Some mathematical and numerical challenges in Density Functional Theory

In this talk, I will present some recent achievements in the mathematical and numerical analysis of Kohn-Sham models.

In the first part of the talk, I will show how to derive a model describing the electronic structure of a crystal with local defects (a system with infinitely many electrons) from a Kohn-Sham model for atoms and molecules, by means of rigorously founded bulk limit arguments [E.C., A. Delerence and M. Lewin, Comm. Math. Phys. 2008 and J. Phys.: Condens. Matter 2008]. The resulting model has a subtle mathematical structure. An interesting feature of it is that the definition of the charge of the defect is not straightforward, and requires mathematical techniques similar to the renormalization techniques used in quantum electrodynamics. This models also allows to recover the electronic component of the macroscopic dielectric permittivity in the RPA approximation (Adler-Wiser formula), using homogenization techniques [E.C. and M. Lewin, Arch. Ration. Mech. Anal. 2009].

In the second part of the talk, I will focus on the construction and use of error estimates for Kohn-Sham calculations in planewave basis sets. I will present optimal a priori error estimates [E.C., R. Chakir and Y. Maday, 2010] and comment on the possible use of these error bounds to lower the computational effort in Kohn-Sham calculations.