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CyberTraining: Modeling Quantum Dynamics of Excited States in Materials in the Era of Machine Learning, 2026

Alexey Akimov

University at Buffalo, SUNY

July 6, 2026

https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2026/

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General Workshop Goals

and

Overview of the CyberTraining Infrastructure

Objectives and Scope

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Workshop Objectives

- Get **familiar with a variety of software packages** relevant to modeling of excited states and nonadiabatic dynamics
- Get an overview of **theoretical background** for corresponding computational methods
- Get **experience** using machine learning tool and applying them to modeling **excited states** or **nonadiabatic dynamics**
- Get a **practical experience** with these tools and packages

2026 (this year!)

- ChemML (Hachmann)
- Prism/SQA+ (Sokolov)
- PySCF / Psi4 (Sokolov)
- PySpawn / OpenMolcas (Levine / Mehmood)
- TENSO (Franco)
- CP2K / DFTB+ / MOPAC (Akimov)
- Libra (Akimov)

CyberTraining: Implementation: Small: Modeling Quantum Dynamics of Excited States in Materials in the Era of Machine Learning

2023 (in person/virtual)

- Nonadiabatic dynamics and quantum-classical methods
- Excited-state electronic structure theory
- Quantum dynamics and open quantum systems
- Charge transfer and excitation energy transfer
- Trajectory surface hopping and ab initio multiple spawning (AIMS)
- Hierarchical equations of motion (HEOM)
- Time-dependent density functional theory (TD-DFT) and TD-DFTB
- Correlated electronic structure methods
- Machine learning methods for excited-state modeling
- Algorithm development and numerical methods
- Reproducible workflows, best practices, Git, and GitHub

2022 (in person/virtual)

- pyUNIxMD (Min)
- CT-MQC (Ibele)
- SHARC (Mai)
- SHARC/COBRAMM (Avagliano
- OpenMolcas (Mai, Avagliano)
- ORCA (Mai)
- Hefei-NAMD (Zhao, Chu)
- Quantum Espresso (Zhao, Chu
- BerkeleyGW and paratec (Zhan
- DynEMol (Rego)
- Libra (Akimov)
- DFTB+ (Shakiba)
- CP2K (Shakiba)
- TBD (Kilin)

2021 (virtual)

- Libra (Akimov)
- NEXMD (Tretiak)
- Newton-X (Barbatti)
- nano-qmflows (Infante, Zapata)
- CAT, auto-FOX (Infante, Zapata)
- COLUMBUS (Lischka)
- DFTB+
- CP2K
- Quantum Espresso
- ErgoSCF

CyberTraining: Pilot: Modeling Excited State Dynamics in Solar Energy Materials

The Plan & Resources

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All the details are here: https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2026/

CyberTraining: Modeling Quantum Dynamics of Excited States in Materials in the Era of Machine Learning, 2026

Join Slack:

- Members can invite new members
- Private and public channels, direct (private) messages, conversations
- Any time, no strings attached

https://join.slack.com/t/quantumdynamicshub/shared_invite/zt-mjbhjssx-GGhsbYHxeBMvhmumK_j7LA

VPN and Accounts:

- 2-factor authentication
- ccr-help@buffalo.edu

Topics and Instructors

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July 6, 2026 (Day 1), Monday, Where: **NSC 201**	**Morning, 9 am - noon** • Worshop Kick Off: goals, logistics, details. Overview of the CCR CyberInfrastructure (30 min) • Getting started with the CCR resources. Hands-on (60 min) • General overview of ML computations (Lecture) (30 min) • General practice with ML computations (Hands on with PyTorch) (60 min) **Noon - 1:30 pm** Lunch break **Afternoon, 1:30 pm - 5:00 pm** • Theory and demos with ChemML I. Lecture and Demos (50 min) • Hands on with ChemML (50 min) • Theory and demos with ChemML II. Lecture and Demos (50 min) • Hands on with ChemML and working on projects (40 min) • Working on projects. Collaborations (20 min)	Alexey Akimov and Johannes Hachmann

ChemML

https://hachmannlab.github.io/chemml/

Prof. Johannes Hachmann (SUNY UB)

https://hachmannlab.cbe.buffalo.edu/

Topics and Instructors

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July 7, 2026 (Day 2), Tuesday, Where:
NSC 210

