An algorithm for electron transport based on planewaves

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We here present an algorithm for the first-principles plane-wave electron transport based on the multiple scattering theories. The pseudopotential method is applied to deal with the electron-ion interactions. Such an algorithm enables us to study the complex band or transport properties of materials under different boundary conditions. Results for a few test systems, e.g. bulk Silicon, Aluminum wire with a hydrogen adatom, are computed and illustrated.