



# Einladung zum Vortrag

## “Materials with tunable properties: a computational design”

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**Termin:** Donnerstag, 10. Oktober 2019, 10:45 Uhr, Lehrvortrag 08:30 Uhr

**Ort:** Victor-Franz-Hess-Hörsaal, Währinger Straße 17,  
1. Stock (Hoftrakt), Raum 112

### Abstract:

Selectively tuning the properties of materials has a great potential in guiding applications and producing materials 'on demand'. Here, we discuss examples of a computational survey of tunable materials. In this survey, we move from the molecular level up to functionalized surfaces and 2D heterostructures exposing their potential to generate novel devices. Our approach is based on exploring the stability, as well as adsorption, optoelectronic, and mechanical properties of the materials. Within this concept, we provide an extended view on their potential and an outlook on modeling materials at different spatiotemporal scales.

Im Rahmen des Vortrages findet eine Lehrprobe zum Thema  
„The quantum harmonic oscillator“ statt.