

# Workshop on Computational *Ab initio* Quantum Thermodynamics

Columbia Global Center, Nairobi, and Technical University of Kenya, Nov. 28 - Dec. 1

## Day 1 (Nov. 29)

Kenya Time	Eastern Time	Sessions
08:45 – 09:00	00:45 - 01:00	Welcome
09:00 – 10:00	01:00 - 02:00	<a href="#">Renata Wentzcovitch</a> – Thermodynamics with QHA overview
10:00 – 11:00	02:00 - 03:00	<a href="#">John Perdew</a> (video) – DFT Introduction
11:00 – 11:15	03:00 – 03:15	Coffee break
11:15 – 12:15	03:15 – 04:15	<a href="#">Pietro Delugas</a> – Introduction to DFPT
12:15 – 13:30	04:15 – 05:30	Lunch
13:30 – 15:30	05:30 – 07:30	Hands-on with QE SCF calculations
15:30 – 15:45	07:30 – 07:45	Coffee break
15:45 – 18:00	07:45 – 10:00	Hands-on with QE SCF calculations and EOS Express workflow ( <a href="#">Qi Zhang</a> )
18:00 – 19:30	10:00 – 11:30	Dinner

## Day 2 (Nov. 30)

Kenya Time	Eastern Time	Sessions
9:00 – 10:00	01:00 - 02:00	<a href="#">John Perdew</a> (video): DFT State-of-the-art
10:00- 11:00	02:00 - 03:00	<a href="#">Pietro Delugas</a> - DFPT and phonon calculations with the Quantum ESPRESSO
11:00 – 11:15	03:00 – 03:15	Coffee break
11:15 – 11:45	03:15 – 03:45	<a href="#">Qi Zhang</a> – The qha Python package
11:45 - 12:15	03:45 – 04:15	<a href="#">Renata Wentzcovitch</a> – Thermoelasticity
12:15 – 13:30	04:15 – 05:30	Lunch
13:30 – 15:30	05:30 – 07:30	Hands-on with QE and Phonon calculations
15:30 – 15:45	07:30 – 07:45	Coffee break
15:45 – 17:30	07:45 – 09:30	Hands-on with QE and Express Phonon workflow ( <a href="#">Qi Zhang</a> )
17:30 – 18:00	09:30 – 10:00	<a href="#">Chenxing Luo</a> – The cij Python package
18:00 – 20:30	10:00 – 12:30	<i>Reception at Columbia Global Center in Nairobi</i>

## Day 3 (Dec. 1)

Kenya Time	Eastern Time	Sessions
09:00 – 10:00	01:00 - 02:00	<a href="#">Zhen Zhang</a> – Phonon Quasiparticle Calculations
10:00 – 11:00	02:00 - 03:00	<a href="#">Renata Wentzcovitch</a> – More applications of quasiparticle calculations
11:00 – 11:15	03:00 – 03:15	Coffee break
11:15 – 12:15	03:15 – 04:15	<a href="#">Zhen Zhang</a> – The phq package
12:15 – 13:30	04:15 – 05:30	Lunch
13:30 – 15:30	05:30 – 07:30	Hands-on with QE and thermoelasticity calculations
15:30 – 15:45	07:30 – 07:45	Coffee break
15:45 – 18:00	07:45 – 10:00	Hands-on with QE and thermoelasticity calculations
18:00 – 19:30	10:00 – 11:30	Dinner