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PWF Tunisia: Computational Materials Science based on Density-Functional Theory for Renewable Energy and Spintronics

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Day 2 (09:30-18:00)

time	title	presenter
09:30	Introduction to solid state theory (Band structure)	STOJIC, Natasa
11:00	Coffee break	
11:20	Basics of density-functional theory DFT (Theorems, basic functionalities)	STOJIC, Natasa
12:45	Lunch break	
14:15	Quantum Espresso (QE) Hands on - scf calculations on Si crystal: parameter convergence, volume relaxation	HSOUNA, Maha STOJIC, Natasa CHIKA, Khouloud JEMAI, Ghassen ARFAOUI, Mehdi
16:00	Coffee break	
16:20	QE Hands on - scf calculations on Si crystal, parameter convergence, volume relaxation	HSOUNA, Maha STOJIC, Natasa CHIKA, Khouloud JEMAI, Ghassen ARFAOUI, Mehdi