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Evaluation of glass transition temperatures based on machine learning of computer simulations: Polymers as the pilot case

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Glass-formers represent an important family of natural and manufactured materials ubiquitous in nature, technology, and our daily lives. Approaching their glass transition temperatures (T_g) makes them resemble solids lacking long-range structural order, similar to liquids. Careful detection of the glass transition and accurate measurement of the T_g-value constitute fundamental steps in both fully resolving the enigma of this phenomenon and making application-oriented choices and advancements for glass-formers. Given the complexities of experimental synthesis and characterization, modern computer simulation methods based on the application of chemically realistic models can play a pivotal role in tackling the glass transition. Based on our previous studies of polymeric systems [1,2], here we will cover common approaches to evaluating the T_g-value from simulations and discuss their pros and cons. We will then introduce promising machine learning (ML) methods that may permit exploration of molecular patterns of the glass transition, fully utilizing available microscopic details within complex high-dimensional datasets from simulations. Finally, we will overview our progress in the development of a novel framework that fuses atomistic computer simulations and several ML methods for computing T_g and studying the glass transition in a unified way from various molecular descriptors for glass-formers.

[1] A.D. Glova, S.G. Falkovich, D.I. Dmitrienko, A.V. Lyulin, S.V. Larin, V.M. Nazarychev, M. Karttunen, S.V. Lyulin, Scale-dependent miscibility of polylactide and polyhydroxybutyrate: molecular dynamics simulations, Macromolecules, 51, 552 (2018)
[2] A.D. Glova, S.V. Larin, V.M. Nazarychev, M. Karttunen, S.V. Lyulin, Grafted dipolar chains: Dipoles and restricted freedom lead to unexpected hairpins, Macromolecules, 53, 29 (2020)

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Keyword-2

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Keyword-3

machine learning

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