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Contrast Behavior of Carbon Adatom Diffusion and Nucleation in the Initial Stage of Graphene Epitaxial Growth on Stepped Metal Surfaces[1] HUA CHEN, WENGUANG ZHU, U of Tennessee-Knoxville, Oak Ridge National Laboratory, ZHENYU ZHANG, Oak Ridge National Laboratory, U of Tennessee-Knoxville — Using first-principles calculations within density functional theory, we study the energetics and kinetics of carbon adatom diffusion and nucleation on three stepped metal surfaces: Ir(111), Ru(0001) and Cu(111). We find that on the flat surfaces, two carbon atoms repel each other on Ir(111) and Ru(0001), while they prefer to form a dimer on Cu(111). Moreover, the step edges on Ir and Ru surfaces cannot effectively trap single carbon adatoms either, whereas it is strongly favorable to form carbon dimers at the step edges. The different behaviors are attributed to the competition between C-C bonding and different types of C-metal bonding, and the picture is generalized to other C/metal systems with predicted results. These findings provide an insight into the understanding of experimentally observed carbon nucleation in the initial stage of graphene epitaxial growth on metal surfaces.

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