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Prediction of direct band gap silicon superlattices with dipole-allowed optical transition[1] SUNGHYUN KIM, Department of physics, KAIST, Daejeon, Republic of Korea, YOUNG JUN OH, Department of Materials Science and Engineering, University of Texas at Dallas, Richardson, TX 75080, USA, IN-HO LEE, Korea Research Institute of Standards and Science, Daejeon, Korea, JOOYOUNG LEE, Center for In Silico Protein Science, School of Computational Science, Korea Institute for Advanced Study, Seoul, Korea, K. J. CHANG, Department of physics, KAIST, Daejeon, Republic of Korea — While cubic diamond silicon (c-Si) is an important element in electronic devices, it has poor optical properties owing to its indirect gap nature, thereby limiting its applications to optoelectronic devices. Here, we report Si superlattice structures which are computationally designed to possess direct band gaps and excellent optical properties. The computational approach adopts density functional calculations and conformational space annealing for global optimization. The Si superlattices, which consist of alternating stacks of Si(111) layers and a defective layer with Seiwatz chains, have either direct or quasi-direct band gaps depending on the details of attacking layers. The photovoltaic efficiencies are calculated by solving Bethe-Salpeter equation together with quasiparticle G0W0 calculations. The strong direct optical transition is attributed to the overlap of the valence and conduction band edge states in the interface region. Our Si superlattices exhibit high thermal stability, with the energies lower by an order of magnitude than those of the previously reported Si allotropes. We discuss a possible route to the synthesis of the superlattices through wafer bonding.

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