

FREE UNIVERSITY

PHYSICS DEPARTMENT

KVV WS 03/04

**V Structural and Electronic Properties of Metal
Oxides and their Surfaces: Theoretical Aspects** (Hermann)
Tu 14.15 - 15.45, Physikbau, Seminarraum Theorie (1.3.21)

First Lecture: Oct. 28, 2003

⇒ **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**

- **V. E. Henrich and P. A. Cox, "The Surface Science of Metal Oxides", University Press, Cambridge 1994.**
- C. N. R. Rao and B. Raven, "Transition Metal Oxides", VCH Press, New York, 1995.
- B. Delmon and J. T. Yates (Eds.), "Transition Metal Oxides: Surface Chemistry and Catalysis", Studies in Surface Science and Catalysis Vol. 45, Elsevier, Amsterdam, 1989.
- B. Grzybowska-Swierkosz, Appl. Catal. A: General 157, 1-420 (1997).
- E. R. Braithwaite and J. Haber, "Molybdenum: An Outline of its Chemistry and Uses", Elsevier, Amsterdam 1994.
- A. Zangwill, "Physics at Surfaces", Cambridge University Press.
- 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.
- C. Giacovazzo et al. "Fundamentals of Crystallography", Oxford University Press, Oxford, 1998.

LECTURE

STRUCTURAL AND ELECTRONIC PROPERTIES OF METAL OXIDES AND THEIR SURFACES: THEORETICAL ASPECTS

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

The lecture will be held weekly (2 hours).

Content:

This lecture deals with theoretical aspects concerning geometric and electronic properties of metal oxides. In particular, physical parameters of the surfaces will be compared with those of the bulk. Tentative subjects are

- **Lattice geometry of metal oxides**
lattice structure, classification schemes, ideal surfaces, defects, imperfections
- **Electronic properties**
bandstructure, metall-insulator transitions,
magnetic insulators, superconductors
- **Surface restructuring**
reconstruction, relaxation, defects
- **Adsorption at metal oxide surfaces**
atomic, molecular adsorbates, reactive adsorption,
catalytic processes

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

Hermann