

# **Engineering of Bulk and Nano Materials for Energy Applications**

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Materials design using first-principles techniques is one of the ultimate goals in computational materials science. Due to the recent advancement in first-principles electronic structure theory and computing power, it is now possible to perform knowledge-based computational design of materials with unique optical, electrical, or magnetic properties that are tuned to specific energy related applications. This vital tool, therefore, has the great potential to accelerate scientific discovery of energy materials. In this talk, selective recent works from my group will be discussed to illustrate how computational methods can be used to design functional materials. Some of the examples include design of (i) solar cell absorber materials through cation mutation, (ii) bipolarly dopable transparent conducting oxides (TCO) for optoelectronic devices, (iii) filled tetrahedron alloys for solid state lighting applications, (iv) low band gap oxides for photoelectrochemical hydrogen production through water splitting, and (v) nano materials for energy storage and production.