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Theoretical dynamics of the S(1D)+H2 reaction in conditions approaching the cold regime.

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The title reaction, widely studied both experimentally and theoretically, has become a benchmark for insertion barrierless reactions [1]. Its dynamics is considered here for collision energies of a few tens of Kelvin. In this energy regime, major quantum effects arise. The aim of the talk is to show how they can be taken into account in the classical trajectory description of the dynamics without modifying the trajectories themselves, so as to keep with the simplicity of the classical trajectory method [2]. These quantum effects are: a) the quantization of reagent and product internal motions [2], b) an original effect called diffraction mediated trapping [2] and c) the quantization of the activated complex states [3]. The inclusion of quantum constraints in the analysis of classical trajectory outcomes is particularly important for polyatomic reactions since quantum scattering calculations are still beyond reach for most of them.

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