Calculating impurity-limited carrier mobility of 2D materials

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Realistic nanoelectronic devices inevitably have some disorder which affect device operation. Unintentional impurities locate at unpredictable positions in the material and predicted physical property should be averaged over the impurity configurations. One may generate many impurity configurations, calculate each of them and average over the results. Unfortunately such a brute force approach is too costly to be practical for first principles simulations. To solve this problem, we have developed a theory of nonequilibrium coherent potential approximation (NECPA) that is integrated with the density functional theory (DFT) and Keldysh nonequilibrium Green's function (NEGF), in which the disorder configuration average is carried out analytically thereby only a single first principles NEGF-DFT computation is necessary to obtain the disorder averaged transport properties. Using NECPA, we have calculated disorder limited carrier mobility of 2D materials including graphene and monolayer black phosphorus.