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

Contribution ID: 1258 Type: not specified

## DFT fundamentals: from theory to practice. Hohenberg-Kohn-Sham theory; variational principle; Hellman-Feynman th and energy derivatives.

Monday, 16 January 2017 09:30 (1:00)

Content

**Summary** 

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Session Classification: Day 1- Monday, January 16