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WIEN2k Hands-On Workshop for New and Existing Users | (smr 3929)

Monday 08 April 2024

notitle - Kastler Lecture Hall (AGH) (08:30-17:30)

time	title	presenter
09:20	Welcome address	PETER BLAHA (TU VIENNA, AUSTRIA), OLEG RUBEL (MCMASTER UNIVERSITY, CANADA), NICOLA SERIANI (ICTP, ITALY)
09:30	Density functional theory (DFT) and the concepts of the augmented-plane-wave plus local orbitals (APW+lo) method	KARLHEINZ SCHWARZ
10:30	Coffee break	
11:00	An overview of the WIEN2k package for beginners	PETER BLAHA
12:30	Registration	
12:30	Lunch	
14:00	Input files of scf programs, Volume optimization	PETER BLAHA
15:00	Coffee break	
15:30	Exercises	LEILA KALANTARI