

Abstract Submitted  
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**Graphene Growth on Cu Surface: A Theoretical Study**<sup>1</sup> ZHENYU LI, PING WU, WENHUA ZHANG, JINLONG YANG, J. G. HOU, University of Science and Technology of China, THE ELECTRONIC STRUCTURE TEAM AT USTC TEAM — Graphene is an important material with many unique properties and a great application potential. A promising way to produce wafer-size graphene is chemical vapor deposition (CVD) on metal surfaces. To improve sample quality, it is important to understand the atomic details during graphene CVD growth. In this talk, some relevant elementary processes on Cu surface have been studied from first principles. Although diffusion of atomic carbon on Cu (111) surface is almost barrierless, coalescence of carbon atoms on the surface is found to be hampered by an intermediate bridging-metal structure. The fact which makes things more complicated is that thermodynamic analysis indicates that the main species on the Cu surface during graphene growth is not the simplest atomic carbon. Therefore, C<sub>x</sub>H<sub>y</sub> species should be explicitly considered for initial stage growth of graphene on Cu surface.

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