TECHNISCHE UNIVERSITÄT WIEN

INSTITUT FÜR THEORETISCHE PHYSIK
WIEDNER HAUPTSTRASSE 8-10, 1040 WIEN

Invitation

Institute for Theoretical Physics – TU Wien

Andreas Grüneis

Max-Planck-Institute for Solid State Research
Stuttgart, Germany

Towards exact many-electron wave functions in real solids

Abstract:

Solving the many-electron Schrödinger equation for real materials exactly is an exponentially hard problem: the required computational cost grows exponentially with respect to the number of electrons. However, thanks to the development of novel theoretical methods and the improvement of numerical algorithms as well as computer hardware over the last decades, significant progress in the study of many-electron systems has been achieved. In this presentation, I will give an introduction to the field of many-electron wave function based theories for the study of periodic systems. I will outline some of our recent developments that push the limits of treatable system sizes substantially and show that wave function based theories can be applied to study molecular adsorption problems on surfaces, pressure-driven phase transitions as well as defects in solids. These applications are paradigmatic for van der Waals interactions and strong correlation effects, and methods that describe their electronic structure accurately are highly sought after.

Date:

Thursday, **12.5.2016**, 8:30

Venue:

Lecture hall – University Library
TU Wien
Resselgasse 4, 5th floor