First principles transport calculations on topological surface states scattering IVAN RUNGGER, AWADHESH NARAYAN, STEFANO SANVITO, Trinity College Dublin — We study the scattering properties of topologically protected states on the Sb(111) and Bi$_2$Se$_3$(111) surfaces by using the ab initio transport code SMEAGOL 1. We consider different types of defects, such as adatoms and extended barriers. In the presence of a strong surface perturbation in the form of a step separating surface terraces we obtain standing-wave states resulting from the superposition of spin-polarized surface states. By Fourier analysis, we identify the underlying two dimensional scattering processes and the spin texture 2. We find evidence of resonant transmission across the surface barrier at quantum well state energies and evaluate their lifetimes. Our results for the Sb surface are in agreement with experimental findings 3. We also show that despite the presence of a step edge along a different direction, the surface states exhibit unperturbed transmission around the Fermi energy for states with near to normal incidence 


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