# Adaptive Finite Element Approximations for Density Functional Models

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**Abstract**

Density functional models are powerful, widely used approaches for computation of ground state electronic energies and densities in chemistry, materials science, biology, and nanosciences. In this presentation, we will talk about adaptive finite element approximations of orbital-free and Kohn-Sham density functional models, including the construction and analysis of the residual type a posteriori error estimators as well as the convergence and complexity of the adaptive finite element approximations. We will demonstrate several typical numerical experiments that show the robustness and efficiency of the adaptive finite element computations in electronic structure calculations. This presentation is based on some joint works with H. Chen, X. Dai, X. Gong, and L. He.