学术报告

初始态选定的量子波包方法及应用：分子反应动力学 & 光谱学

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Abstract ： The initial state specific wave packet method is briefly introduced and applied to study the dynamics of tetra-atomic and polyatomic reactions within full-dimensional and/or reduced dimensional models and mimic experimental photoelectron-photofragment coincidence spectra. Three examples are given to present interesting findings. 1) For the early barrier HCl + OH reaction, vibrational excitation of HCl promotes the reaction much more than translational energy, which is in sharp contrast to the naively extended Polanyi's rules to polyatomic reactions. On the other hand, fundamental and overtone excitations of HCl change the reaction mechanism from a direct barrier crossing process to a capture-like process. 2) For the H_2 + H_2O^+ reaction, rotational excitation of H_2O^+ greatly enhances the reaction at low collision energies and the enhancement effect decreases with the increase of collision energy. The enhancement effect results from the reorientation of H_2O^+ caused by the chemical force in the short range .These dynamical features agree well with experimental observations. 3) The experimental photoelectron-photofragment coincidence spectrum of NH_4^- is well mimicked and explained by theoretical calculations.

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