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Understanding the Growth of Carbon Nanotubes by Catalyst-Assisted Chemical Vapor Deposition ELIF ERTEKIN, UC Berkeley, JEFFREY GROSSMAN, COMPUTATIONAL NANOSCIENCE GROUP TEAM — In catalyst-assisted chemical vapor deposition, carbon nanotubes are formed when a curved graphene island lifts off the surface of the catalyst particle on which it is growing. While this growth technique offers effective control over patterning and alignment, control over nanotube radius and chirality is ultimately tied to understanding the point at which lift-off occurs. We use atomistic approaches to model the lift-off process via the interplay between the excess energy required to grow a curved (and thus, necessarily defected) graphene island and the interaction energy between the growing island and the underlying catalyst. The atomistic approach combines Monte Carlo methods with *ab initio* total energy electronic structure methods to explore island formation, growth, and lift-off on a catalyst surface. Using this approach, we are able to systematically study the effect of incident atomic flux rate, growth temperature, and catalyst curvature. The different defect topologies in the growing graphene cap that result from different growth conditions are a key parameter in determining the chirality of the nanotubes.

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