Chemical Engineering Doctoral Defense

Utilization of Computational Techniques in the Development of Functional Materials

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Abstract

Functional materials are a class of materials that encompass tunable properties desirable in various fields of science and engineering. Through tailoring and altering these materials, their characteristics can be fine-tuned for specific applications. Computational modeling proves to be a crucial methodology in the design and optimization of such materials. Herein, we report the utilization of molecular dynamics simulations and quantum calculations in two fields of functional materials: electrolytes and semiconductors.

Molecular dynamics simulations were performed on ionic liquid-based electrolyte systems to identify molecular interactions, structural changes, and transport properties that are often reflected in experimental results. The simulations aid in the development process of the electrolyte systems and can be invoked as a complementary or predictive tool to laboratory experiments. The theme of this study stretches further to include computational studies of the reactivity of atomic layer deposition (ALD) precursors. Selected aminosilane-based precursors were chosen to undergo density functional theory (DFT) calculations to determine surface reactivity and viability in an industrial setting. The calculations were expanded to include the testing of a semi-empirical tight binding program to predict precursor reactivity with a high surface coverage model. Overall, the implementation of computational methodologies and techniques within these applications improves materials design and process efficiency while streamlining the development of new functional materials.

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