Density Functional Theory Calculations of the Role of Defects in Amorphous Silicon Solar Cells

ERIC JOHLIN, LUCAS WAGNER, TONIO BUONASSISI, JEFFREY C. GROSSMAN, MIT — Amorphous silicon holds promise as a cheap and efficient material for thin-film photovoltaic devices. However, current device efficiencies are severely limited by the low mobility of holes in the bulk amorphous silicon material, the cause of which is not yet fully understood. This work employs a statistical analysis of density functional theory calculations to uncover the implications of a range of defects (including internal strain and substitution impurities) on the trapping and mobility of holes, and thereby also on the total conversion efficiency. We investigate the root causes of this low mobility and attempt to provide suggestions for simple methods of improving this property.

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