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Electronic Transport in Graphene on hBN with impurities: DFT-NEGF Study[1] TOMOAKI KANEKO, TAKAHISA OHNO, National Institute for Materials Science, MATERIALS RESEARCH CONSORTIUM FOR EFFICIENT ELECTRONIC DEVICES TEAM, UNIVERSITY OF TOKYO TEAM — Graphene on hBN substrate shows much higher mobility compared with graphene on SiO_2 substrate. However, such good performance can be seen only for high quality hBN substrate. To understand such property, we performed the transport calculation of graphene adsorbed on hBN with impurities based on the density functional theories (DFT) and nonequilibrium Green's function method (NEGF). In this study, we consider the graphene adsorbed on monolayer hBN and we introduced carbon and oxygen impurities in hBN by replacing the B or N atoms. We employed PHASE code for the structure optimization and ASCOT code for transport calculation. We found that doping from hBN and impurity levels reduce the conductance. For the scattering by impurity levels, the stacking structure of graphene and hBN plays importance role.

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