Abstract Submitted
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Carbon atom bonding processes in CVD graphene growth on copper surface: A first principles study[1] TAKAHISA OHNO, National Institute for Materials Science, University of Tokyo, NOBUO TAJIMA, TOMOAKI KANEKO, JUN NARA, National Institute for Materials Science — Graphene has attracted considerable research interest due to potential application to future electronic devices. Large area and high-quality graphene is needed for device applications. Chemical vapor deposition using copper surface with hydrocarbon source is one of the practical methods to produce graphene. This method is appropriate for creating large area graphene, and the graphene growth control to obtain high quality product is a challenge. The carbon atom nucleation and cluster growth processes in the CVD reactions have been studied extensively as key steps to control graphene growth. In the present study, first principles molecular dynamics calculations are performed to obtain fundamental insight into these C-C bonding process. First principles simulation code PAHSE (http://www.ciss.iis.u-tokyo.ac.jp/english/project/device/) was used in these calculations.

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