Compressed Sensing in Electronic Structure Calculations

Niklas Menzel

Fritz-Haber-Institut Berlin

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Abstract

Electronic structure theory models the many-electron systems which are used to describe and predict properties of molecules and matter. Starting point in many applications are Schroedinger-like equations $\hat{H}\Psi = \epsilon\Psi$, with the Hamiltonian $\hat{H}$ describing the many-body system. The accuracy of the approximated solutions depends highly on the underlying basis. One of the most-widely used basis-sets in molecular simulations are Gaussian-type basis sets. In this talk we will discuss methods for Gaussian basis set selection using ideas from compressed sensing.