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**Electronic transport properties of nano-scale Si films: an ab initio study**[1] JESSE MAASSEN, YOUQI KE, FERDOWS ZAHID, HONG GUO, McGill University — Using a recently developed first principles transport package, we study the electronic transport properties of Si films contacted to heavily doped n-type Si leads. The quantum transport analysis is carried out using density functional theory (DFT) combined with nonequilibrium Green's functions (NEGF). This particular combination of NEGF-DFT allows the investigation of Si films with thicknesses in the range of a few nanometers and lengths up to tens of nanometers. We calculate the conductance, the momentum resolved transmission, the potential profile and the screening length as a function of length, thickness, orientation and surface structure. Moreover, we compare the properties of Si films with and without a top surface passivation by hydrogen.

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