The research and development of functional polymer materials encounter huge chemical complexity and multi-scale characteristics making it critical to construct the mapping between chemical formula, chain morphology, processing technology, and physical properties. The applicant plans to build high-throughput molecular dynamics software by integrating tools of quantum, all-atom, coarse-grained, and microscopic resolutions. The software will simulate multi-dimensional dynamics from conformational changes to a continuous migration, exploring mechanisms such as thermal transport in chains of different entanglements, mechanical response on shearing, and the chain dissolving in blends. It will also predict macroscopic properties such as thermal conductivity, viscosity, solubility, and dielectric constant. Combined with databases and machine learning, the software will provide a new blueprint for the design of functional polymers. When universities lead the software development and hold the intellectual property rights, technologies will evolve with reliability, accuracy, continuity, and versatility by removing the information barrier and retaining transparency. Our software will act as a fundamental tool for energy materials, multi-scale transport mechanisms, energy storage and conversion, and other fields of major national needs. The progress and completion of the project are guaranteed by the applicant's 10,000-line demo code, more than 20 closely related journal publications, and six years of work experience in software development.