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Advanced Workshop on High-Performance & High-Throughput Materials Simulations using Quantum ESPRESSO | (smr 3102)

Thursday 26 January 2017

Day 9 - Thursday, January 26

- Adriatico Guest House - Kastler Lecture Hall (09:00-18:30)

time	title	presenter
09:00	Advanced Molecular Dynamics. Thermostats, Barostats and Nuclear Quantum Effects	M. CERIOTTI
10:30	Coffee Break	
11:00	Hands-on: Advanced Molecular Dynamics using i-PI and QE	M. CERIOTTI, R. PETRAGLIA
12:30	Lunch Break	
14:00	Levels & Hierrachy of Parallelism in QE.	S. DE GIRONCOLI, P. GIANNOZZI
16:00	Coffee Break	
16:30	Hands-on: Levels & Hierarchy of Parallelism in QE.	S. DE GIRONCOLI, P. GIANNOZZI