Genetic engineering of band-edge optical absorption in Si/Ge superlattices

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 [(Si)$_n$(Ge)$_m$]$_p$ (i.e. a single repeat unit) grown on Si can form direct-gap heterostructures with weak optical transitions as a result of zone folding and quantum confinement. The much richer space of multiple-period superlattices [(Si)$_{n_1}$(Ge)$_{n_2}$(Si)$_{n_3}$(Ge)$_{n_4}$…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 $\Gamma$ yielded by this search. We show this pattern is robust against known difficulties during experimental synthesis.

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