

Abstract Submitted
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Computational study of the Effect of Sulfur Passivation on GaAs Heterojunction Solar Cells¹ TED YU, UCLA, Department of Mathematics, RAMESH LAGHUVAMARAPU, UCLA, Department of Electrical Engineering, LIANG YAN, WEI YOU, UNC, Chapel Hill, Department of Chemistry, DIANA HUFFAKER, UCLA, Department of Electrical Engineering, CHRISTIAN RATSCH, UCLA, Department of Mathematics — We report DFT calculations that study the effect of sulfur passivation ($(\text{NH}_4)_2\text{S}$ and octanethiol) on GaAs surfaces. Sulfur passivation of GaAs solar cells is an area of interest, as it improves the I-V characteristics of heterojunctions by decreasing the density of surface states. We elucidate the fundamental mechanism of sulfur passivation on GaAs by showing how the sulfur species react with different reconstructed GaAs (100) and (111B) surfaces. Using state of the art hybrid functionals to calculate band structures and density of states, we find that a reconstructed GaAs surface does not have mid-gap surface states. Therefore, we show that sulfur passivation does not reduce surface states on reconstructed surfaces. We also study arsenic vacancies and adatoms on these surfaces to determine the energies of creating these imperfections. They lead to mid-gap surface states that are shown to be energetically plausible in certain GaAs surface reconstruction. We study the most energetically favorable surface reconstructions with As vacancies and show how sulfur passivation plays a role in removing surface states. These results will guide in the selection of passivating agents for GaAs solar cells and lead to a better understanding of such systems.

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