Doctoral dissertation

An evidence-based framework to reveal uncertainties for decision support in materials discovery

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Abstract

Searching for new materials is challenging and multifaceted, with countless potential candidates to explore. While data-driven approaches have shown promise in narrowing down the search space, their effectiveness is limited by certain factors. This doctoral thesis addresses these limitations and proposes a data-driven frame- work for quantitatively measuring the similarities between materials while accounting for uncertainty. The framework focuses on two scenarios: binary properties and continuous properties. For binary properties, the material similarity is assessed by evaluating the differences in compositions and their impact on the property of interest. For continuous properties, the similarity is determined by examining the correlation between occurrences of specific physical properties in the materials. The goal is to identify materials that exhibit similar behavior and characteristics, despite variations in composition. This framework provides a basis for informed decision- making in materials discovery and offers insights into the underlying mechanisms governing material behavior. This research contributes to more reliable and robust material discovery processes by incorporating uncertainty in similarity measurements. The proposed framework offers a valuable tool for materials science re- searchers, aiding in identifying and understanding materials with desirable proper- ties and paving the way for advancements in materials discovery and development.

Keywords: Materials discovery, Decision-making, Data-driven approach, Simi- larity measurement, Dempster-Shafer theory