

# Eigensolvers for Large Electronic Structure Calculations

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The solution of the single particle Schrödinger equation that arises in electronic structure calculations often requires solving for interior eigenstates of a large Hamiltonian. The states at the top of the valence band and at the bottom of the conduction band determine the band gap that relates to important physical characteristics such as optical or transport properties.

In order to avoid the explicit computation of all eigenstates, a folded spectrum method has been usually employed to compute only the eigenstates near the band gap. In this talk, we compare the conjugate gradient minimization, the optimal block preconditioned conjugate gradient, the implicit restarted Lanczos, and variants of the (Jacobi-)Davidson algorithms applied to the folded spectrum matrix for the computation of eigenstates of interest. We also show results when some of these algorithms are applied to the unfolded spectrum.

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