Using Atomically-detailed Computations to Accelerate Materials Screening For Energy Applications

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There are many examples of energy technologies where the development of breakthrough materials can be characterized as a search through a space containing huge numbers of distinct materials. When appropriately applied, computational modeling can accelerate efforts to locate the "nuggets" in these search spaces that warrant detailed experimental study. Understanding the multiple objectives that define that success or failure of a material in a practical, applied context is crucial to these modeling efforts. I will discuss example of using modeling the search for high performance materials for use in hydrogen purification, hydrogen storage, and carbon dioxide capture.