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Stability of Carbyne: First Principles Approach KEVIN KWON, COLIN HOLMES, SEUNG SOON JANG, School of Materials Science and Engineering, Georgia Institute of Technology 771 Ferst Drive, Atlanta, GA 30332-0245 — Over the last decade, carbon based nanomaterials have gained attention due to the discovery of graphene and its extraordinary properties. This has inspired new research into other carbon allotropes to obtain their unique properties. Carbyne is one such allotrope composed of linear sp-hybridized carbon bonds that has promising results and characteristics to surpass graphene's mechanical strength and possess novel electrical properties. It has two semi-stable conformations: Polyyne (alternating triple and single bonds) and Polycumulene (repeating double bonds). We investigated the stability of these forms with infinite chain lengths by employing periodic boundary conditions. Geometric optimization was performed using DMoL3 with GGA PBE. After comparing the energies, the most stable form alternated between Polyyne and Polycumulene as the number of carbon atoms within each boundary increased; furthermore, every odd carbon atoms showed Polyyne as the most stable form, while every even number of carbon atoms showed Polycumulene as the most stable form. Considering k-point sampling resulted in the Polycumulene structure being the most stable as the number of k-points increased.

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