Abstract Submitted
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**Role of catalytic metals on formation process of carbon nanotube and graphene: ab initio molecular dynamics study** YASUSHI SHIBUTA, The University of Tokyo, KOHEI SHIMAMURA, Kumamoto University, TOMOYA OGURI, The University of Tokyo, RIZAL ARIFIN, WATARU HASHIZUME, FUYUKI SHIMOJO, Kumamoto University, SHU YAMAGUCHI, The University of Tokyo — The growth mechanism of carbon nanotubes and graphene has been widely discussed from both the experimental and computational points of view. At the present, most of numerical studies focuses on the aggregation of isolate carbon atoms on the catalytic metal surface, whereas the initial dissociation of carbon source molecules should affect the yield and quality of the products [1]. Under such circumstance, we have investigated the dissociation of carbon source molecules on the metal surface using the ab initio molecular dynamics simulation in order to discuss the initial stage of graphene growth via a chemical vapor deposition (CVD) technique [2,3]. In the presentation, we performed the ab initio MD simulations of the dissociation process of methane on Ni(111) surface to discuss initial dissociation process of the graphene formation, and the dissociation process of ethanol on Ni32 cluster to discuss that for the carbon nanotube formation. [1] Y. Shibuta, Diamond and Related Materials, 20 (2011) 334-338. [2] Y. Shibuta, R. Arfin, K. Shimamura, T. Oguri, F. Shimojo, S. Yamaguchi , Chem. Phys. Lett. 565 (2013) 92. [3] T. Oguri, K. Shimamura, Y. Shibuta*, F. Shimojo, S. Yamaguchi, J. Phys. Chem. C 117 (2013) 9983.

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