Abstract Submitted
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Breaking of symmetry in graphene growth on metal surfaces VASILII I. ARTYUKHOV, Rice University, Houston, TX, YUFENG HAO[1], RODNEY S. RUOFF[2], University of Texas at Austin, Austin, TX, BORIS I. YAKOBSON, Rice University, Houston, TX — Understanding and controlling the factors that define the morphology of graphene crystals is crucial for improving CVD-produced graphene quality. First-principles atomistic calculations linked to crystal growth theory have successfully explained[3] the striking polygonal (hexagons, dodecagons) graphene island shapes. However, more recently, islands with broken symmetry that is lower than the intrinsic symmetries of both graphene and the substrate were observed in our experiments as well as by other groups. Here we examine the effect of metal surface symmetry on graphene crystal shapes via first-principles calculations and Monte Carlo modeling, focusing primarily on Ni and Cu substrates. For equilibrium shape, edge energy variations δE manifest in distorted hexagons with different ground-state edge structures. In growth or nucleation, energy variation enters exponentially as $\sim e^{\delta E/k}\mathrm{B}^T$, strongly amplifying the symmetry breaking, up to completely changing the shapes to triangular, ribbon-like, or rhombic.[4]

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[3]V. I. Artyukhov, Y. Liu, and B. I. Yakobson, *Proc. Natl. Acad. Sci. U.S.A.* 109, 15136 (2012).
[4]V. I. Artyukhov, Y. Hao, R. S. Ruoff, and B. I. Yakobson, *arXiv*:1405.5799 (2014)

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