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Towards Continuum Modeling from Atomistic Principles

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Summary

Molecular modeling can provide a detailed understanding of structures, properties, and processes for materials as diverse as organic molecules, polymer blends, or alloys. Yet, these methods have generally been restricted to length scales of {}{}100 nm and time scales of {}{}10-6 seconds, which limits their usefulness for research problems on the engineering scale. In this work, we discuss several approaches for extending their domain of applicability to the macro-scale.

Enhancements to atomistic modeling methods make it possible to apply accurate atomistic models to problems in electronics materials, alloys, and polymers. Statistical methods such as Quantitative Structure-Activity Relationships (QSAR) extend this even further by uncovering relationships between molecular and macroscopic quantities. Predictive analytics can create totally empirical models that predict material properties by leveraging the data that research teams have already accumulated.

We illustrate these approaches with applications to design of catalysts for fuel cells, alloys for automotive applications, and structural polymers for aircraft. The results demonstrate how these methods are rapidly becoming indispensible tools in the design of materials at all length and time scales.