Ab-initio scattering-state based method for calculating transport in nanostructures

IVAN P. DAYКОV, TOMÁS A. ARIAS, Department of Physics, Cornell University, Ithaca, NY, 14853 — We will present an ab-initio computational method for calculating the transport properties of nanostructures. In contrast to the commonly employed scattering-state approaches it directly utilizes supercells with periodic boundary conditions, which makes it ideal for use with planewave density functional codes.