# First Principles-based Atomistic Modeling of Nanomaterials for Renewable Energy and Electronics: Opportunities and Challenges

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A variety of nanostructured materials have been successfully synthesized and characterized. However, in many cases little is known about their synthesis, structure and property relationships; although such fundamental understanding is essential for further advances in nanotechnology. Experiments may yield many clues to the behavior of nanomaterials, but their interpretations are often controversial due largely to the difficulty of direct characterization. Under such circumstances, first principles-based atomistic modeling has emerged as an increasingly important area of research in nanoscale science and engineering. My research group has been active in atomistic modeling of nanomaterials, with particular emphasis on developing a better understanding of the relationships between their synthesis, structure and properties for various applications in catalysis, batteries, electronics, and photonics. This presentation will focus on introducing our ongoing efforts, with some recent progress on uncovering molecular mechanisms underlying the alloying effects of multi-metallic nanocatalysts on heterogeneous oxidation/hydrogenation reactions.