

15.03.2018

INDUSTRIAL FORUM. SESSION 8

SIESTA: professional open source code ready for industry

Program

11:30-11:40 Introduction to SIMUNE and SIESTA

11:40-11:50 SIESTA-PRO: SIESTA code ready for the industry

Federico Marchesin

11:50-12:00 SIESTA code: main technical features

Mónica García-Mota

12:00-12:30 Excited states properties for SIESTA calculations: time-dependent density functional theory and beyond.

Peter Koval

12:30-13:00 Hints to perform an accurate and well-converged siesta calculation

- input file. Principal siesta input parameters
- pseudopotential
- basis set. The delta-test

Monica García-Mota and Federico Marchesin

13:00-13:15 Analyzing the results. Post-processing siesta output

Monica García-Mota

13:15-13:30 Round table discussion and closing remarks