





## Seminar announcement

Tuesday, June 21, 2022 1:30 pm

## WSI, Seminar room S 101

also ONLINE via ZOOM https://tum-conf.zoom.us/j/63032060135 Meeting-ID: 630 3206 0135 Kenncode: 934720

## "Origin, consequences, and analysis of Fermi energy limits in ionically bonded semiconductors"

The function of semiconductor devices relies on the spatial variation of the Fermi energy. In classical elemental and covalently bonded semiconductors, the Fermi energy can often be varied throughout the whole energy gap, enabling a plethora of applications. This is very often not the case in ionically bonded semiconductors, which often lack ambipolar dopability. The related confinement of the Fermi energy constitutes a fundamental limitation for many applications, in particular for processes relying on interfacial charge transfer. The origin of the Fermi energy limits is often assigned to self-compensation, which is the formation of compensating crystallographic point defects, which can be traced back to the dependence of defect formation enthalpies on the Fermi energy. However, self-compensation is not the only mechanism, which can lead to a limitation of the Fermi energy. The oxidation or reduction of lattice species can occur for Fermi energies deep inside the energy gap. In addition, dopants or defects may change their valence and become activated or deactivated by moving the Fermi energy across their charge transition level or by segregation. After an introduction to the different charge compensation mechanisms, the presentation will illustrate several examples using the analysis of materials and their interfaces, mostly Schottky barriers, by means of photoelectron spectroscopy with in-situ sample preparation. Although this approach has been applied recently mostly to oxides, examples of chalcogenide photovoltaic materials, such as Cu(In,Ga)Se2 and SnS are also included. The importance of selecting materials with a suitable variation of the Fermi energy will be emphasized.

Prof. Andreas Klein Institute of Materials Science, Electronic Structure of Materials Technische Universität Darmstadt Germany