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

Wednesday 10 April 2024

notitle - Kastler Lecture Hall (AGH) (09:00-17:30)

time	title	presenter
09:00	Advanced DFT: mGGA, Hybrid-DFT, vdW-DFT, LDA+U, EECG, mBJ, KTBM-meta-GGAs	FABIEN TRAN
10:00	Coffee break	
10:30	Mixing + force minimization	LAURENCE MARKS
11:30	Exercises	LEILA KALANTARI
12:30	Lunch	
14:00	Wien2k at the command line	PETER BLAHA
15:00	Coffee break	
15:30	Exercises	LEILA KALANTARI