

Abstract IOM

Dr. Sarah Glaß, Institut für Membranforschung



How Machine Learning Can Support the Design Process of Membranes

Surface properties are crucial for the performance of membranes for water purification. They can cause the formation of fouling, wanted or unwanted adsorption and improve the separation performance. Therefore, designing membranes with specific surface properties for particular applications is very promising. However, predictive structure-preparation-property relations between the preparation strategies of the membranes and their performance are often very complex and, therefore, barely known. One possibility to tackle this issue is the application of data-driven methods such as machine learning to predict new materials. These machine learning models can generalize from the information in a data set and recognize patterns, allowing them to prognosticate to new (similar) data.

To do this, machine learning methods typically use large data sets. In chemistry and materials science, however, data sets are often limited to a few dozen or a few hundred. Nevertheless, machine learning has also shown excellent predictive ability in this field. Methods, which can be used for those small data sets, as well as their limitations, will be discussed in this study.