Ingo Barth博士講演会

Max Planck Institute of Microstructure Physics, Halle, Germany

Quantum Hydrodynamics Approach for Calculations of Electronic Current Densities

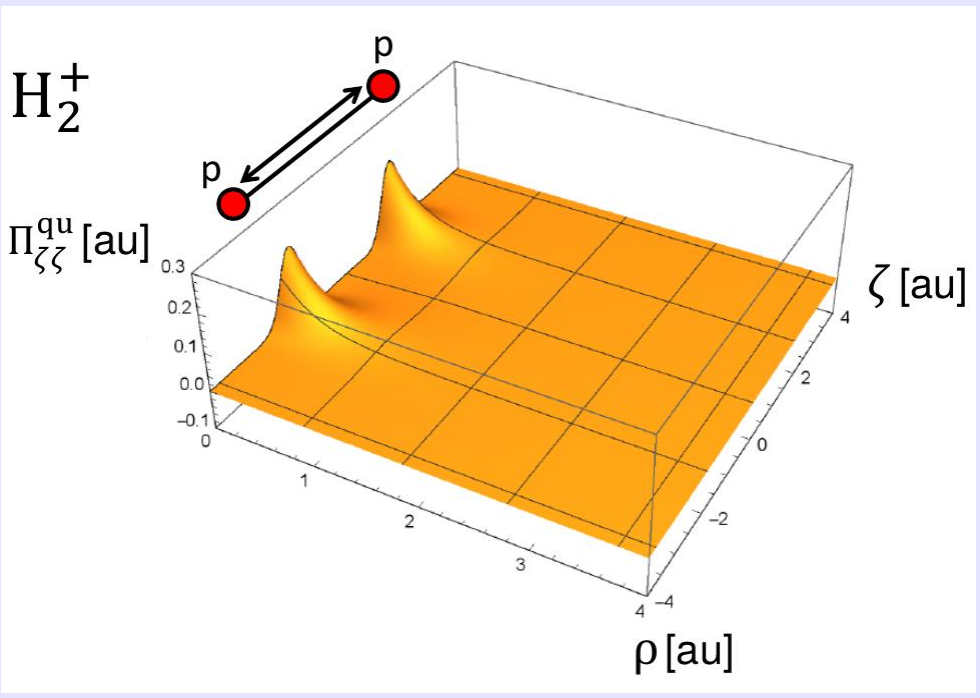
日時 : 2017年 3月13日(月)　15:30 ～17:00
場所 :化学専攻第4講義室(大学院講義棟H23)

Barth博士は量子動力学研究の第一人者で，分子の反応中の電子移動に関する新しい理論について話していただきます。

Very recently, we have developed the theory of many-particle quantum hydrodynamics for different quantum systems. In particular, we have derived, without any approximations, the many-particle Ehrenfest equation of motion directly from the time-dependent Schrödinger equation for many-particle systems consisting of several particle sorts [1]. First, I will show some simple examples for dynamics of Gaussian wave packets and compare the numerical results of current densities with exact ones. Then, I will show using this approach even within the Born-Oppenheimer approximation, how to obtain non-zero electronic current densities for vibrating molecules (for example H2+) or even chemical reactions in a single electronic non-degenerate ground state.

[1]K. Renziehausen, I. Barth, *Derivation of many-particle quantum hydrodynamics and discussion about different versions of the pressure tensor*, in preparation.

講演は独語手話から英語への翻訳で行われます。



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