High-throughput In-silico Synthesis, Characterization, and Design of Organic Polymer Materials

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Polymer design is a vital part of a wide range of applications including identifying suitable sustainable and recyclable plastics, improving polymer-biopolymer interfaces for biomedical engineering and therapeutics, and designing self-healing materials with dynamic covalent networks. The vast polymer design space over all chemical domains far exceeds the practical amount of experimental capital and research effort available and would greatly benefit from computational structure-function models for systematic exploration. Molecular dynamics (MD) approaches are some of the most attractive of such models due to their speed and interpretability and are becoming sufficiently rapid to evaluate polymer properties on a large scale. However, current open-source MD tools lacks automated, high-throughput, and general infrastructure for constructing and representing polymer systems (so-called "*in-silico* synthesis") which is instrumental in generating structural datasets for bulk physical property evaluation and validation. Here we expand our existing work in polymer modeling to enable high-accuracy polymer design across diverse chemistries and applications using these approaches. The tools we have implemented to these ends have been incorporated into the Open Force Field MD toolkit (https://github.com/openforcefield/openff-toolkit), as well as a purpose-built Python library for general polymer structure generation (https://github.com/timbernat/polymerist), and are described in greater detail in our recent preprint (https://doi.org/10.26434/chemrxiv-2023-f2zxd-v2).