



Nano structures of amorphous silicon: localization and energy gap

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Abstract

Renewable energy research has created a push for new materials; one of the most attractive material in this field is quantum confined hybrid silicon nano-structures (nc-Si:H) embedded in hydrogenated amorphous silicon (a-Si:H). The essential step for this investigation is studying a-Si and its ability to produce quantum confinement (QC) in nc-Si: H. Increasing the gap of a-Si system causes solar cell efficiency to increase. By computational calculations based on Density Functional Theory (DFT), we calculated a special localization factor, [G Allan *et al.*, *Phys. Rev. B* **57** (1997) 6933.], for the states close to HOMO and LUMO in a-Si, and found most weak-bond Si atoms. By removing these silicon atoms and passivating the system with hydrogen, we were able to increase the gap in the a-Si system. As more than 8% hydrogenate was not experimentally available, we removed about 2% of the most localized Si atoms in the almost tetrahedral a-Si system. After removing localized Si atoms in the system with 1000 Si atoms, and adding 8% H, the gap increased about 0.24 eV. Variation of the gap as a function of hydrogen percentage was in good agreement with the Tight -Binding results, but about 2 times more than its experimental value. This might come from the fact that in the experimental conditions, it does not have the chance to remove the most localized states. However, by improving the experimental conditions and technology, this value can be improved.

Keywords: density functional theory, amorphous structure, silicon, localization, energy gap, HOMO, LUMO, DOS, quantum confinement

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