FREE UNIVERSITY

PHYSICS DEPARTMENT **KVV WS 06/07**

V **Basics of Theoretical Crystallography for Surface Scientists** (Hermann)
Tue 14.15 - 15.45, Physikbau, Seminarraum Theorie T1 (1.3.21)

First Lecture: Oct. 17, 2006

⇒ **TARGET GROUP**

Advanced physics and chemistry students, PhD students

⇒ **TYPE OF PRESENTATION**

Lecture (2 hours weekly)

⇒ **REQUIREMENTS**

Basics of solid state physics/chemistry and surface science

⇒ **LITERATURE**

- M.A. Van Hove, W.H. Weinberg, and C.M. Chan, "Low Energy Electron Diffraction", Springer Series in Surface Science, Vol. 6, Heidelberg 1986.
- D.P. Woodruff and T. A. Delchar, "Modern Techniques of Surface Science", Cambridge University Press 1986 (2nd Ed. 1996).
- C. Giacovazzo et al., “Fundamentals of Crystallography”, IUCr Texts on Crystallography 2, Oxford Science Publishing 1998, ISBN 0 19 855578 4.
- J.C. Slater, "Symmetry and Energy Bands in Crystals", Dover Publications, New York 1972.
- R.W.G. Wyckoff, "Crystal Structures" Vol. I-VI, Interscience Pub., New York 1963.
- T. Hahn (Ed. 1983, 1965, 1987), “International Tables for Crystallography”, Vol. A, Reidel Publishing, Boston.
- J.F. Nicholas in Landold-Börnstein, New Series, "Physics of Solid Surfaces, Subvolume a, Structure", Bd. III/24a, Springer 1993.
- G. Burns and A. M. Glazer, “Space Groups for Solid State Scientists”, 2nd Ed., Academic Press, New York 1990.

LECTURE

BASICS OF THEORETICAL CRYSTALLOGRAPHY FOR SURFACE SCIENTISTS

Prof. Dr. Klaus Hermann, Theory Department, Fritz-Haber-Institut der MPG, Berlin

The lecture will be given weekly (2 hours).

Content

This lecture covers important methods of theoretical crystallography applied to systems in two and three dimensions. It will provide students and researchers with a good understanding of local geometries and symmetries at ideal single crystal surfaces. This knowledge is important for many experimental and theoretical studies of physical as well as chemical phenomena at surfaces. The lecture covers amongst other subjects

- **3-dimensional crystal lattices**
  classification schemes, lattice basis representation, 3-dim. symmetry, neighbor shells, number theoretical methods, Minkowski reduction
- **Netplanes**
  reciprocal lattice, netplane-adapted lattice basis, Miller indices, cubic and 4-index notation, 2-dim. symmetry, netplane stacking, densest netplanes
- **Ideal single crystal surfaces**
  primitive vs. non-primitive lattices, vicinal stepped and kinked surfaces, Miller index decomposition, warped surfaces (faceting)
- **Real crystal surfaces**
  reconstruction, relaxation, imperfections, experimental studies, NIST surface structure database
- **Adsorbate systems**
  atomic and molecular adsorbates, periodic overlayers (commensurate, incommensurate), 2x2 matrix nomenclature, Wood notation

Basic knowledge of solid state physics/chemistry and surface science is required.

Hermann