Morning, 9 am - noon

Alexander Sokolov

- Electronic structure methods overview. Lecture and Demos (30 min)
- Hands on with basic calculations with PySCF/Psi4 (60 min)
- Advanced electronic structure methods with PySCF/Psi4. Lecture and Demos (50 min)
- Hands on exercises (40 min)

Noon - 1:30 pm Lunch break **Afternoon, 1:30 pm - 5:00 pm**

- Second quantization algebra and its application to Multireference Algebraic Diagrammatic Construction (MR-ADC) Theory. Lecture (50 min)
- Hands on exercises with second quantization algebra using SQA+ (60 min)
- N-electron valence perturbation theory (NEVPT) and multireference algebraic diagrammatic construction theory (MR-ADC). Lecture and Demos (40 min)
- Spectroscopic calculations with Prism. Hands on exercises (40 min)
- Working on projects. Collaborations (20 min)

PySCF https://pyscf.org/

Psi4 https://psicode.org/

SQA+ https://github.com/sokolov-group/sqa_plus

PRISM https://github.com/sokolov-group/prism/

Prof. Alexander Sokolov (Ohio State U)

https://research.cbc.osu.edu/sokolov.8/

Topics and Instructors

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July 8, 2026 (Day 3), Wednesday, Where: **Clemens 120**	**Morning, 9 am - noon** • Basics of excited state calculations with OpenMolcas. Lecture and Demo (50 min) • Hands on exercises with excited state calculations with OpenMolcas. (60 min) • Advanced electronic structure calculations with OpenMolcas. Lecture and Demo (40 min) • Hands on exercises with excited state calculations with OpenMolcas. (30 min) **Noon - 1:30 pm** Lunch break **Afternoon, 1:30 pm - 5:00 pm** • Theory of nonadiabatic dynamics with multiple spawning/muliple cloning. Lecture (60 min) • Hands on exercises with PySpawn using model Hamiltonians (60 min) • Demonstration of atomistic AIMS calculations with PySpawn/OpenMolcas (30 min) • Hands on exercises with PySpawn/OpenMolcas (30 min) • Working on projects. Collaborations (30 min)	Benjamine Levine and Arshad Mehmood

OpenMolcas
https://gitlab.com/Molcas/OpenMolcas

https://github.com/compchem-cybertraining/Tutorials_OpenMolcas

https://github.com/compchem-cybertraining/Tutorials_PySpawn

pySpawn17 https://github.com/blevine37/pySpawn17

Dr. Arshad Mehmood
(Stony Brook U)

https://arshadmehmood118.github.io/

Prof. Benjamin Levine
(Stony Brook U)

https://levinegroup.org/

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July 9, 2026 (Day 4), Thursday, Where:
NSC 201

Morning, 9 am - noon — Alexey Akimov

- Overview of quantum-classical methodologies. Lecture and demos (100 min)
- Hands on exercises with quantum-classical calculations of model Hamiltonians using Libra. (80 min)

Noon - 1:30 pm Lunch break **Afternoon, 1:30 pm - 5:00 pm**

- Trajectory surface hopping calculation for atomistic systems using Libra interfaces with DFTB+, MOPAC etc. Lecture and demos (60 min)
- Hands on exercises on atomistic simulations using Libra (120 min)
- Working on projects. Collaborations (30 min)

Libra

https://github.com/Quantum-Dynamics-Hub/libra-code

https://github.com/compchem-cybertraining/Tutorials_Libra
https://github.com/compchem-cybertraining/Tutorials_DFTB_plus
https://github.com/compchem-cybertraining/Tutorials_CP2K

Prof. Alexey Akimov
(UB, SUNY)

https://akimovlab.github.io/

Dr. Mohammad Shakiba
(UC Merced)

https://mohammadshakiba.github.io/

Topics and Instructors

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July 10, 2026 (Day 5), Friday, Where: **Clemens 120**	**Morning, 9 am - noon** • Theory of quantum dynamics in open systems. Lecture (90 min) • Hands on exercis with dissipative quantum dynamics simulations using TENSO (90 min) **Noon - 1:30 pm** Lunch break **Afternoon, 1:30 pm - 5:00 pm** • Hands on exercis with dissipative quantum dynamics simulations using TENSO (30 min) • Working on projects. Collaborations (120 min) **Evening 6:30 pm** Optional trip to Niagara Falls	Ignacio Franco

