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MaX School on Advanced Materials and Molecular Modelling with Quantum ESPRESSO | (smr 3622)

Monday 17 May 2021

notitle - Online (08:00-12:30)

time	title	presenter
08:00	Participant's computer setup check	
08:20	Opening remarks and general instructions	STEFANO BARONI (SISSA, ITALY), RALPH GEBAUER (ICTP, ITALY)
08:30	QUANTUM ESPRESSO: overview and basic functionalities. The self-consistent cycle. PBC: supercells and k-point sampling	RALPH GEBAUER
10:00	Break and participant's computer setup check	
10:30	Hands-on: How to compile Quantum ESPRESSO. SCF calculations + post-processing – part 1. XCrySDen, PWgui, QE-emacs-modes, and PWTK	PIETRO DELUGAS (SISSA, ITALY)