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What are new when Si nanowires get small: magic numbers and square shape[1] RUQIAN WU, Department of physics and astronomy, UCI, CA — Through systematic density functional studies, we found the existence of "magic numbers" for Si nanowires grown along the <100> axis. Strikingly, Si nanowires prefer the sharp square cross-section with corner atoms when the diameter is smaller than 1.7 nm. This is promoted by two facts: (1) the presence of the corner atoms permits formation of benign reconstruction pattern to maximally saturate the dangling bonds; and (2) the corner atoms develop pairs and strongly interact with each other across nanowires.

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