

**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 IURI TIMROV

Session Classification : Day 1- Monday, January 16