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SPRING COLLEGE IN CONDENSED MATTER
ON
"THE INTERACTION OF ATOMS & MOLECULES WITH SOLID SURFACES"
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THE KINETICS AND DYNAMICS OF GAS-SURFACE PROCESSES

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Outline

This will be a course of 5 lectures aimed at establishing theoretical foundations which will facilitate a study of topical problems in surface dynamics and kinetics. It is not my intention here to present large volumes of experimental kinetic data for every conceivable system and attempt to catalogue them according to standard (or non-standard!) kinetic models. Instead I will go back to basics and build upon elementary concepts in chemical physics (potential energy surfaces, transition state theory etc, etc) and address classes of problems in the literature which appear to be in some sense 'generic'. Let me begin by outlining the overall structure of my lectures.

- L(i) An introduction to kinetics and dynamics at surfaces. The potential energy surface (PES). The Born-Oppenheimer approximation. Electronic representations. Transition state theory (TST).
- L(ii) Elementary surface processes. An experimental example, the H_2/Cu system as a prototype for kinetics of adsorption, desorption and reaction. Activated processes, the Van Willigen model.
- L(iii) Calculating desorption rates. Molecular dynamics of infrequent events. Crossing surfaces and transition states at surfaces. Detailed balance and microscopic reversibility. Examples, atomic desorption of Ar/Pt and molecular associative desorption of H_2/Cu .
- L(iv) Early and late activation barriers and their influence on surface processes. Probing the PES by scattering experiments. Sticking coefficients and their dependence on beam properties. Molecular precursors to adsorption. Normal vs. total energy scaling, $N_2/W(110)$.
- L(v) Multiple activation barriers and their consequences on kinetic and dynamic measurements. Quantum effects in H_2 scattering from surfaces. When is classical molecular dynamics not enough? Vibrationally enhanced sticking. Surface resonances.

REFERENCES

References will be given on a lecture-by-lecture basis. I shall attempt to include most of the standard works and reviews as well as original papers where possible.

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