Iterative Solution of self-consistent-field equations – Modern Approaches

Introduction
Much of electronic structure theory today relies on the solution of the famous Kohn-Sham equations in the density functional theory framework. These equations constitute a set of non-linear partial differential equations and they must be solved using iterative methods. The final solution called is the self-consistent-field solution and it should exhibit consistent electron density and effective potential.

Standard procedures for finding the self-consistent-field solution is to use linear or Pulay mixer with a suitable preconditioner when needed. While this poses no problem for materials with large band gaps and tightly bound electrons other cases can prove problematic due to, e.g., charge sloshing. Recently more ambitious methods have been proposed but their implementation to real electronic structure theory codes is still missing. [1,2]

Project description
In this project the student will implement modern iterative methods and preconditioners to an existing electronic structure theory code, FHI-aims. [3] In addition, the implementation will be tested for efficiency and accuracy in cases where traditional approaches fail.

Requirements
Some experience in programming is required. FHI-aims is written in Fortran90/95 so that some familiarity with modern Fortran is a benefit.

Gains
After the project the student will be familiar with a modern electronic structure code as well as state-of-the-art methods in solving the self-consistent-field equations.

Contact
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