

Abstract Submitted
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Direct band gap silicon crystals predicted by an inverse design method¹ YOUNG JUN OH, Korea Advanced Institute of Science and Technology, IN-HO LEE, Korea Research Institute of Standards and Science, JOOYOUNG LEE, Korea Institute for Advanced Study, SUNGHYUN KIM, KEE JOO CHANG, Korea Advanced Institute of Science and Technology — Cubic diamond silicon has an indirect band gap and does not absorb or emit light as efficiently as other semiconductors with direct band gaps. Thus, searching for Si crystals with direct band gaps around 1.3 eV is important to realize efficient thin-film solar cells. In this work, we report various crystalline silicon allotropes with direct and quasi-direct band gaps, which are predicted by the inverse design method which combines a conformation space annealing algorithm for global optimization and first-principles density functional calculations. The predicted allotropes exhibit energies less than 0.3 eV per atom and good lattice matches, compared with the diamond structure. The structural stability is examined by performing finite-temperature ab initio molecular dynamics simulations and calculating the phonon spectra. The absorption spectra are obtained by solving the Bethe-Salpeter equation together with the quasiparticle G_0W_0 approximation. For several allotropes with the band gaps around 1 eV, photovoltaic efficiencies are comparable to those of best-known photovoltaic absorbers such as CuInSe₂.

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