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PWF Sri Lanka - Advancing Computational Material Science: A Workshop on Density Functional Theory (DFT)

Sunday 20 April 2025

<u>Day 1</u> - E-resources room (05:00-13:00)

time	title	presenter
05:00	Introductory Remarks	
05:30	Lecture 1: Basics of Quantum Mechanics (Recap of Schrödinger Equation, Bra-ket notation, Matrix formulation, Variational Principle, Applications to the H-atom)	
07:00	Coffee break	
07:30	Lecture 2: Introduction to Variational Principle and H-atom Calculation	
09:00	Lunch break	
09:30	Lecture 3: Many-Electron Systems and Approximations (Born-Oppenheimer Approximation, Hartree, Hartree-Fock	
11:00	Coffee break	
11:30	Hands-on Session: Solving quantum mechanical toy problems using the variational principle	