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

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 elec Ψ . tronic functions on single-crystal silicon wafe[rs](#page-4-0) 21. 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 dipoleallowed direct-gap material.

There are three main routes to integrating optical functions—and speci cally light emission—onto a silicon wa-11 fer. The "device" route relies on a strong external magnetic eld to instigate electron-hole recombination despite silicon's indirect gap through either eld 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 ϕ achieved through rare-earth doping, such as erbisinor by [e](#page-4-0)ngineering dislocations into the silicon wafer.

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 $gap \nightharpoonup \nighth$ \mathbf{A}

 \mathbf{A} is γ

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as germanium (and unlike silicon), uniaxial tensile strain

explicit goal of finding a direct-gap and optically active material. Using a combination of genetic algorithms \mathcal{I}_1 and \mathcal{I}_2 algorithms \mathcal{I}_1 and \mathcal{I}_2 and band-structure calculation [\[12\]](#page-4-11), we identify a motif with a 50-fold increase of the dipole matrix element of the dipole matrix element over t_{max} record set by Si6Ge4. This motion is a dipoleallowed direct-gap material with a light effect g defined by the momentum matrix) of 10% compared to the direct transition at

the growth direction of the dipole matrix element reported in Table [I](#page-2-0). Indeed, whereas the overall magnitude of the directed is fairly constant for any \mathcal{C} -any \mathcal{C} any \mathcal{C} any \mathcal{C} strate, for any concentration x , the component along the component \mathcal{X} $g\circ g=\bigvee_{i=1}^n g_i\circ g_{i+1-i+1-i+1} = g_{i+1-i+1-i+1-i+1} = g_{i+1-i+1-i+1}$ to almost extinct on the Germanium substrate. Finally, we can extend the Germanium substrate. Finally, we can $f(x) = \frac{1}{2} \int_{-\infty}^{\infty} f(x) \, dx$ the magic sequence will not the magic sequence be ill affected by the superlattice construction, since its

effective masses are quite specific squarely between those of sili---sili---sili---sili---sili---sili---sili--con and Germanium (see Table [II\)](#page-3-0). Mechanism of the interband coupling leading to a dipole-allowed transition.—To understand how the magic s equence becomes direct and optically-active, we analyze and optically \sim in the middle panel of Fig. [2](#page-2-1) the orbital character of the band-edges Fourier space. The orbital character, also called $m_{\rm e}$ is represented to origin of the origin of th superlattice's CBM in the unfolded Brillouin zone of the zinc blende. In other words it tells us which states from the bulk-components hybridize through folding at in the superlattice Brillouin zone. We find that in both the $m_{\rm eff}$ sequence and $\Delta_{\rm eff}$ Ge4 the CBM at $\frac{d}{dx}$ constructed from X and S states, with however a much larger contribution \mathcal{C} tion in the case of the latter. This result is in line with the much larger absorption from the magic sequence. The lower $t \approx 2$ $t \approx 2$ plot the wave function density of the w CBM and VBM averaged over the epitaxial plane. In both materials, the VBM is delocalize over the whole superlat $t_{\rm max}$ is principally located over S^{\sharp} rich region. However, in the magic sequence, the magic sequence, the magic sequence, this region \tilde{Y} is fairly small (two monolayers). mostly contained within the active motif itself. \mathcal{S} the results to deviation from the optimal structure. And the accuracy of the growth method \mathcal{A} could result slight variations from the optimal structure predicted in this Letter. How much would this affect the optical transition across the electronic gap $\mathfrak{g}_{\mathbb{C}}$ the effect of changing both the virtual substrate and α mutations in the magic sequence upon the optically active direct gap. In the following, α $n \sim 1$ with a Ge buffer of n monolayers, while β $S_1 = \mathbf{G}_{1} + \frac{1}{2}\mathbf{G}_{2} + \frac{1}{2}\mathbf{G}_{3} + \frac{1}{2}\mathbf{G}_{4} + \cdots$ $\mathbf{G}=\left\{ \mathbf{G}=\left\{ \begin{array}{ll} 2\mathbf{G}=\left\{ 2\mathbf{G}=\left\{ 2\mathbf{G}\right\} \right\} \end{array}\right.\right.\left.\left.\begin{array}{ll} \mathbf{G}=\left\{ \begin{array}{ll} 2\mathbf{G}=\left\{ 2\mathbf{G}\right\} \end{array}\right.\right.\left.\begin{array}{ll} \mathbf{G}=\left\{ 2\mathbf{G}\right\} \end{array}\right.\left.\begin{array}{ll} \mathbf{G}=\left\{ 2\mathbf{G}\right\} \end{array}\right.\left.\begin{array}{ll} \mathbf{G}$ \mathcal{A} is directed vertical axis—solid lines)—solid lines. t difference between the folder c and the C $\Delta_{x,y}$ and the dipole matrix element between the valence \sum_{x} A A \cdots A \pm ∞ ∞ ∞ A A lines) as a function of the choice of substrate in-plane n 21

the case of indirect gaps in reciprocal space. For reference, \mathcal{A}_max

 $1'$ w. U. Louis Co., S. Louis R. R. R. \mathcal{A} , G. Le $S_{\rm c}$, and $S_{\rm c}$ is equal to Δ , nature (London) 410, 192