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**Stable Carbon Nanoarches in the Nucleation of Graphene on Cu(111)**[1] ROBERT VAN WESEP, HUA CHEN, WENGUANG ZHU, Phys Dept, U of Tennessee; Materials Science & Engineering Division, ORNL, ZHENYU ZHANG, Phys Dept, U of Tennessee; Materials Science & Engineering Division, ORNL; ICQD, USTC — To fully exploit the device potential of graphene, reliable production of large-area, high-quality samples is required. Epitaxial growth on transition metal surfaces have shown promise in this regard, but further improvement would be facilitated by a more complete understanding of the nanoscale processes involved. Using density functional theory calculations, we have investigated the energetics and kinetics of graphene nucleation and growth on a Cu(111) surface. Our calculations have revealed an energetic preference for the formation of stable 1D carbon nanoarches consisting of 3-13 atoms when compared to 2D compact islands. Our findings may provide the structural link between nucleated carbon dimers [1] and larger carbon nanodomes [2], and may also explain some recent experimental observations. We will also present results on estimating the critical cluster size that marks the transition from nanoarch dominance to island dominance in the growth sequence.

[1] Hua Chen, et al., Phys. Rev. Lett. 104, 186101 (2010).
[2] Paolo Lacovig, et al., Phys. Rev. Lett. 103, 166101 (2009).

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Robert Van Wesep
Phys Dept, U of Tennessee;
Materials Science & Engineering Division, ORNL

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