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Transferable tight binding model for strained group IV and III-V heterostructures YAOHUA TAN, Dr, MICHEAL POVOLOTSKYI, TILLMANN KUBIS, TIMOTHY BOYKIN, GERHARD KLIMECK, Prof — Modern semiconductor devices have reached critical device dimensions in the range of several nanometers. For reliable prediction of device performance, it is critical to have a numerical efficient model that are transferable to material interfaces. In this work, we present an empirical tight binding (ETB) model with transferable parameters for strained IV and III-V group semiconductors. The ETB model is numerically highly efficient as it make use of an orthogonal sp3d5s* basis set with nearest neighbor inter-atomic interactions. The ETB parameters are generated from HSE06 hybrid functional calculations. Band structures of strained group IV and III-V materials by ETB model are in good agreement with corresponding HSE06 calculations. Furthermore, the ETB model is applied to strained superlattices which consist of group IV and III-V elements. The ETB model turns out to be transferable to nano-scale hetero-structure. The ETB band structures agree with the corresponding HSE06 results in the whole Brillouin zone. The ETB band gaps of superlattices with common cations or common anions have discrepancies within 0.05eV.

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