CLUSTERS IN CONTACT WITH SUBSTRATES - THE EFFECT OF THE INTERFACE ON CLUSTER DYNAMICS

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The talk presents theoretical studies of coupled ionic and electronic dynamics of metal clusters in contact with an inert environment (insulator substrates as rare gases or MgO) and compares it with the behavior of free clusters. The theoretical tool for these investigations is time-dependent density-functional theory at the level of the local-density approximation. The scheme includes a self-interaction correction to describe properly electron emission. The treatment resolves the fully detailed electronic dynamics at femtosecond scale and proceeds up to several picoseconds to track the consequences on the slow ionic and atomic motion in these complex compounds.

Observable signatures from various dynamical scenarios are discussed. As a basic feature we consider optical response and its modification through the environment. In the non-linear regime, we will consider the dynamics of cluster deposition and excitation by short laser pulses. For embedded and deposited clusters, there emerges the particularly interesting question of energy and particle transport from the highly excited cluster (acting as chromophore) to the inert environment. The various transport processes and corresponding time scales will be analyzed. We will also address the remarkable difference in the dynamics of free clusters and clusters embedded in rare-gas matrix.