

Table of contents

Tuesday 22 April 2025	1
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PWF Sri Lanka - Advancing Computational Material Science: A Workshop on Density Functional Theory (DFT)

Tuesday 22 April 2025

Day 3 - E-resources room (05:00-13:00)

time	title	presenter
05:00	Lecture 7: DFT in Practice (Overview, Basis Sets, Pseudopotentials, Brillouin Zone Sampling and k-points)	
06:30	Coffee break	
07:00	Hands on Session: Bulk Silicon: Optimizing Basis Set Size, k-grid, Computing Lattice Parameters, Visualize charge density	
08:30	Lunch break	
09:30	Lecture 9: Introduction to Stress, Forces, and Geometry Optimization in DFT + handling finite systems	
11:00	Coffee break	
11:30	Hands on Session Continuation: Lattice parameter (vc-relax and EOS) and geometry optimization, setting up and doing surface calculation, VESTA introduction	