PL-5

Ab-initio molecular dynamics

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In the last few decades, computational physics has established itself as a discipline that parallels more traditional experimental and theoretical physics in its importance. Numerical simulations are able to describe phenomena of increasing complexity, guiding experimental work, predicting new phenomena and providing invaluable insights. Of special significance in this context is the recent development of ab-initio molecular dynamics. This approach allows complex physical and chemical systems to be described with great accuracy and without adjustable parameters. Calculation of the dynamical and static properties of electrons and ions in condensed matter systems has become accessible. We will describe the principle of this methodology and illustrate its power with examples of great scientific and practical relevance. Present limits and future perspectives of ab-initio molecular dynamics will also be discussed.

PL-6

The Flexible Surface: Development and Frontiers of Molecular Surface Science

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The development of surface science techniques in physics permitted atomic level studies of structure, composition, and dynamics at surfaces of metals, oxides, halides, molecular crystals (ice), and polymers. The reconstruction of clean surfaces and adsorbate induced restructuring were discovered. The nature of the surface chemical bonds of adsorbed monolayers was elucidated along with the role of surface defects (vacancies, steps and kinks) in breaking chemical bonds. The atomic and molecular foundation of applications of chemical and mechanical surface properties to catalysis and tribology are being established, and this will be discussed through examples. Improvements in time and spatial resolution of the various surface probes are at the frontier of surface instrumentation developments. Studies of the buried interfaces, solid-liquid, solid-gas at high pressure, and solid-solid, represent the experimental frontiers.