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First Principles Design of Functional Materials for Energy Applications

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Materials design using first-principles techniques is one the ultimate goals in computational materials science. Due to the recent advancement in first-principles electronic structure theory and computer 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 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 (1) design PV absorber materials through cation atomic mutation; (2) design bipolar dopable transparent conducting oxides; (3) design nitride alloys for LED to fill the green gap; and (4) design oxides for hydrogen production through PEC water splitting.