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Genetic engineering of band-egde optical absorption in Si/Ge superlattices[1] MAYEUL D'AVEZAC, JUN-WEI LUO, NREL, THOMAS CHANIER, University of Iowa, ALEX ZUNGER, University of Colorado — Integrating optoelectronic functionalities directly into the mature Silicon-Germanium technology base would prove invaluable for many applications. Unfortunately, both Si and Ge display indirect band-gaps unsuitable for optical applications. It was previously shown (Zachai *et al.* PRL **64** (1990)) that epitaxially grown $[(\mathrm{Si})_n(\mathrm{Ge})_m]_p$ (i. e. a single repeat unit) grown on Si can form direc-gap heterostructures with weak optical transitions as a result of zone folding and quantum confinement. The much richer space of *multiple-period* superlattices $[(\mathrm{Si})_{n_1}(\mathrm{Ge})_{n_2}(\mathrm{Si})_{n_3}(\mathrm{Ge})_{n_4}\ldots Ge_{n_N}]_p$ has not been considered. If $M = \sum n_i$ is the total number of monolayers, then there are, roughly, 2^M different possible superlattices. To explore this large space, we combine a (i) genetic algorithm for effective configurational search with (ii) empirical pseudopotential designed to accurately reproduce the inter-valley and spin-orbit splittings, as well as hydrostatic and biaxial strains. We will present multiple-period SiGe superlattices with large electric dipole moments and direct gaps at Γ yielded by this search. We show this pattern is robust against known difficulties during experimental synthesis.

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