

## O 1: Overview Talk: Claudia Draxl

Time: Monday 9:30–10:15

Location: S054

**Invited Talk**

O 1.1 Mon 9:30 S054

**From surfaces and molecules to interfaces and hybrid materials: Theoretical spectroscopy of low-dimensional systems**

— •CLAUDIA DRAXL — Humboldt-Universität zu Berlin, Berlin, Germany — Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany

*Ab initio* spectroscopy is a powerful combination of quantum-based theories and computer simulations. It covers a wide range of theoretical and computational methods, which go beyond density-functional theory by incorporating many-body effects and interactions that show

up in the excited state. This methodology not only allows for analyzing data obtained by experimental probes like photoemission, optical absorption, Raman, infrared, X-ray, and electron-loss spectroscopy, but also for shining light onto the underlying processes. These may be distinctively different depending on the nature and dimensionality of the material. Low-dimensional systems and interfaces challenge our theoretical concepts and numerical approaches. A series of selected examples – from surfaces and molecules to interfaces and organic-inorganic hybrid materials – will show how we can explore exciting new phenomena, where we are in our theoretical understanding, and what the major issues are that need to be tackled.