

2026 Quantum Multiscale Hackathon

A week of collaborative coding at the Rutgers University Inn and Conference Center — an ACS Fall 2026 satellite event, by invitation only.

DETAILS

When: August 27 – September 1, 2026

Where: Rutgers University Inn and Conference Center, New Brunswick, NJ

[Accommodation details](#)

[Download program \(PDF\)](#)

THEMES

TBD

SOFTWARE (A-Z)

- Anvil
- ce-TDDFT
- DFTpy
- eDFTpy
- Environ
- FHI-aims
- MBX
- QEpy
- Quantum ESPRESSO
- SHRED

- SigML

ACS Fall 2026 satellite. The hackathon begins on **August 27**, the final day of the ACS Fall 2026 meeting in Chicago, so participants can travel directly from the meeting. Participation is **by invitation only**.

Accommodation details

- **Hotels.** Due to constraints at the Rutgers University Inn, most participants will spend the first night (**August 27**) at the **Heldrich Hotel** in downtown New Brunswick. All other nights (**August 28–September 1**) will be at the RU-Inn. See the [Heldrich-to-Inn map](#). The organizers will run shuttles on the first two days so everyone can travel between the Inn and the Heldrich as needed.
- **Getting around.** The RU-Inn is on the Douglass campus. All participants can use the Rutgers bus system for free to move around (e.g., between the RU-Inn and downtown). See the [RU bus map](#) and the [hours of operation](#) (detailed, but accurate).
- **Gym.** The **Cook/Douglass Recreation Center** will be open. Hours are posted on the [Rutgers Recreation operating status](#) page.
- **Move-in weekend.** The hackathon coincides with Rutgers move-in weekend, so expect many students and families around campus helping with dorm move-in.

Confirmed Participants (A–Z)

AIMS (Volker Blum), Duke

Caricato Research Group (Marco Caricato), University of Kansas

Hoffmann Group (Norah Hoffmann), NYU

Li Zhu, Rutgers University–Newark

MATERIALab (Oliviero Andreussi), Boise State

Paesani Research Group (Francesco Paesani), UCSD

PRG (Michele Pavanello), Rutgers–Newark

Scientific AI (Fred Hamprecht), Heidelberg University, Germany

Urban Research Group (Alex Urban), Columbia

Remote Participants (A–Z)

Alexander White, Los Alamos National Laboratory

Davide Ceresoli, CNR Milano

Sergei Manzhos, Science Tokyo

Wenhui Mi, Jilin University

Xuecheng Shao, Jilin University

Schedule

Thursday, August 27

- | | |
|---------------------|--|
| All day | Final day of the ACS Fall 2026 meeting (Chicago) — travel to New Brunswick, NJ |
| 4:30 pm | Check-in at the Rutgers University Inn and Conference Center (New Brunswick, NJ), or to other assigned hotel |
| 6:00–9:00 pm | Hors d'oeuvres and drinks in the Dining Room (Rutgers Inn) |

Friday, August 28

- | | |
|----------------------------|---|
| 8:00 am | Breakfast |
| 8:45 am | Opening remarks |
| 9:00 am | Introductions and flash presentations of hackathon projects |
| 10:00 am | Hackathon begins |
| 12:30 pm | Lunch and presentation (35 min) · Speaker: Volker Blum (Duke) |
| After lunch–2:30 pm | Free |
| 2:30 pm | Hackathon |
| 6:30 pm | Hackathon day 1 wrap-up and set goals for day 2 |
| Evening | Free |

Saturday, August 29

8:00 am	Breakfast
8:45 am	Flash presentations about goals for day 2
9:30 am	Hackathon
12:30 pm	Lunch and presentation (35 min) · Speaker: Li Zhu (Rutgers University–Newark) · "Making Correlated-Electron Simulations Affordable: Machine-Learned Self-Energies and Entropy-Driven Interatomic Potentials"
After lunch–2:30 pm	Free
2:30–5:30 pm	Frisbee Golf at the Rutgers Disc Golf Course
5:30 pm	Free
6:30 pm	Hackathon Dinner · Keynote speaker: Alex Urban (Columbia)

Sunday, August 30

8:00 am	Breakfast
8:45 am	Flash presentations about goals for day 3
9:30 am	Hackathon
12:30 pm	Lunch and presentation (35 min) · Speaker: Oliviero Andreussi (Boise State) · "MapSy: Mapping and Learning Electrochemical Reactivity"
After lunch–2:30 pm	Free
2:30 pm	Hackathon
6:30 pm	Hackathon day 3 wrap-up and set goals for day 4
Evening	Free

Monday, August 31

8:00 am	Breakfast
8:45 am	Flash presentations about goals for day 4
9:30 am	Hackathon
12:30 pm	Lunch and presentation (35 min) · Speaker: Marco Caricato (University of Kansas) · "CCResPy: a Coupled Cluster Response Program in Python for Molecules and Periodic Systems"
After lunch–2:30 pm	Free
2:30 pm	Hackathon
6:30 pm	Hackathon day 4 wrap-up and set goals for day 5
Evening	Free

Tuesday, September 1

8:00 am Breakfast

9:30 am Hackathon

12:00 pm Hackathon Wrap-up and Concluding Remarks

2:00 pm Check-out

Coffee will be available at any time during the day!