Genetic-Algorithm Discovery of a Direct-Gap and Optically Allowed Superstructure from Indirect-Gap Si and Ge Semiconductors

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The fact that silicon is the paradigm semiconductor—readily dopable by either electrons or holes and protected from environmental scatterers by a native oxide passivation layer—is unfortunately not matched by the additional virtue of being able to strongly emit and absorb light. Nevertheless, one of the outstanding projects of the semiconductor industry is the integration of optical and electronic functions on single-crystal silicon wafers [1,2]. We provide a new and unexpected solution to a classic problem, showing how two indirect-gap materials (Si and Ge) can be spatially melded together into one strongly dipole-allowed direct-gap material.

There are three main routes to integrating optical functions—and specifically light emission—onto a silicon wafer. The "device" route relies on a strong external magnetic field to instigate electron-hole recombination despite silicon's indirect gap through either field emission—e.g., tuneling between electron and hole bands—or electron avalanches [2]. The second route relies on introducing local recombination centers into the material, thus bypassing altogether the constraints imposed on the optical spectra by silicon's band structure. In practice, this has been achieved through rare-earth doping, such as erbium [3], or by engineering dislocations into the silicon wafer [4].

The third route prefers to manipulate the band structure of silicon directly to create a material with optically active band edges. For example, in an indirect material where the gap at γ

[illegible] X [illegible] G [illegible]

[illegible] α_n [illegible] n [illegible] β [illegible] G 2G 2G 2G [illegible] γ [illegible] G 2G 2G 2G 2G [illegible] c [illegible] $\Delta_{x,y}$ [illegible]

[illegible] 1G x [illegible] x [illegible] G 0 [illegible]