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Density Functional Calculation of Quantum Wire CHIN-SHENG WU, Yuan Ze University — Quantum wire displays quantum effects on the electrical transport properties. If the diameter of a wire is in the nanometer dimension, the energy and momentum of free electrons will be limited to a series of discrete values. Following from the quantization of electron energy, the electrical conductance is found to be quantized in multiples of $2^2_{e/h}$ where e is the electron charge and h is the Planck constant. The conductance of a ballistic quantum channel is equal to the summation of each electron conductance. We apply density functional theory to calculate the electron structure of quantum wire. To perform a calculation for a specific case, we take Al ($r_s = 2$) atoms for the quantum wire, which behave as potential quantum well with the barrier plus biased voltage between the two boundaries. The number of electrons is determined by the cross section and length of the quantum wire. The current density j is equal to electron charge density multiplying velocity. The quantizations of conductance corresponding to the lowest energy states are only observed for atom-size wires. Their corresponding wavelength being thus extremely small they have a very large energy separation which makes resistance quantization observable even at room temperature.

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