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First Principles Study of Carbyne Structural Stability[1] KEVIN KWON[2], COLIN HOLMES[3], KI CHUL KIM[4], SEUNG SOON JANG[5], Georgia Institute of Technology — Carbyne is composed of linear sp-hybridized carbon bonds and yields promising results to surpass graphene's mechanical and electrical properties. Carbyne has two semi-stable conformations: Polyyne (alternating triple and single bonds) and Polycumulene (repeating double bonds). This study investigated the stability of these forms at infinite chain lengths by using periodic boundary conditions. Geometric optimization was performed via DFT calculations using DMoL3 and PBE GGA functional group. Each configuration's chain was stretched or compressed until the most stable form – lowest energy - was obtained. After comparing the energies, the most stable form alternated between Polyyne and Polycumulene as the number of carbon atoms within each boundary increased. Polyyne was the most stable form for odd number of carbons and Polycumulene was the most stable for even number of carbons. Finally, K-point sampling was increased in the direction of the chain axis to obtain a more accurate depiction of structural stability. As the number of k-points increased, the Polycumulene structure became more stable compared to Polyyne.

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