# Digital foundry: Predicting new materials and their properties with supercomputers

A talk by Silvana Botti

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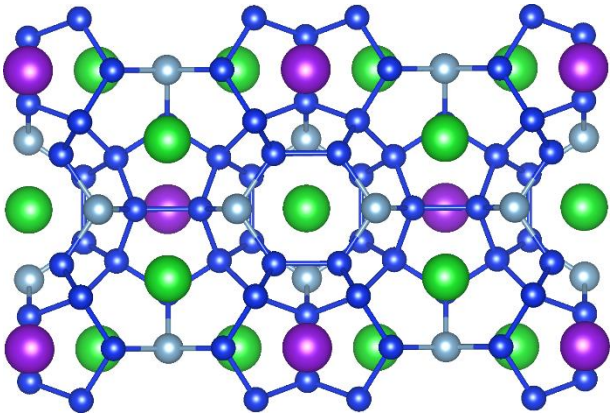
DATE / TIME: Monday, Dec 18th 2017, 4:00 p.m.

LOCATION: TU Wien, Seminarraum 138C (Freihaus, Turm B/yellow, 9. OG)



In this lecture I will discuss how first-principles calculations can efficiently speed up the discovery of new materials.

Theoretical approaches based and going beyond density functional theory ally today accuracy and efficiency, and are therefore suitable tools for understanding the physics not only of simple perfect crystals, but also of nanostructured materials, doped semiconductors, interfaces, alloys, etc. As a result, *ab initio* simulations of spectroscopic properties can finally account for the complexity of "real" experimental samples, allowing accurate comparison of calculated and measured structural and excitation properties. The powerful combination of theoretical spectroscopy with high-throughput calculations and structural prediction can therefore provide a precious guide to experimentalists in the search of new materials.