimov Co-Instructors: Juliette Zito, Mohammad Shakiba ● Introduction to DFT and TD-DFT calculations with CP2k ● Computing nonadiabatic couplings and performing other types of calculations with **nano-qmflows** *Break (1:00 pm - 2:00 pm)* **Second half of the day:** (2:00 pm - 5:00 pm) Instructors: Alexey Akimov ● Trajectory surface hopping and Ehrenfest methods for nonadiabatic dynamics ● TSH and Ehrenfest dynamics calculations with **Libra** with model Hamiltonians ● TSH dynamics calculations with **Libra** with atomistic Hamiltonians with 1-particle (KS) and many-body (TD-DFT) states
Day 3 Wednesday, 16 (11 am - 5 pm)	**First half of the day:** (11:00 am - 1:00 pm) Instructors: Amber Jain (lecture), Alexey Akimov ● Lecture of Hierarchy of equations of motion (HEOM). ● Demonstration of HEOM calculations with **Libra** code *Break (1:00 pm - 2:00 pm)* **Second half of the day:** (2:00 pm - 5:00 pm) Instructors: Alexey Akimov ● Lecture and hands-on with DVR and wavepacket dynamics with

	Libra.
Day 4 Thursday, 17 (11 am - 5 pm)	**First half of the day:** (11:00 am - 1:00 pm) Instructors: Ivan Infante Co-Instructors: Bas van Beek, Roberta Pascazio ● Building structures molecular structures of QDs: **FOX** and **CAT** *Break (1:00 pm - 2:00 pm)* **Second half of the day:** (2:00 pm - 5:00 pm) Instructors: Alexey Akimov Co-Instructors: Mohammad Shakiba ● Electronic structure with **ErgoSCF**, **DFTB+**, **cp2k**, and **QE/eQE** ● Nonadiabatic dynamics of atomistic systems: Libra/ErgoSCF, Libra/DFTB+, Libra/QE, Libra/eQE, Libra/cp2k. ● Analysis and auxiliary functions of Libra package
Day 5 Friday, 18 (11 am - 5 pm)	**First half of the day:** (11:00 am - 1:00 pm) Instructors: Sergei Tretiak ● Lecture on NA-MD in large organic molecules. Discussions. Simple demonstrations. *Break (1:00 pm - 2 pm)* **Second half of the day:** (2:00 pm - 5:00 pm) Instructors: Walter Malone ● Hands-on with **NEXMD**
Days 6 and 7 Weekend	**Home Projects**
Day 8 Monday, 21 (11 am - 5 pm)	**First half of the day:** (11:00 am - 1:00 pm) Instructors: Aiichiro Nakano (lecture) ● Lecture on NA-MD calculations with **QXMD** *Break (1:00 pm - 2 pm)* **Second half of the day:** (2:00 pm - 5:00 pm) Instructors: Alexey Akimov ● Hands-on with **QXMD**
Day 9 Tuesday, 22 (11 am - 5 pm)	**First half of the day:** (11:00 am - 1:00 pm) Instructors: Hans Lischka Co-instructors: Reed Nieman ● Lecture: Accurate calculations of excited states with **COLUMBUS** *Break (1:00 pm - 2 pm)* **Second half of the day:** (2:00 pm - 5:00 pm) Instructors: Hans Lischka

	Co-instructors: Reed Nieman, Bhumika Jayee ● Hands on with accurate calculations of excited states with **COLUMBUS**
Day 10 Wednesday, 23 (11 am - 5 pm)	**First half of the day:** (11:00 am - 1:00 pm) Instructors: Mario Barbatti Co-Instructors: Ljiljana Stojanovic, Alexey Akimov ● Excited states dynamics with **Newton-X** (interfaces with **DFTB+**, and abstract Hamiltonians) *Break (1:00 pm - 2 pm)* **Second half of the day:** (2:00 pm - 5:00 pm) Instructors: Hans Lischka Co-Instructors: Reed Nieman, Bhumika Jayee ● Hands on with accurate calculations of excited states with **COLUMBUS**
Day 11 Thursday, 24 (11 am - 5 pm)	**First half of the day:** (11:00 am - 1:00 pm) Instructors: Mario Barbatti Co-Instructors: Hans Lischka, Alexey Akimov ● Excited states dynamics with **Newton-X** (interfaces with **COLUMBUS**) *Break (1:00 pm - 2 pm)* **Second half of the day:** (2:00 pm - 5:00 pm) Instructors: Mario Barbatti Co-Instructors: Hans Lischka, Alexey Akimov ● Excited states dynamics with **Newton-X** (interfaces with **COLUMBUS**), continued
Day 12 Friday, 25 (11 am - 5 pm)	● Participants' projects presentations ● Awards and Closing