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The Origin of Negative Thermal Expansion in sp-sp^2 Hybridized Carbon Systems: Rigid Unit Modes CHEOL-WOON KIM, SEOUNG-HUN KANG, YOUNG-KYUN KWON, Kyung Hee University — Based on first-principles density functional theory, we investigate the thermal expansion behaviors of three kinds (α, β, and γ) of graphyne, which is two-dimensional carbon allotrope composed of sp- and sp^2-hybridized bonds. Using quasi-harmonic approximation, their Gibbs free energies are calculated as a function of 2D area and temperature to evaluate their temperature-dependent area variations. We find that all three kinds of graphyne exhibit negative thermal expansion behaviors up to quite high temperature as similarly seen in graphene. Their thermal contraction can be explained partially by the ripple effect as observed in graphene, which seems, however, somewhat insufficient for their much larger thermal contraction than that of graphene. Their anomalously huge thermal contraction behaviors are attributed mainly to unusual phonon modes with a frequency of a few hundreds of cm^{-1}, which do not exist in graphene. These modes are identified to "rigid unit modes (RUMs)", the librational modes of "rigid units" composed only of sp^2-bonds. RUMs are unusual in 2D materials, but known to be resposible for the negative thermal expasion in various metal oxides composed of rigid polyhedra, such as MO_6, where M is a metal cation.

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