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Fundamental understanding and computational design of thin-film photovoltaics materials

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The search for abundant and clean energy sources has placed photovoltaics at the focus of research over a variety of disciplines spanning physics, chemistry and materials science. However, the quest for more cost-efficient photovoltaics is challenged by limitations in efficiency of charge excitation and collection in the materials and their interfaces. We will present our recent *ab initio* calculations aimed at understanding important microscopic mechanisms in solar photovoltaic materials. Our goal is to predict accurately key properties that govern the efficiency in these materials, including structural and electronic effects, interfacial charge separation, electron and hole traps, excited state phenomena, band level alignment, and binding energies. Examples of our work in the areas of organic and other thin-film photovoltaics will be presented. We use these examples to illustrate how accurate electronic structure approaches can improve our understanding and lead to more efficient materials.