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

## Tuesday 24 January 2017

**Day 7- Tuesday, January 24 - Adriatico Guest House - Kastler Lecture Hall (09:00-23:00)**

time	title	presenter
09:00	Solvent and Environment Effects: Continuum Models	O. ANDREUSSI
10:30	Coffee Break	
11:00	Hands-on: Environment Effects (Solvation, Electrochemistry, PBC) via Continuum Models	O. ANDREUSSI, I. TIMROV
12:30	Lunch Break	
14:00	Introduction to AiiDA, the ADES model and the concept of provenance	G. PIZZI
15:00	Hands-on: Introduction to AiiDA & browsing through the graph	G. PIZZI, F. GARGIULO, S. HUBER, L. KAHLE, S. WAYCHAL
16:30	Coffee Break	
17:00	Hands-on: Running SCF Calculations in QE using AiiDA	G. PIZZI, F. GARGIULO, S. HUBER, L. KAHLE, S. WAYCHAL
20:30	RECEPTION	