Topologically protected transport in two-dimensional topological insulators from first principles

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Abstract: The outstanding transport properties expected in time-reversal invariant topological insulators whose helical edge states promise to be immune to backscattering even in the presence of impurities have proven to be challenging to realize experimentally, and have so far only been demonstrated in very short devices. In search for an explanation to this puzzling observation, we here report a full first-principles calculation of topologically protected transport at the edge of novel quantum spin Hall insulators specifically, Bismuth and Antimony halides based on the non-equilibrium Green's functions formalism. Our calculations unravel two different scattering mechanisms that may affect two-dimensional topological insulators, namely spontaneous time-reversal symmetry breaking at vacancy defects and inter-edge scattering mediated by multiple co-operating impurities, possibly non-magnetic. We discuss their drastic consequences for typical non-local transport measurements as well as strategies to mitigate their negative impact. Finally, we give more relevance to our observations by comparing the transport properties of topologically protected edge states to those of the trivial edge states in MoS2 ribbons. Our results provide insights about the limitations of topological protection and shed light on previously underestimated mechanisms that may be at the basis of anomalous experimental results.