FREE UNIVERSITY

PHYSICS DEPARTMENT

KVV WS 07/08

V Metal Oxides and their Surfaces: Theory of Structure and Electronic Properties (Hermann)

Tu 14.15 - 15.45, Physikbau, Seminarraum Theorie (1.3.21)

First Lecture: Oct. 23, 2007

\Rightarrow TARGET GROUP

Advanced physics and chemistry students, PhD students

\Rightarrow TYPE OF PRESENTATION

Lecture (2 hours weekly)

\Rightarrow **REQUIREMENTS**

Basics of solid state physics/chemistry and surface science

\Rightarrow 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.

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