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A first principles study on CVD graphene growth on copper surfaces: C-C bonding reactions at graphene edges NOBUO TAJIMA, TOMOAKI KANEKO, JUN NARA, National Institute for Materials Science, Materials Research Consortium for Energy Efficient Electronic Devices (MARCEED), OHNO TAKAHISA, National Institute for Materials Science, Materials Research Consortium for Energy Efficient Electronic Devices (MARCEED),University of Tokyo —
Graphene has attracted considerable research interest owing to its potential application to future electronic devices. Large area and high quality graphene is needed for device applications. Chemical vapor deposition (CVD) using a copper surface with a hydrocarbon source is one of the practical methods to produce graphene. This method is appropriate for creating large area graphene with low cost, and the graphene growth control to obtain a high quality product is a remaining challenge. The carbon atom nucleation and cluster growth processes in the CVD reactions have been studied extensively as key steps that affect the graphene growth behavior. We have been studying the carbon atom reactions in these processes by theoretical approaches In the present study, we have focused on the later stage of CVD reaction, that is, carbon atom reactions at graphene edges by which carbon clusters grow in the Cu-CVD We have found that these reactions have energy barriers of $\sim$1 eV. First principles simulation code PHASE http://www.ciss.iis.u-tokyo.ac.jp/riss/english/project/device/) was used in the theoretical calculations.

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