

Agenda

Material Science codes on innovative HPC architectures: from electronic structure to spectra with Quantum ESPRESSO and Yambo

3-5 December 2018

Cineca - Casalecchio di Reno (Bologna)

Day 1

08:45 - 09:00	Registration	
09:00 - 10:30	Welcome Introduction talk on Material Science and DFT	F. Affinito
10:30 - 11:00	Coffe break	
11:00 - 13:00	QE basics (including access to HPC, building)	F. Affinito
13:00 - 14:30	Lunch break	
14:30 - 16:00	QE basics	F. Affinito P. Bonfa'
16:00 - 16:30	Coffe break	
16:30 - 18:00	QE (less) basics	F. Affinito P. Bonfa'

Day 2

09:00 - 10:30	QE on HPC machines: parallelism	P. Bonfa'
10:30 - 11:00	Coffe break	
11:00 - 13:00	Yambo: introduction & getting started (yambo in general, QE + p2y)	A. Ferretti
13:00 - 14:30	Lunch break	
14:30 - 16:00	GW Lecture I+II (ARPES: from exp to computer simulations)	A. Ferretti
16:00 - 16:30	Coffe break	
16:30 - 18:00	Yambo: LinRes hands on	All

Day 3

09:00 - 10:30	Yambo: GW hands on	A. Marini A. Ferretti
10:30 - 11:00	Coffe break	
11:00 - 13:00	Yambo: GW hands on	A. Marini A. Ferretti
13:00 - 14:30	Lunch break	
14:30 - 16:00	Yambo: parallel tutorial I	A. Marini
16:00 - 16:30	Coffe break	
16:30 - 18:00	Yambo: parallel tutorial II	A. Marini

NB: the agenda may be subject to changes that will be communicated to the students as soon as possible.