Do density changes affect Kohn-Sham results?

Andreas Savin
Laboratoire de Chimie Théorique
CNRS and UPMC (Université Paris 6)
Paris, France

The Kohn-Sham model is a system of non-interacting fermions having the same density as a given system of interacting fermions. Density functional approximations are seen as to reliably simulate Kohn-Sham systems. However, the density of approximate Kohn-Sham systems is not exact, and the error made in the density seems to play a role. A careful analysis shows, however, that the way density functionals are constructed, namely by using models of the pair density for all one-particle densities, allows to circumvent this problem.