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Electronic properties of grain boundaries in III-V materials JONNY DADRAS, Univ of California - Los Angeles, CHRISTIAN RATSCH, Institute of Pure and Applied Mathematics — III-V semiconductors, have many applications in the field of optoelectronics. InAs, in particular, is known for its high electron mobility and narrow band gap (˜0.4 eV) and is commonly used in infrared detectors as well as a terahertz radiation sources. Grain boundaries (GBs) generally degrade a material's performance by introducing *interface-states* that reduce charge carrier mobility. The present work employs state of the art all-electron DFT calculations, using the FHI-AIMS code. The GBs are modeled as interfaces between several low-index planes. Hence, the relevant electronic structure is seen to arise from *surface-surface interactions* between thermodynamically favorable surface reconstructions. The recently developed Interface Builder is used to guide construction of surface interfaces. Detailed Projected Density of States (PDOS) difference and charging analyses are performed in order to understand the nature of the local bonding that can arise and, therefore, how best to dope or alter the material to minimize the defective electronic structure. The research is extended to a few cases of the ternary In-As-Sb system.

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