Second Sharjah Regional Workshop on Computational Science and Engineering
December 11-13, 2016
Centre for Advanced Materials Research
Research Institute of Sciences and Engineering
University of Sharjah

	Lecture Title	Time	Lecturer
Day 1	○ Welcome	09:00 - 09:15	
	○ Overview on ab-initio Molecular Dynamics (MD)	09:15 – 09:30	Oliviero Andreussi
	○ Molecular dynamics: general theory and analysis of the trajectories	09:30 – 10:30	Oliviero Andreussi
	○ Introduction to Density Functional Theory (DFT)	10:45 – 11:45	Qteish Abdallah
	○ Ab initio MD: algorithms and applications	11:45 -12: 45	Davide Ceresoli
	Lunch	12:45 – 14:00	
	○ Tutorial 1 Born-Oppenheimer MD with the PW code	14:00 – 17:00	Oliviero & Davide
Day 2	○ Tutorial 2 Large-scale AIMD with the CP code	09:00 – 12:45	Oliviero & Davide
	Lunch	12:45 – 14:00	
	○ Tutorial 3 Transport properties from MD simulations and advanced techniques	14:00-17:00	Oliviero & Davide

- ✓ Morning and afternoon coffee breaks are served at 10:30 -10: 45 and 15:30 – 15: 45
- ✓ Day 3 for face to face and informal discussion if needed.