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WORKSHOP ON

"SURFACE SCIENCE AND CATALYSIS"

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ELECTRONEGATIVE ADDITIVES AND POISONING OF METAL CATALYSTS

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I. INTRODUCTION

- Influence of the surface srtucture and composition on the catalytic activity and selectivity
- Deactivation of the catalysts, chemical deactivation /poisoning/
- Stages of the metal catalyst poisoning and the origin of the poisons
- The relevance of the surface science model studies to the fundamental understanding of the mechanism of the poison action

II. ADSORPTION AND INTERACTION OF ELECTRONEGATIVE ATOMS /Cl,S,N,C,O,P/ ON SINGLE CRYSTAL METAL SURFACES

- Deposition and surface concentration
- Adsorption site occupation and ordering
- Bond lenghts, bond angles and effective adatom radius
- Work function changes and charge transfer
- Adatom induced perturbations in the surface electronic structure
- Adatom induced reconstruction, or formation of a surface compound

III. THE CHEMISORPTIVE PROPERTIES OF THE MODIFIED SURFACES TOWARDS MOLECULES WITH ACCEPTOR BEHAVIOUR /CO, NO, O_2, H_2/

- Adsorption rate on modified surfaces
- Adsorption states and corresponding binding energies
- Capacity of the surface for adsorption in the presence of a modifier
- Dissociation probability on modified surfaces
- Changes in the electronic structure of the coadsorbate in the presence of a modifier
- Possible mechanisms of the modifier's action /e.g. steric blocking, electrostatic interactions, via the substrate interactions, etc./
- Strenght of the effect and the contribution of the local geometry, electronegativity and effective radii of the modifier

IV. MODEL STUDIES OF SOME SURFACE REACTIONS AND CORRELATIONS BETWEEN THE EFFECT OF THE MODIFIER ON THE REACTION RATE AND THE CHEMISORPTIVE PROPERTIES

- examples with CO oxidation on Pt /110/, NO reduction on Pt/100/ and CO hydrogenation on Ni /100/
- Comparison with data for the effect of poisons in the "real" catalysis

V. CONCLUSIONS

The application of the results obtained with model systems in explainng the poison action in the "real" catalysis works satifactorily in the cases of metal catalysed reactions, which are structural insensitive. The mechanism ofpoisoning is rather complex, involving site blockage due direct repulsive interactions at short modifier - reagent distances, and indirect via modification of the electronic structure of the substrate.

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