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

## Friday 20 September 2024

### Day 5 (09:30-18:00)

time	title	presenter
09:30	Computational materials science for functional materials: fundamental science for development	SERIANI, Nicola
11:00	Coffee break	
11:20	Ab-initio simulations of materials for energy applications	SERIANI, Nicola
12:50	Lunch break	
14:15	QE Hands on - molecular adsorption on Al(100)	YADAV, Anita HSOUNA, Maha STOJIC, Natasa CHIKA, Khouloud JEMAI, Ghassen ARFAOUI, Mehdi
16:00	Coffee break	
16:20	QE Hands on - magnetism and DFT+U calculations of FeO	YADAV, Anita HSOUNA, Maha STOJIC, Natasa CHIKA, Khouloud JEMAI, Ghassen ARFAOUI, Mehdi