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An investigation of dopping profile for a one dimensional heterostructure ZHAOHUI HUANG, DRAGAN STOJKOVIC, PAUL LAMMERT, VINCENT CRESPI, Department of Physics, The Pennsylvania State University — A one-dimensional junction is formed by joining two silicon nanowires whose surfaces are terminated with capping groups of different electronegativity and polarizability. If this heterostructure is doped (with e.g. phosphorous) on the side with the higher bandgap, the system becomes a modulation doped heterostructure with novel one-dimensional electrostatics. We use density functional theory calculations in the pseudopotential approximation, plus empirical model calculations, to investigate doping profiles in this new class of nanostructures.

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