PyTENSO https://github.com/ifgroup/pytenso

Prof. Ignacio Franco
(U of Rochester)

https://sas.rochester.edu/chm/groups/franco/

Mr. Juan, Camilo
Rodríguez Betancourt
(U of Rochester)

Dr. Michelle Anderson
(U of Rochester)

Organizational and Preparatory

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Prof. Alexey Akimov
(UB, SUNY)

Ms. Layla Heydarizadeh
(UB, SUNY)
- paperwork

Ms. Anna Akimova
- inspirational

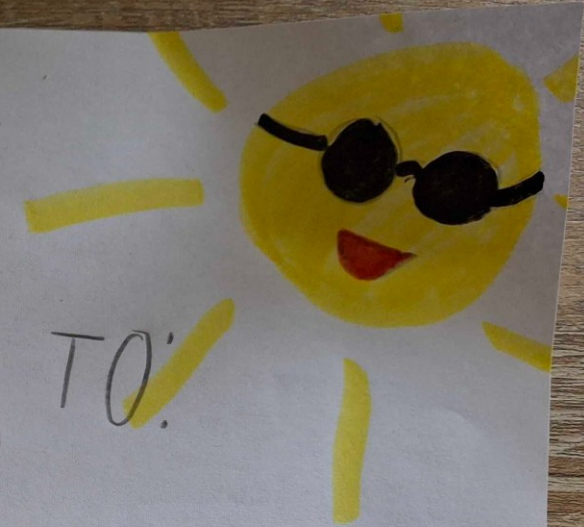
University at Buffalo

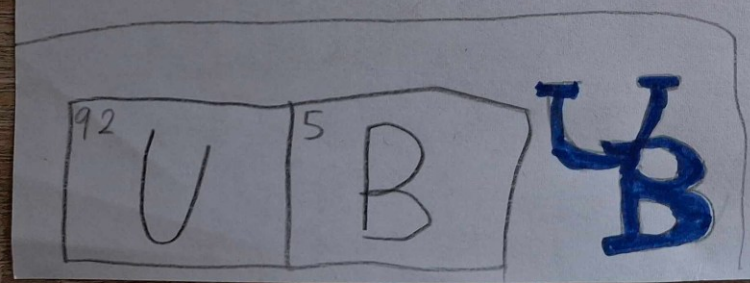
WELCOME TO:

the SUMMER WORKSHOP!

Monday 7/6/26 - 7/11/26

2026





waterfall day:
7/11/26

Please Introduce Yourself

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- Name, position, affiliation, research group
- Research interests and expertise
- Anything else you would like to share with us

More Resources

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Codes: https://github.com/Quantum-Dynamics-Hub
Training: https://github.com/compchem-cybertraining

