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Computational Design of Solar Energy Harvesting Materials Made of Earth-Abundant Elements[1]

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Very large-scale deployment of photovoltaic (PV) technology based on both the first and second generation solar cells posts serious questions on the materials supply as they rely on either high-purity and high-quality silicon crystals or rare elements such as indium and tellurium. "Ancient" PV materials made of earth-abundant elements, such as oxides and sulfides of copper and iron, have attracted resurgent interests. There is also intensive research devoted to the search for "modern" earth-abundant PV materials, with a recent promising example being $Cu_2ZnSnSe_4$. Computational approaches play a key role in this endeavor by guiding the screening and optimization of the materials toward high device performance. In this paper, I will focus on two aspects of computational design of earth-abundant PV materials. First, I will discuss the methods for accurately predicting band gaps of semiconductor materials. The emphasis will be on the performance of hybrid functional method on different classes of materials. Based on these understandings, I will discuss how to tune the band gap of a material to match the solar spectrum. For example, one could reduce of the band gap of anatase to 1.5 eV by the chemical codoping approach. Second, I will discuss the methods for accurate computation of defect properties, which is important as the defectiveness is intrinsic to the low-cost synthesized materials. I will introduce a method for calculation of defect formation energies by minimizing the error due to the "band-gap problem" of the density functional theory. I will also discuss approaches to mitigating the effects of defects, e.g., by passivation.

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