Density functional theory and its applications to contemporary problems in physics

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Since its proposition in 1964 by Hohenberg and Kohn, density functional theory has seen a tremendous amount of development both in terms of its theoretical foundations and with recent advances in computational resources also in practical applications. The method, shifting the focus from a wavefunction-based description of the many-particle problem to the particle density, has provided a much more affordable treatment of numerous physical systems. A search in ISI Web of Knowledge reveals some 38000 publications on density functional theory between the years of 2005 and 2010.

Traditionally utilized heavily for atomistic problems such as those in quantum chemistry and solid state physics, other many-particle applications in physics have recently been tackled with density functional theory, uncovering new insight that has been absent in models previously developed.

In this talk, I will first give a brief description of the density functional theory, including its foundations and some practical concerns. I will then give several examples currently under investigation in our group. The range of applications I will present ranges from dipolar fermions in a harmonic two-dimensional trap to practical materials science problems such as zeolites.