

Dynamics of chemical reactions in the gas phase

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In this talk I will discuss available options for theoretical investigations of the dynamics of chemical reactions in the gas phase. This will include a comparison between standard time-dependent wave-packet and time-independent scattering calculations and also Multi Configurational Time Dependent Hartree (MCTDH) calculations [1]. I will then exemplify this by specifically showing theoretical and experimental results for the reaction between a hydrogen atom and methane forming a hydrogen molecule and a methyl radical. The focus will be on the thermal reaction rate constant [2,3].

[1] Nyman, G., Yu, H-G. *Int. Rev. of Phys. Chem.*, 32:39-95, 2013.

[2] Yu, H-G., Nyman, G. *J. Chem. Phys.*, 111:3508-3516, 1999.

[3] Andersson, S., Nyman, G., Arnaldsson, A., Manthe, U., Jonsson, H. *J. Phys. Chem. A.*, 113:4468-4478, 2009.