

"Computational Chemistry and Spectroscopy" Workshop

Date: Thursday, 24.02.2022

Venue: Online via Zoom

Link: <https://uni-due.zoom.us/j/68259809514?pwd=RWZmY3k3OFFpK29sUWV4V2NobGFkQT09>

Meeting-ID: 682 5980 9514

Kenncode: 588796

Host: Prof. Dr. Frank Neese & Dr. Dimitrios Manganas (MPI Kofo)

Agenda

9:00-10:00	Prof. Dr. Frank Neese Introduction to computational chemistry
10:00-10:15	Coffee break
10:15-11:00	Dr. Dimitrios Manganas Theoretical spectroscopy beyond DFT
11:00-11:15	Coffee break
11:15-12:00	Dr. Dimitrios Manganas Developing computational protocols for solids and surfaces
12:00-13:00	Lunch
13:00-13:45	Dr. Dimitrios Manganas Core level spectroscopy for solids