On behalf of the group of

Electronic Properties of Materials

we cordially invite you to the following talk

Gergö Kukucska

Eötvös-Loránd-University, Budapest, Hungary

Simulation of Raman spectra based on first principles methods

Abstract:

Raman spectroscopy is undoubtedly one of the most widespred non-destructive optical method of our days. Despite its versatility from experimental point of view, theoretical modeling of Raman peak intensities can be hardly found in the literature. The available theoretical works usually utilize the Placzek approximation based on the response for a time independent electric field. In this talk we present our method based on the built in algorithms of the Vienna Ab-initio Simulation Package (VASP) to calculate Raman intensities, using the excitation energy dependent Placzek approximation and we show its applications for various systems.

Date: Tuesday, 2nd October 2018, 11:30

Location: Josef-Stefan-Lecture-Hall, 3rd floor, Faculty of Physics, Boltzmanngasse 5, 1090 Wien

Prof. Paola Ayala, Prof. Hans Kuzmany,
Prof. Wolfgang Lang, Prof. Thomas Pichler