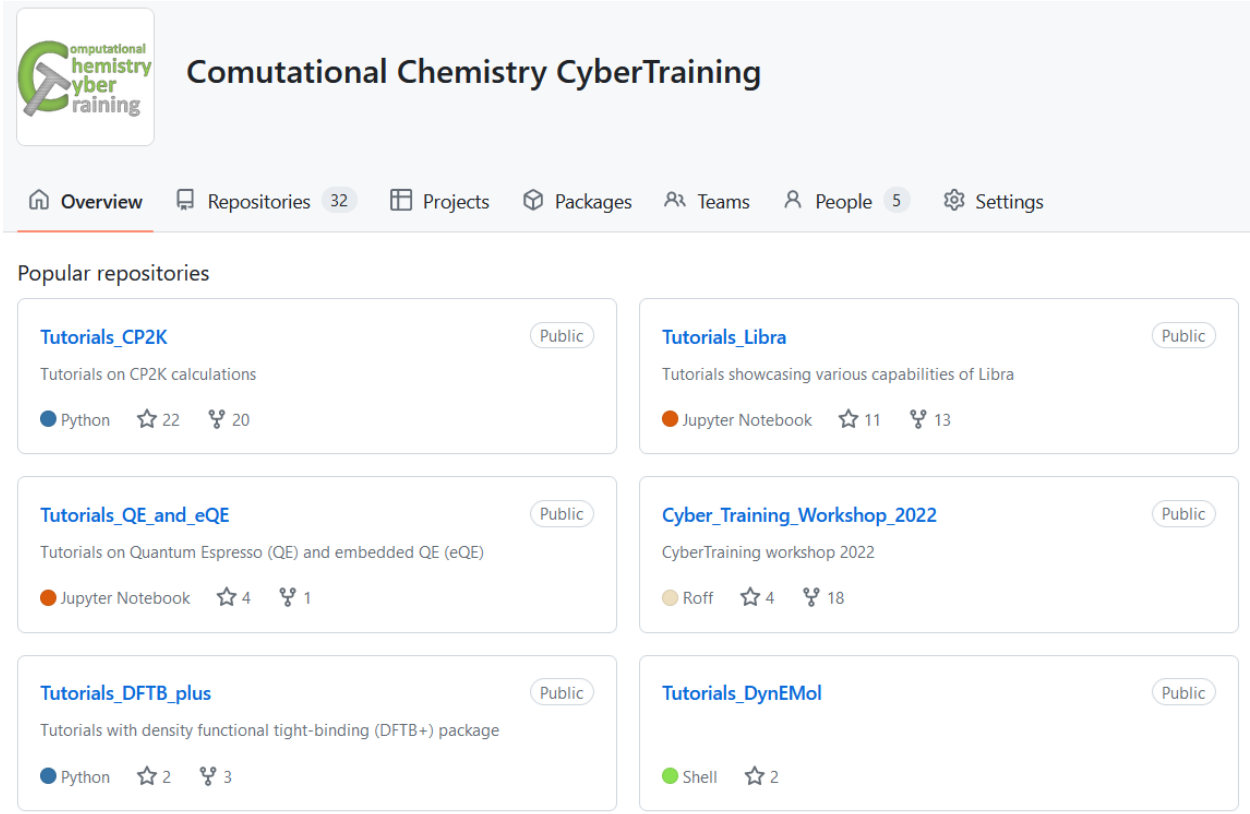
Quantum Dynamics Hub: https://quantum-dynamics-hub.github.io/

Summer 2021 workshop: https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2021/

Libra Winter school: https://compchem-cybertraining.github.io/Libra_Winter_School_2022/

Summer 2022 workshop: https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2022/

Summer 2023 workshop: https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2023/



Summer 2026 workshop (this!) https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2026/

Daily Schedule

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Daily

- Breakfast = hotel
- 9:00 am – 12:00 pm: Morning session (Recording)
- 12:00 – 1:30 pm Working lunch/rest – on your own at “Commons”, rest, discuss, collaborate
- 1:30 pm – 5:00 pm: Afternoon session (Recording)
- After 5:00 pm: collaborations/on your own, dinner on your own

