



INTERNATIONAL ATOMIC ENERGY AGENCY  
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION



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WORKSHOP ON  
"SURFACE SCIENCE AND CATALYSIS"  
(4 - 8 May 1987)

OUTLINE OF LECTURES

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These are preliminary lecture notes, intended only for distribution to participants.

ICTP Trieste Workshop on Surface Science and Catalysis

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LECTURE I      THEORY OF CHEMISORPTION

- Introduction: The adiabatic potential energy surface
- Density functional theory and the variational principle
- "Ab initio" calculations of potential energy surfaces
- Effective medium theory
- Trends in chemisorption energies
- Trends in activation energies for dissociation
- Dynamics

LECTURE II      THE AMMONIA SYNTHESIS

- Background
- UHV studies of  $N_2$ ,  $H_2$ , and  $NH_3$  adsorption on Fe surfaces
- The reaction mechanism
- Statistical mechanics of competitive chemisorption
- The rate equation
- Comparison to experiment and understanding:
  - rates
  - reaction orders
  - overall activation energies
  - coverages
- An analog: Hydro-desulphurization and denitrogenation over "CoMoS"
- Trends in the ammonia activity along the transition metal series

LECTURE III      POISONING AND PROMOTION

- The phenomena
- Models proposed
- Effective medium theory applied to this problem
- Density of states effects
- Electrostatic effects
- The promotion of the ammonia synthesis by K
- The poisoning of the ammonia synthesis by  $H_2O$
- Other examples