Theoretical study of conductance in kinked nanowires

BRANDON COOK, KALMAN VARGA, Vanderbilt University — Controlled growth of single-crystalline kinked semiconductor nanowires has recently been observed experimentally. The wires could be key in the integration of nano-scale devices. The conductance of a perfect nanowire is an integer multiple of the quantum unit of conductance. Using first-principles transport calculations we have studied how the conductance properties of nanowires change due to kinks and turns. We used monoatomic chains as well as 1-4 nm diameter Si nanowires as prototypical examples. We have found that the transmission strongly depends on the geometry of the kinks, especially for thin nanowires.

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Brandon Cook
Vanderbilt University

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