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Understanding electronic band-edge properties of GaSbAs/GaAs nanostructures through k.p theory simulations CHRISTINA JONES, EM-MANOUIL KIOUPAKIS, University of Michigan - Ann Arbor — Gallium antimonide (GaSb) nanostructures embedded in gallium arsenide (GaAs) have been predicted by theory and have been found experimentally to demonstrate both type-I and type-II band alignment. The ability of GaSb nanostructures to exhibit two band alignment types makes them versatile in applications such as LEDs, photodetectors, and charge-based memory elements. We present a systematic study of the mechanisms behind the band alignment type in order to understand the underlying physics behind the alignment transition and allow for prediction and optimization of electronic properties. We employ the eight-band k.p. method through a commercially available software package (nextnano) to calculate the band structure by self-consistently solving the Schroedinger and Poisson equations and including strain and polarization charges. Results obtained for GaSbAs/GaAs quantum wells show both type-I and type-II band alignment depending on strain and composition. Calculated band-edges are compared to published experimental results.

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