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Genomic design of strong direct-gap optical transition in Si/Ge core/multishell nanowires[1] LIJUN ZHANG, MAYEUL D'AVEZAC, JUN-WEI LUO, National Renewable Energy Laboratory, ALEX ZUNGER, University of Colorado — Converting the electronically superior but optically impractical indirect-gap Si and Ge semiconductors into a strongly light-absorbing system has been a long-standing challenge, given that the phonon-assisted optical transition of the indirect gap has weak intensity, requiring thick absorbers. One of main strategies has been the use of two-dimensional (2D) layer-by-layer growth of Si/Ge superlattices (SLs). However, the maximum thickness of SLs that can be grown coherently on a substrate is limited by the lattice-mismatch-induced strain. This limitation can be greatly relaxed by changing from 2D SLs to one-dimensional quantum nanowire (NW), where much higher strain can be accommodated. With developed Vapor-Liquid-Solid based technique, experimental growth of Si/Ge core-multishell NWs has recently demonstrated a significant level of synthetic control. However, the number of possible core/multishell sequences and thicknesses might easily reach an astronomic value. We will present here a genomic search for targeted core/multishell NW geometries that give both a direct gap and a significantly enhanced dipole-allowed optical transition in the Si/Ge system, by using a combination of genetic algorithm with atomistic pseudopotential electronic-structure calculations.

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