

**O 68: Invited Talk (Klaus Heinz)**

Time: Friday 13:30–14:15

Location: HSZ 02

**Invited Talk** O 68.1 Fri 13:30 HSZ 02  
**Surface Structure Analysis – Present Status and Future**  
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The knowledge of the crystallographic structure of a surface, that is the positions of atoms within a certain slab of a surface, is essential for the quantitative understanding of its physical properties. Hereby, the item "surface" stands for clean and adsorbate covered surfaces as well as interfaces, which all are crucial components of nanostructures.

The current status of surface crystallography is reviewed including the limitations involved. Emphasis is on quantitative low-energy diffraction (LEED) but the strength of other and competing methods as, e.g., photoelectron diffraction (PED) and surface x-ray diffraction

(SXR) is also illuminated. Today's state of the art techniques which use TensorLEED combined with structural search routines as well as recent progress made by so called holographic-type direct methods or the valuable use of Patterson-type maps will be described. It will also be shown that a single method may be unable to resolve the (full) structure or even to get only an idea about the proper model. Instead, the application of several methods can be necessary. These include in particular scanning tunneling microscopy (STM) with its real-space information and first-principles methods as density functional theory (DFT) which minimizes the system's energetics rather than an R-factor. It will also be discussed whether or not crystallographic precision in the picometer range – which we are used to achieve for simple structures – is necessary for complex structural phases.