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

Contribution ID : 1261 Type : not specified

DFT hands on: total energy scf calculations, optimizations, bands, dos, and post-processing; insulators vs metals (k-points); SCs: defects, isolated systems, surfaces.

Monday, 16 January 2017 16:30 (2:00)

Content

Summary

Presenter(s): P. GIANNOZZI (University of Udine); PRESENTED BY IURII TIMROV

Session Classification: Day 1- Monday, January 16