Location

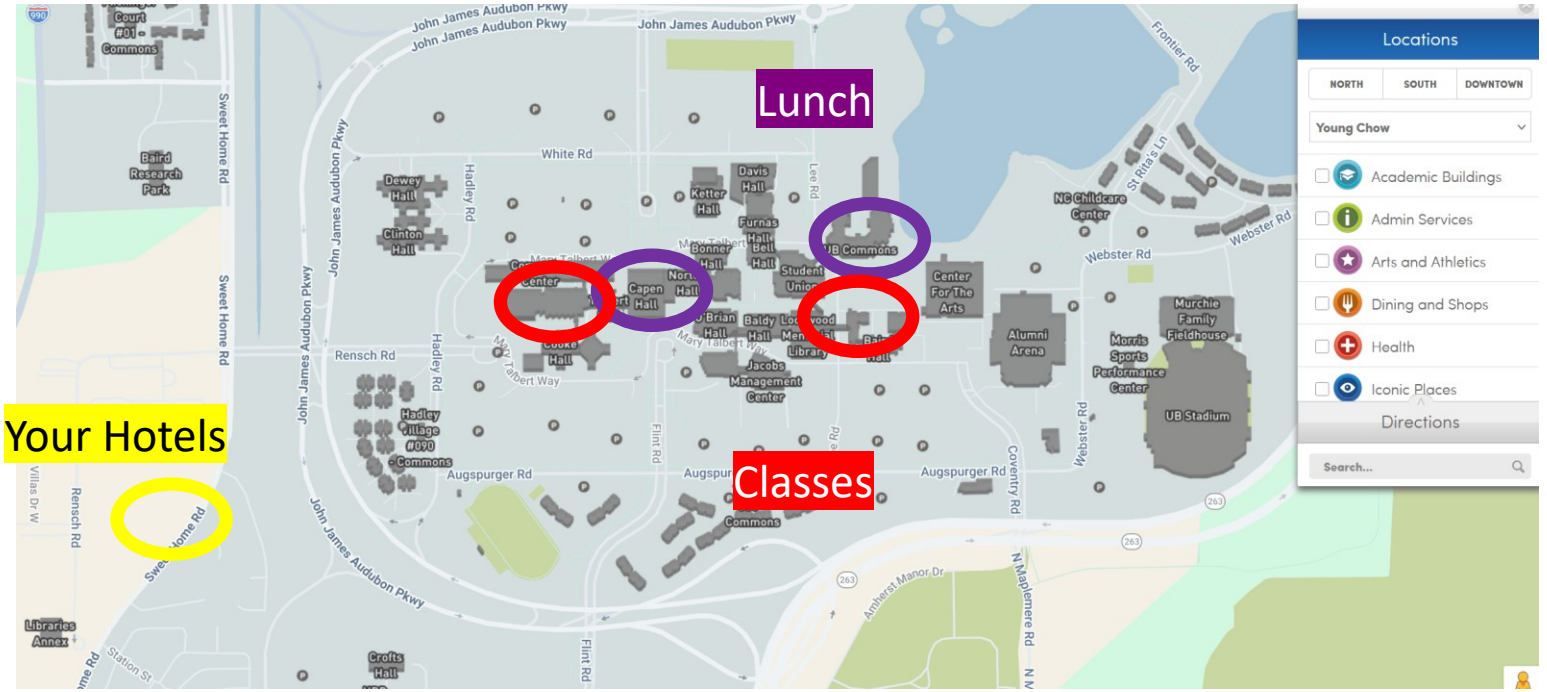
Classes are @:

Monday, Thursday: NSC 201

Tuesday: NSC 210

Wednesday, Friday: Clemens 120

Campus Map:
https://www.buffalo.edu/home/visiting-ub/map.html



Logistic

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- We cover your hotel stay (except for the local folks). Stipends also cover the rest of expenses, please keep your receipts just in case. Let me know your flight expenses via the Google form provided on Slack channel.

- Travel for the US participants to a reasonable amount, partially the international participants (as the funds allow), except for local/UB-affiliated folks.

- Paperwork: All trainees will need to fill in the RF Participation Stipend form and one of the other two forms: W-9 - for the US residents and W-8BEN for the non-residents. The forms are distributed to you **via Slack** – please **DON't send them back via e-mail** – upload to the form provided or via Slack.

- A lot of paperwork later – likely it'll be just me handling most of the stuff

- Prizes: $300 (1 first prize), $200 (3 second prizes), $100 (5 first prizes) – the project competition. Online and in-person participants are eligible. UB-affiliated participants are eligible too.

- Reimbursement/honoraria to the instructors – a separate paperwork. Will send you instructions via the Instructors Channel on Slack.

Course Project

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Project rules https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2026/CODE_OF_CONDUCT.html

- Consist of: a) short written report, b) presentation at the last day of workshop; c) set of input/output files deposited on the GitHub repository
- Should actively involve one of the packages discussed over the workshop period
- Preferably not something you have an extensive experience with
- Doesn't have to be a full-scale research project, but can be a step towards this direction
- Projects completed using local or home institution resources are eligible
- Can be an application or a coding project
- The consistency in your course work during this school will contribute to your chances to win the awards
- The awards decisions will be made based on the committee evaluation. The awards will be: 1 first prize ($300), 3 second, and 5 third prizes.

Project Timeline: https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2026/_episodes/07-project

- Have your work accepted to the GitHub repo by **July 18 (Saturday), 5 pm Buffalo time**
- First stage winners are selected by **July 22**
- Zoom oral presentations - **July 24-26 (the exact dates are to be determined)**

Check out the past years' projects:

https://github.com/compchem-cybertraining/Cyber_Training_Workshop_2021/tree/gh-pages/course_work

https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2021/_episodes/13-projects

https://github.com/compchem-cybertraining/Cyber_Training_Workshop_2022/tree/gh-pages/course_work

https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2022/_episodes/15-projects

https://github.com/compchem-cybertraining/Cyber_Training_Workshop2023_course_projects

https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2023/_episodes/08-projects

