

Role of Atomic-Scale Modeling in Materials Design and Discovery

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The discovery and design of new materials is the limiting factor to improve many existing technologies or to enable new applications. Material modeling methods across length scales are now widely applied and show promise for fulfilling the ultimate goal contained within the phrase “materials by design”. This presentation will review the evolution of some common material modeling methods and their integration with cutting-edge experimental methods as well as data informatics. Illustrative applications will be discussed within the context of metal/piezoelectric interfacial systems for electronic devices, new metal alloy design, novel two-dimensional and nanostructured systems, and the role of strain and dopants in the design of multifunctional materials. A future outlook of materials modeling within the context of material design and discovery will also be provided.