Electron-hole recombination enhanced by lone-pairs in kesterite solar cells

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Abstract

In solar cells, photogenerated charge carriers (electrons and holes) can be annihilated by recombination processes, limiting the performance. Under solar illumination, trap-assisted non-radiative recombination process is often a dominant mechanism as described by Shockley-Read-Hall (SRH) statistics. While the radiative recombination is well understood, it has been difficult to predict the non-radiative recombination rate of a certain material theoretically. In this work, we calculate the non-radiative recombination rate in kesterite solar cells (Cu2Zn(Ge,Sn)(S,Se)4) mediated by the native point defects using first-principles density functional theory (DFT) calculations. We find that Sn-related defects exhibit both deep levels and large lattice distortion after the carrier captures induced by the formation of inert lone pairs. Hence, the sulfur vacancy (V_S), sulfur vacancy-donor complex and Sn antisites (Sn_Zn) have large carrier capture cross-sections resulting in low open-circuit voltage and poor solar-to-electricity conversion efficiency. Since the thermal equilibrium concentrations of harmful native defects are intrinsic properties of the material, they determine the fundamental limit of solar cell efficiencies.

Keywords: *Solar cell, Defect, DFT*

References

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Biography

Dr Sunghyun Kim is currently a postdoctoral researcher funded by the European H2020 project STARCELL (http://www.starcell.eu) on electron trapping at defects in semiconductors. Dr Kim studied physics at the Korean Advanced Institute of Science and Technology (KAIST) and specialised in computational physics for his PhD on the first-principles electronic structure of semiconductors. A full list of publications can be found on https://scholar.google.co.uk/citations?user=v438vEAAAAAJ.