

Workshop Schedule

Day	Package(s) and Instructor(s)
Day 1 Monday, 14 (11 am - 5 pm)	<p>First half of the day: (11:00 am - 1:00 pm) <u>Instructors:</u> Alexey Akimov, Jeanette Sperhac, Sudhakar Pamidighantam <u>Co-Instructors:</u> Alexey Akimov</p> <ul style="list-style-type: none"> • Introductions • Overview of UB CCR & OnDemand, SEAGrid • Submitting jobs on UB CCR HPC and via SEAGrid <p><i>Break (1:00 pm - 2:00 pm)</i></p> <p>Second half of the day: (2:00 pm - 5:00 pm) <u>Instructors:</u> Alexey Akimov</p> <ul style="list-style-type: none"> • 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)	<p>First half of the day: (11:00 am - 1:00 pm) <u>Instructors:</u> Ivan Infante, Felipe Zapata, Alexey Akimov <u>Co-Instructors:</u> Juliette Zito, Mohammad Shakiba</p> <ul style="list-style-type: none"> • Introduction to DFT and TD-DFT calculations with CP2k • Computing nonadiabatic couplings and performing other types of calculations with nano-qmflows <p><i>Break (1:00 pm - 2:00 pm)</i></p> <p>Second half of the day: (2:00 pm - 5:00 pm) <u>Instructors:</u> Alexey Akimov</p> <ul style="list-style-type: none"> • 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)	<p>First half of the day: (11:00 am - 1:00 pm) <u>Instructors:</u> Amber Jain (lecture), Alexey Akimov</p> <ul style="list-style-type: none"> • Lecture of Hierarchy of equations of motion (HEOM). • Demonstration of HEOM calculations with Libra code <p><i>Break (1:00 pm - 2:00 pm)</i></p> <p>Second half of the day: (2:00 pm - 5:00 pm) <u>Instructors:</u> Alexey Akimov</p> <ul style="list-style-type: none"> • Lecture and hands-on with DVR and wavepacket dynamics with

	Libra.
Day 4 Thursday, 17 (11 am - 5 pm)	<p>First half of the day: (11:00 am - 1:00 pm) <u>Instructors:</u> Ivan Infante <u>Co-Instructors:</u> Roberta Pascazio, Bas van Beek</p> <ul style="list-style-type: none"> Building structures molecular structures of QDs: FOX and CAT <p><i>Break (1:00 pm - 2:00 pm)</i></p> <p>Second half of the day: (2:00 pm - 5:00 pm) <u>Instructors:</u> Alexey Akimov <u>Co-Instructors:</u> Mohammad Shakiba</p> <ul style="list-style-type: none"> 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)	<p>First half of the day: (11:00 am - 1:00 pm) <u>Instructors:</u> Sergei Tretiak</p> <ul style="list-style-type: none"> Lecture on NA-MD in large organic molecules. Discussions. Simple demonstrations. <p><i>Break (1:00 pm - 2 pm)</i></p> <p>Second half of the day: (2:00 pm - 5:00 pm) <u>Instructors:</u> Walter Malone</p> <ul style="list-style-type: none"> Hands-on with NEXMD
Days 6 and 7 Weekend	Home Projects
Day 8 Monday, 21 (11 am - 5 pm)	<p>First half of the day: (11:00 am - 1:00 pm) <u>Instructors:</u> Aiichiro Nakano (lecture)</p> <ul style="list-style-type: none"> Lecture on NA-MD calculations with QXMD <p><i>Break (1:00 pm - 2 pm)</i></p> <p>Second half of the day: (2:00 pm - 5:00 pm) <u>Instructors:</u> Thomas Linker, Alexey Akimov</p> <ul style="list-style-type: none"> Hands-on with QXMD
Day 9 Tuesday, 22 (11 am - 5 pm)	<p>First half of the day: (11:00 am - 1:00 pm) <u>Instructors:</u> Hans Lischka <u>Co-instructors:</u> Reed Nieman</p> <ul style="list-style-type: none"> Lecture: Accurate calculations of excited states with COLUMBUS <p><i>Break (1:00 pm - 2 pm)</i></p> <p>Second half of the day: (2:00 pm - 5:00 pm) <u>Instructors:</u> Hans Lischka</p>

	<u>Co-instructors:</u> Reed Nieman, Bhumika Jayee <ul style="list-style-type: none"> 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) <u>Instructors:</u> Mario Barbatti <u>Co-Instructors:</u> Ljiljana Stojanovic <ul style="list-style-type: none"> Excited states dynamics with Newton-X (interfaces with DFTB+, and abstract Hamiltonians) <i>Break (1:00 pm - 2 pm)</i> Second half of the day: (2:00 pm - 5:00 pm) <u>Instructors:</u> Hans Lischka <u>Co-Instructors:</u> Reed Nieman, Bhumika Jayee <ul style="list-style-type: none"> 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) <u>Instructors:</u> Mario Barbatti <u>Co-Instructors:</u> Hans Lischka, Alexey Akimov <ul style="list-style-type: none"> Excited states dynamics with Newton-X (interfaces with COLUMBUS) <i>Break (1:00 pm - 2 pm)</i> Second half of the day: (2:00 pm - 5:00 pm) <u>Instructors:</u> Mario Barbatti <u>Co-Instructors:</u> Hans Lischka, Alexey Akimov <ul style="list-style-type: none"> Excited states dynamics with Newton-X (interfaces with COLUMBUS), continued
Day 12 Friday, 25 (11 am - 5 pm)	<ul style="list-style-type: none"> Participants' projects presentations Awards and Closing