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Predicting the Glass Transition Temperature of Amorphous Polymers via Integration of Cheminformatics and Molecular Dynamics Simulations

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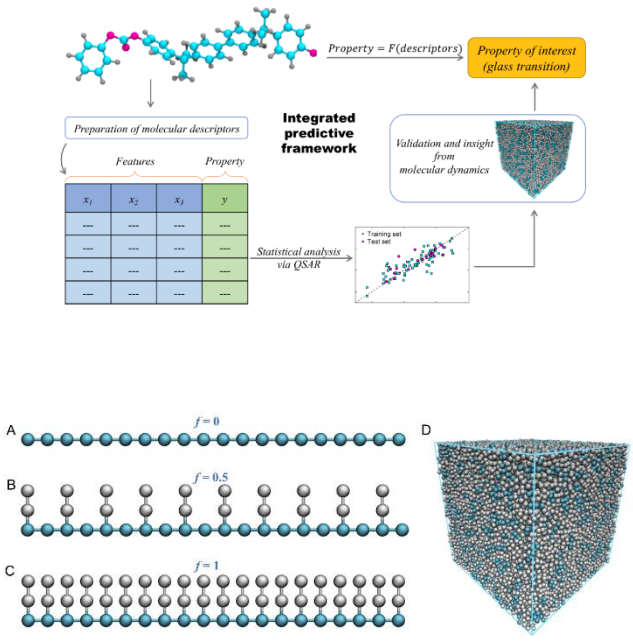
Graphical Abstract



Glass transition temperature T_g is one of the most important thermophysical properties of amorphous polymers. The substantial change in polymer dynamics at glass-transition temperature causes a major change in physical properties, including mechanical modulus, density, specific heat, damping characteristics, dielectric properties of the polymer[1-5]. The cheminformatics approach based on machine learning algorithms is often applied to predict the quantitative relationships between key molecular descriptors and the glass transition temperature T_g of investigated polymers. In this work, we discussing an innovative modeling framework by integrating cheminformatics and coarse-grained molecular dynamics simulations to predict T_g of diverse set of more than hundred polymers[6-10]. This synergistic approach provides valuable insights into the roles of key molecular features (i.e., cohesive interactions, chain stiffness, and topology) influencing the of polymers, paving the way to establish a materials-by-design framework for polymeric materials [11-12]. By harnessing the power of this unprecedented computational efficiency provided by this novel framework, we can successfully predict properties of not only the

	polymeric materials, but also other classes of organic and inorganic materials

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