Defect-limited efficiency of chalcogenide solar cells

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I will discuss our development of a computational approach to connect the calculated defect properties of semiconductors to their solar cell performance. The case study is antimony selenide (Sb_2Se_3). Solar cells based on this material have the potential to achieve earth-abundant and environmental-friendly alternatives among thin-film photovoltaic light absorbers, due to their promising electronic and optical properties [1,2]. Despite notable developments over the past decade, the light-to-electricity conversion efficiency of Sb_2Se_3 reached a plateau these years (~ 10%) [3]. The origin of the efficiency bottleneck remains controversial. A significant potential cause can be attributed to the considerable trap density in Sb_2Se_3. Defects could largely limit the device performance through trap-assisted carrier recombination. I will present our most recent work [4-6] investigating the trap-limited conversion efficiency in Sb_2Se_3. I will first introduce the structures and energetics of intrinsic point defects in Sb_2Se_3 calculated by a global structure searching method, ShakeNBreak [7]. Then I will present the nonradiative carrier capture processes and the upper limit to the conversion efficiency in Sb_2Se_3 considering both radiative and nonradiative processes. The most harmful defect species will be identified.

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