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Accelerating materials discovery through the development of polymer databases

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Efficient materials discovery can be greatly aided by access to databases that tabulate material property measurements and that allow for the exploration of material-property relationships. Such databases are less prevalent for polymers than other materials such as metals, in part due to the variety of structures associated with a single polymer identifier. For example, polyethylene could be branched or linear; it could also have a narrow or broad molecular weight distribution. I will discuss initial efforts towards generating a polymer property database in collaboration with Prof. Juan de Pablo and colleagues at the University of Chicago. Specifically, we focused on tabulating the Flory-Huggins chi parameter, describing the miscibility of polymer blends, using a course-based approach coupled with specialty software. In the context of a class setting, the undergraduate students learned about the field of polymer physics and used the software to identify chi parameters and related quantities, such as the method of measurement, from previously identified articles from literature. Both successes and challenges of this approach are measured through metrics of the resulting database and feedback from the students.