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New Eigensolvers for Large Scale Nanoscience Simulations

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We present results for state-of-the-art iterative eigensolvers based on conjugate gradients and variants of Davidson in the context of semi-empirical plane wave electronic structure calculations. These new methods give significant speedup over existing conjugate gradient methods used in electronic structure calculations. The new methods are demonstrated for CdSe quantum dots as well as quantum wires (single electron devices) constructed from layers of InP and InAs. These systems are studied in the context of a semi-empirical potential where we typically solve for a few states around the gap allowing us to study large scale nanosystems. The parallelization of this approach is discussed as well as scaling results to large processor counts.