**Workshop Schedule**

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| **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 |