Anomalous transport and spin filtering effect in graphene nanojunctions

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Electronic transport properties of zigzag graphene nanoribbons with defects are explored by using nonequilibrium Green's functions method in combination with density functional theory. The defects are found to generally decrease the conductance of graphene nanoribbons and the conductance decreases further with the increase of the defect size. Anomalous transport, however, appears when the defects break the symmetry of the nanoribbons: the current of the ribbons with this kind of defects can be much larger than that of the perfect graphene ribbons. This behavior is ascribed to more conducting channels along the edges, provided in asymmetrical graphene ribbons. Perfect spin filtering effect is achieved in zigzag-edged graphene flakes sandwiched between two gold electrodes. The orientation of the spin current is found to be flipped if the flake is doped with N, O, or F atoms. The results indicate that the transport properties of graphene can be tuned flexibly and are potentially useful in future nanoelectronic applications.