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Getting Started on UB CCR

Accessing UB Computing Resources

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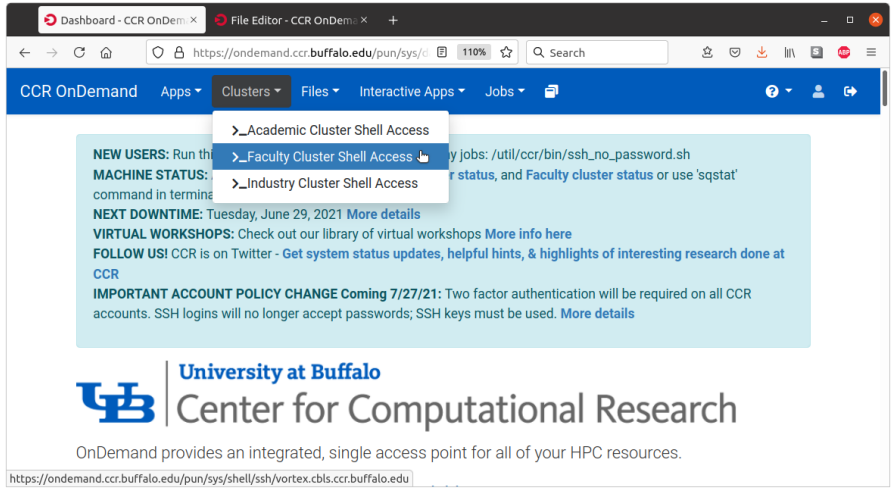
Before the Workshop

https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2026/setup.html

OnDemand (not Firefox, use Chrome)

On campus – nothing special;
Off-campus – use UB VPN

https://ondemand.ccr.buffalo.edu/

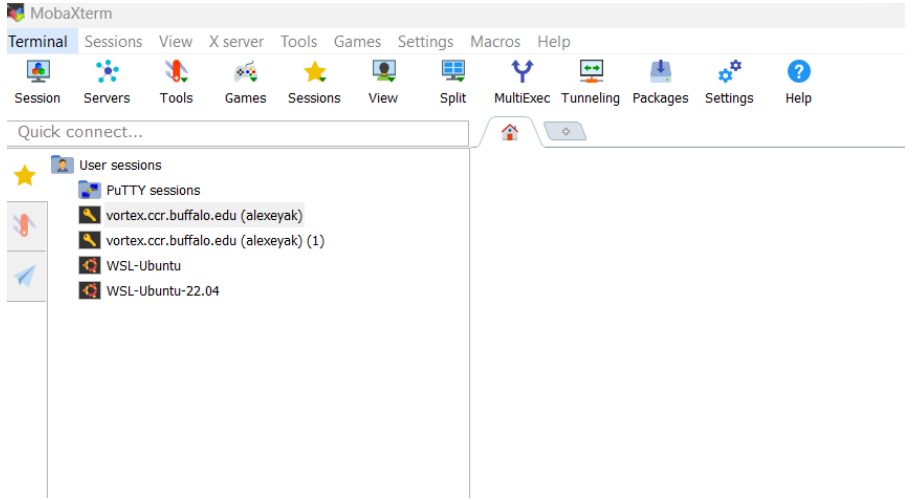


Moba Xterm

Generate the SSH public/private key.

- Use Moba Tools -> MobaKeyGen
- Coordinate it with your UB credentials

https://docs.ccr.buffalo.edu/en/latest/portals/idm/



Accessing UB Computing Resources

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Your **.bashrc** file (in your home directory)

```
# .bashrc

# User specific aliases and functions

# Source global definitions
if [ -f /etc/bashrc ]; then
        . /etc/bashrc
fi
module use /projects/academic/cyberwksp21/MODULES
module load libra_ava/devel
```

- Restart terminal or `source .bashrc`
- For terminal-based operations: Activate conda environment: `conda activate libra2`
- For Jupyter – just launch it

Projects directory: /projects/academic/cyberwksp21 - slower, smaller, but permanent, **limited space**!
Scratch space: /vscratch/grp-cyberwksp21 - faster, larger, but temporary; content will be purged in 60 days
Home directory: convenient to use, but others can not access it in case you need them check something

Using Jupyter Notebooks

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https://compchem-cybertraining.github.io/Cyber_Training_Workshop_2026/_episodes/04-tsh