Abstract Submitted
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**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 $Bi_2Se_3$(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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