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Machine learning in polymer informatics

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Abstract

Abstract Polymers have been widely used in energy storage, construction, medicine, aerospace, and so on. However, the complexity of chemical composition and morphology of polymers has brought challenges to their development. Thanks to the integration of machine learning algorithms and large data resources, the datadriven methods have opened up a new road for the development of polymer science and engineering. The emerging polymer informatics attempts to accelerate the performance prediction and process optimization of new polymers by using machine learning models based on reliable data. With the gradual supplement of currently available databases, the emergence of new databases and the continuous improvement of machine learning algorithms, the research paradigm of polymer informatics will be more efficient and widely used. Based on these points, this paper reviews the development trends of machine learning assisted polymer informatics and provides a simple introduction for researchers in materials, artificial intelligence, and other fields. image

Keywords: polymer informatics, machine learning, polymer property prediction, polymer databases, data-driven m

Full text

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