

A theoretical model for the selective subsurface absorption of atomic hydrogen in a Pd(111) surface by infrared (IR) laser pulses is presented. The dynamics of the adsorbate is studied within the reduced density matrix approach. Energy and phase relaxation of the hydrogen atom are treated using the semi-group formalism. The vibrational excitation leading to subsurface absorption is performed using rationally designed pulses as well as infrared laser pulses optimized on-the-fly. It is shown that dissipation can be used as a tool to transfer population to an otherwise unaccessible state via a mechanism known as "laser distillation". We demonstrate that, when the reaction path is generalized from a reduced one-dimensional to full three-dimensional treatment of the system, the laser control strategy can prove very different