Recommender Systems in Materials Science: Methods and Applications

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A recommender system based on experimental databases aids in the efficient discovery of inorganic compounds. This presentation reviews studies on discovering unknown compounds using such systems. Two primary methods are highlighted: one using compositional descriptors derived from elemental features for machine learning and binary classification of chemical compositions registered in the inorganic crystal structure database (ICSD), and the other employing tensor decomposition techniques without descriptors. Predictive performance for unknown chemically relevant compositions (CRCs) was assessed by checking their presence in other databases.

Additionally, a synthesis-condition recommender system was developed using machine learning on a parallel experimental dataset collected through a polymerized complex method. This system's recommendation scores for unexperimented conditions were evaluated, leading to the discovery of two new pseudo-binary oxides.

Recommender systems are increasingly popular in fields like e-commerce and social networking, where they suggest products and content based on user data. This methodology is also applicable to materials discovery, where recommendation scores indicate the likelihood of finding relevant chemical compositions and synthesis conditions. The reviewed studies highlight the advantages of both tensor-based and descriptor-based approaches. Tensor-based methods are preferred when data is uniformly distributed, while descriptor-based approaches help avoid cold-start problems when few known CRCs are available.

For synthesis-condition recommender systems, data acquisition speed is critical. Combining these systems with high-speed, automated synthesis robots can iteratively improve recommendation quality. Although still in its infancy, the application of recommender systems to various problems in materials science and technology holds significant potential.