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The effects of silicon on the electronic properties of the clathrates $A_8Ga_{16}Si_xGe_{30-x}$ (A= Ba, Sr) EMMANUEL NENGHABI, CHARLES MYLES, Texas Tech University — We have studied the structural and electronic properties of the Ba and Sr guest-containing type-I semiconductor clathrates $Ba_8Ga_{16}Si_xGe_{30-x}$ and $Sr_8Ga_{16}Si_xGe_{30-x}$ for Si compositions x = 0, 5 and 15. Our calculations are based on the generalized gradient approximation (GGA). Starting with stable structures of the Ge-based Type I clathrate semiconductors $Ba_8Ga_{16}Ge_{30}$ and $Sr_8Ga_{16}Ge_{30}$ containing no Ga-Ga bonds, we have constructed unit cells of $Ba_8Ga_{16}Si_xGe_{30-x}$ and $Sr_8Ga_{16}Si_xGe_{30-x}$ by replacing appropriate numbers of the framework Ge atoms with Si. For the values of x that we have considered, we find that the fundamental band gap of $Ba_8Ga_{16}Si_xGe_{30-x}$ decreases with increasing x but that the band gap of $Sr_8Ga_{16}Si_xGe_{30-x}$ increases with increasing x. We also find that several electronic states near the top of the valence band and near the bottom of the conduction band in both materials are modified by the Si p states. The trends in the structural and electronic properties of these materials as x is varied are discussed, and our results are compared to experiment where possible.

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