We present an ab initio multiscale study of electronic and transport properties of two-dimensional graphene after epoxide functionalization via ozone treatment[1,2]. The orbital rehybridization induced by the epoxide groups triggers a strong intervalley scattering and changes dramatically the conduction properties of graphene. A DFT-parametrized tight-binding model within the Kubo formalism[3] allows us to simulate mesoscopic-sized systems up to 2 million atoms. By varying the random coverage density of epoxide defects from 0.1 to 4%, charge conduction can be tuned from a diffusive to a strongly localized regime, with localization lengths down to a few nanometers long. Experimental results[4] supporting the interpretation as a metal-insulator transition are also provided.

References


Figures