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**Intermediate band in type-II silicon clathrate with Cu/Ag guest atoms** ZHAOHUI HUANG, HUASHAN LI, ZHIGANG WU, MARK T. LUSK, Colorado School of Mines — We investigate the structural and electronic properties of type-II clathrate with guests of Cu and Ag atoms, and our first-principles calculations demonstrate that an intermediate band (IB) would exist in the originally forbidden gap if one or two isolated Cu or Ag atoms located in a cage. These IBs have nearly ideal energy separations to VBM and CBM of the host clathrate, thus they would be useful for making highly-efficient solar cells. However, Cu and Ag atoms tend to form clusters larger than two atoms, which lead to a heavily doped semiconductor instead of generating useful IBs. We will discuss possible approaches to overcome this severe problem.

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