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氟原子与氢分子共线反应几率的量子散射计算

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摘要 基于最新的6SEC势能面,用邓从豪等提出的LCAC-SW方法计算得到了共线反应F+H~2(v=0)→HF(v')+H的态-态反应几率,计算结果准确地反映出势能面的特点,进一步证明LCAC-SW方法是一成功的量子散射方法。

关键词 氟 氢 量子反应散射 势能面 国家自然科学基金委员会基金

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A quantum scattering study of collinear reaction probabilities for the fluorine atom and hydrogen molecule system

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Abstract A new quantum scattering approach (linear combination of arrangement channels-scattering wavefunction, LCAC-SW) proposed by Deng and his co-workers is used to calculate collinear state-to-state reaction probabilities for the F+H~2(v=0)→HF(v')+H system on the 6SEC potential energy surface. The calculated results reflect the character of potential energy surface accurately (there is a "shallow hollow" along reaction coordinate on 6SEC potential energy surface). They are compared with other theoretical investigations reported in the literature. It is shown that the LCAC-SW approach is the successful one of quantum scattering methods.

Key words FLUORINE HYDROGEN POTENTIAL ENERGY SURFACES FOUNDATION OF NATIONAL SCIENCE FOUNDATION COMMITTEE

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