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

# Wednesday 18 January 2017

## Day 3 -Wednesday, January 18

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

| time | title | presenter |
|---|---|---|
| 09:00 | Basics of ab-initio Molecular Dynamics: dynamics on the Born-Oppenheimer surface, energy conservation, ensembles, thermostats and barostats | S. SCANDOLO |
| 10:30 | Coffee Break | |
| 11:00 | Car-Parrinello Molecular Dynamics: adiabaticity, metals, thermostats and barostats, correlation times and averages | SCANDOLO, S. |
| 12:30 | Lunch Break | |
| 14:00 | Hands-on: Ab-initio Molecular Dynamics: starting the dynamics, computing averages | GIANNOZZI, P. |
| 16:00 | Coffee Break | |
| 16:30 | Hands-on: Ab-initio Molecular Dynamics: computing correlations and thermodynamic properties, using thermostats | GIANNOZZI, P. |