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Mechanical Tuning of Molecular Carbon Chains

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Polymers and macromolecules typically act as weak flexible chains in compression, buckling and coiling like strands of spaghetti. One of the newest carbon allotropes being investigated is the bare minimum possible molecular structure – a one-dimensional chain of carbon atoms know as carbyne, consisting of repeating *sp*-hybridized groups. Clearly, this molecular "rod" or "wire" had potential as a structural or transport element, and its mechanical behavior is of critical importance. While exhibiting exemplary mechanical properties in tension (a 1D modulus on the order of 313 nN and a strength on the order of 11 nN), its use as a structural component at the molecular scale is limited due to its relative weakness in compression and the immediate onset of buckling under load.

To circumvent this effect, here, we probe the effect of confinement to enhance the mechanical behavior of carbyne chains in compression. The confinement can be thought of as a virtual carbon nanotube, where carbyne chains have been observed. This is similar to bracing a column to prevent buckling at the macroscale. Through full atomistic molecular dynamics (MD), implementing the quantum-based ReaxFF potential and LAMMPS software, we characterize the mechanical properties of a free (unconfined chain) and explore the effect of confinement radius (R), free chain length (L) and temperature (T) on the effective compressive stiffness of the chains. We further define the upper and lower bounds via axial compression and entropic stiffness theories. We demonstrate that the stiffness can be tuned over an order of magnitude by geometric control. Confinement may inherently stabilize the chains, potentially providing a platform for the synthesis of extraordinarily long chains (tens of nanometers) with variable compressive response. Such control and understanding of mechanical response is of critical importance if carbnyne is to be introduced in nanoscale devices and applications.

Keywords: carbon; carbyne; molecular dynamics; confinement; stiffness

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