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Data-Driven Design of Liquid-Crystalline Polyimides by Interplay with Expert Knowledge

Stephen Wu
The Institute of Statistical Mathematics, Tokyo, Japan

Abstract

Light responsive polyimides with liquid crystal (LC) alignment capability are often used in display devices. Meanwhile, a typical polyimide exhibits a low thermal conductivity, which is not suitable for applications in heat-prone flexible electronics. Recent research has reported successful fabrication of high intrinsic thermal conductivity LC polyimide films that the in-plane thermal conductivity exceeds 2 W/(mK). In this study, we exploited expert knowledge and the rapidly increasing amount of polymer data driven by the new interdisciplinary research field, called polymer informatics, to accelerate the discovery of LC polyimide with desired thermal properties. We began with a newly designed template for building the backbone of polyimides based on experience from polymer scientists. Purchasable molecules from the ZINC database that match the components in our template were exhaustively searched and extracted to construct a large virtual library of polyimides. Then, a machine learning model for LC classification was trained with data from PoLyInfo, the largest polymer property database, and used to screen out promising candidates of LC polyimide. Thermal conductivity of the screened candidates was predicted by another machine learning model trained with data from molecular dynamics simulations. Finally, guided by the predicted thermal properties of the candidates, we aimed to demonstrate the effectiveness of our design approach by synthesizing new LC polyimides from our selected candidates.

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Polymer Informatics.