Polyyne Chains and Derivatives: A Pathway to Superior Thermoelectric Performance

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Thermoelectricity has garnered significant attention in addressing growing environmental challenges and the demand for efficient energy conversion from dissipated heat. The trend toward device miniaturization highlights the need for smaller material systems with minimal energy dissipation while maintaining high efficiency in converting thermal energy to electrical energy. This study presents a low-dimensional, carbon-based material system comprising one-dimensional (1D) polyyne chains and their derivatives (two, three, and four chains) tailored for thermoelectric applications. The investigation includes a detailed analysis of doping and strain effects on the thermoelectric figure of merit (ZT) across various temperatures. Comprehensive thermodynamic and structural stability analyses—encompassing formation energy evaluations, phonon dispersion studies, and *ab-initio* molecular dynamics simulations—confirm the robustness of these materials. The results reveal exceptional structural stability even under prolonged high-temperature conditions, underscoring their suitability for practical applications. Peak ZT values, ranging from 1.5 to 3.1, were computed for different derivative systems under varied doping scenarios and temperature conditions. Additionally, the cumulative lattice thermal conductivity as a function of phonon frequency and mean free path was calculated, alongside critical phonon properties such as heat capacity, phonon lifetime, and group velocity at different temperatures. These findings establish the potential of polyyne chain systems to significantly enhance thermoelectric efficiency and drive advancements in energy harvesting technologies.