**First principle investigation of defect properties in energy materials**

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First-principles study of semiconductor energy materials plays an important role in developing clean energy technologies because it can provide useful physical insights, fresh perspective and new design principles for developing innovative clean energy materials with high solar power conversion efficiency and reduced cost. Similar to other semiconductors, one of the most important issues in energy material is to control the defects, either for introducing charge carrier, improving charge transport, or reducing non-radiative carrier recombination. For example, a good solar cell material should have good defect properties so that it can be doped well such that charge carriers can be created easily to generate the required electric field and has less defect-induced recombination centers such that it has high carrier life time and minority carrier mobility, so photo-generated charge can be easily collected. In this talk, using thin-film solar cell absorber materials CdTe, CIGS and CZTS as examples, I will discuss how theoretical first-principles studies can be used to better understand and improve the solar cell performance. Control of doping in other optoelectronic energy materials such as TCOs will also be discussed.