

# Perturbo Workshop Program

September 21-22, 2023

Organizers: Bernardi research group at Caltech (<http://bernardi.caltech.edu>).

## Day1, Thursday, September 21st:

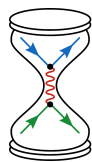
(in Pacific Time, each lecture and tutorial is followed by 5-10 minutes of Q&A)

9:00 - 9:45 AM	<b>Lecture 1:</b> Introduction, overview, and selected results.	Prof. Marco Bernardi
9:45 - 10:25 AM	<b>Tutorial 1:</b> The Perturbo code. Download and installation. Perturbopy postprocessing suite. Testsuite.	Shaelyn Iyer
10:25 - 10:30 AM	<b>Break</b>	
10:30 - 11:15 AM	<b>Lecture 2:</b> Electron-phonon (e-ph) interactions. Short vs. long-range, interpolation, SOC, DFT+U.	Jinsoo Park
11:15 AM - 12:00 PM	<b>Tutorial 2:</b> Preliminary steps: DFT, DFPT, Wannier90. Interface with Perturbo. Interpolation.	Yao Luo
12:00 - 1:00 PM	<b>Lunch Break</b>	
1:00 - 1:45 PM	<b>Lecture 3:</b> Transport in the Boltzmann transport equation (BTE) framework. Perturbo implementation.	Dhruv Desai
1:45 - 2:25 PM	<b>Tutorial 3:</b> Calculations of e-ph scattering rates and mobility vs. temperature / doping.	Khoa Le
2:25 - 2:30 PM	<b>Break</b>	
2:30 - 3:15 PM	<b>Lecture 4:</b> Ultrafast electron dynamics in the BTE framework, high-field dynamics.	Ivan Maliyov
3:15 - 4:00 PM	<b>Tutorial 4:</b> Nonequilibrium ultrafast carrier dynamics.	Kelly Yao

## Day2, Friday, September 22nd:

(in Pacific Time)

9:00 - 10:00 AM	<b>Flash Talks on New Results &amp; Frontiers</b>	Jinsoo Park Yao Luo Kelly Yao Ivan Maliyov
10:00 - 11:00 AM	<b>Hands-on 1:</b> Using Perturbo via Docker. Testsuite.	Sergei Kliavinek
11:00 AM - 12:00 PM	<b>Hands-on 2:</b> Running preliminary calculations, generating the HDF5 file of e-ph elements in the Wannier basis. Interpolation.	Shiyu Peng
12:00 - 1:00 PM	<b>Lunch Break</b>	
1:00 - 2:00 PM	<b>Hands-on 3:</b> Transport calculations, magnetotransport. Using Perturbopy to read the output files and plot data.	Dhruv Desai
2:00 - 3:00 PM	<b>Hands-on 4:</b> High-field carrier dynamics: calculation of velocity-field curves.	Ina M. Sorensen
3:00 - 3:15 PM	<b>Closing remarks</b>	Prof. Marco Bernardi



# Perturbo

