Generating topological insulator gap in graphene with heavy adatoms

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Graphene was the first material predicted to realize a topological insulator (TI) in seminal work by Kane and Mele, though unfortunately the gap is unobservably small due to carbon's exceedingly weak spin-orbit coupling. It is hence important to search appropriate adatoms and/or substrates to expand the spin-orbit coupling gap through hybridization. We found that heavy In or Tl adatoms may dramatically enhance the gap to 7 or 20 meV. These gaps are large enough for the realization of quantum spin Hall effect in graphene in most experimental conditions.

We also have a new proposal for generating a two-dimensional spin-orbit coupling gap with impurity bands arising from heavy adatoms that are mediated through graphene. First principles calculations predict that spin-orbit coupling induced gaps as large as 200 meV can be generated by placing Re, Os and Ir adatoms on graphene over a broad range of coverage. Furthermore, tuning the Fermi level is not required to enter the TI state. The mechanism at work is expected to be rather general and may open the door to designing new two-dimensional TI phases in many materials.