

PWF Uzbekistan: School on Materials Modeling and Simulation

DFT and Molecular Dynamics Approaches

Location: Uzbekistan • Dates: 6–10 Oct 2025 • Hours: 09:00–19:00 (local)

Day 1 — Monday, 6 Oct 2025

Time	Session	Speaker/Facilitator
10:00 – 11:00	Opening remarks	Umedjon Khalilov Bakhromjon Abdulazizov
11:00 – 11:30	Introduction to ICTP and the PWF Program	Natasa Stojic
11:30 – 12:30	Introduction to Computational Materials Science	Natasa Stojic
12:30 – 14:00	Lunch	—
14:00 – 15:30	First-Principles Materials Modeling (overview of DFT concepts)	S. Javad Hashemifar
15:30 – 16:00	Coffee/Tea Break	—
16:00 – 17:00	Introduction to Molecular Dynamics (motivation, potentials, workflow)	S. Mehdi Vaez Allaei
17:00 – 18:00	Meet the Participants & Project Introductions / Social Interaction	All participants

Day 2 — Tuesday, 7 Oct 2025

Time	Session	Speaker/Facilitator
09:00 – 10:30	Kohn–Sham Density Functional Theory (energy functionals, pseudopotentials)	S. Javad Hashemifar

10:30 – 11:00	Coffee/Tea Break	—
11:00 – 12:30	MD Algorithm (time integration, PBC, etc.)	S. Mehdi Vaez Allaei
12:30 – 14:00	Lunch	—
14:00 – 15:30	Hands-on DFT #1 (basic input files, cutoffs, k-points)	S. Javad Hashemifar
15:30 – 16:00	Coffee/Tea Break	—
16:00 – 17:30	Hands-on MD #1 (temperature control, RDF, MSD analysis)	S. Mehdi Vaez Allaei
17:30 – 18:00	Daily Wrap-up & Discussion	Chair of the Day

Day 3 — Wednesday, 8 Oct 2025

Time	Session	Speaker/Facilitator
09:00 – 10:30	DFT Lecture (exchange–correlation, convergence, DOS)	S. Javad Hashemifar
10:30 – 11:00	Coffee/Tea Break	—
11:00 – 12:30	Characterization of Material Phases in MD (structural identifiers, RDF, order parameters)	S. Mehdi Vaez Allaei
12:30 – 14:00	Lunch	—
14:00 – 15:30	Hands-on DFT #2 (band structure, DOS, charge analysis)	S. Javad Hashemifar
15:30 – 16:00	Coffee/Tea Break	—
16:00 – 17:30	Hands-on DFT #3 (phonon calculations, stability tests)	S. Javad Hashemifar

Day 4 — Thursday, 9 Oct 2025

Time	Session	Speaker/Facilitator
09:00 – 10:30	Equilibrium & Non-equilibrium MD (Green–	S. Mehdi Vaez Allaei

	Kubo & NEMD methods)	
10:30 – 11:00	Coffee/Tea Break	—
11:00 – 12:30	DFT Lecture (optical and electronic properties)	S. Javad Hashemifar
12:30 – 14:00	Lunch	—
14:00 – 15:30	Hands-on MD #2 (heat flux, autocorrelation analysis)	S. Mehdi Vaez Allaei
15:30 – 16:00	Coffee/Tea Break	—
16:00 – 17:30	Hands-on MD #3 (non-equilibrium setup and post-processing)	S. Mehdi Vaez Allaei

Day 5 — Friday, 10 Oct 2025

Time	Session	Speaker/Facilitator
09:00 – 10:30	Potentials and Force Fields in MD (EAM, AIREBO, ReaxFF)	S. Mehdi Vaez Allaei
10:30 – 11:00	Coffee/Tea Break	—
11:00 – 12:30	DFT Lecture (solid structures, case studies and advanced applications)	S. Javad Hashemifar
12:30 – 14:00	Lunch	—
14:00 – 16:00	Hands-on MD #4 (force-field comparisons and validation)	S. Mehdi Vaez Allaei
16:00 – 17:00	Closing Ceremony	Organizers
17:00 – 19:00	Hands-on MD #5 (extended Q&A and mini-projects)	S. Mehdi Vaez Allaei