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First principles analysis of quantum transport in Bi2Se3 3D topological insulators YONGHONG ZHAO, YIBIN HU, LEI LIU, YU ZHU, HONG GUO — By carrying out density functional theory (DFT) within the Keldysh nonequilibrium Green's function formalism (NEGF), we have investigated quantum transport properties of the Bi2Se3 topological insulator from atomistic first principles without any phenomenological parameters. Using the scattering states, our results vividly reveal the surface Dirac fermions and helical edge spin states in the momentum space. We have also determined the real-space distribution of the helical edge spin states which provide the penetration depth of the surface topological conducting channels into the bulk Bi2Se3 crystal. Our first principles calculations take into account the full non-collinear spin structure and spin-orbit interaction, the details of these technical advances within the NEGF-DFT quantum transport formalism will also be briefly discussed.

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