

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Magic structures of H-passivated $\langle 110 \rangle$ silicon nanowires TZU-LIANG CHAN, Ames Laboratory and Physics Department, Iowa State University, CRISTIAN V. CIOBANU, Division of Engineering, Colorado School of Mines, FENG-CHUAN CHUANG, NING LU, CAI-ZHUANG WANG, KAI-MING HO, US. DOE Ames Laboratory and Physics Department, Iowa State University — We report a genetic algorithm approach combined with ab initio calculations to determine the structure of hydrogenated $\langle 110 \rangle$ Si nanowires. As the number of atoms per length increases, we find that the cross section of the nanowire evolves from chains of six-atom rings, to fused pairs of such chains, to hexagons bounded by $\{001\}$ and $\{111\}$ facets. Our calculations predict that hexagonal wires become stable starting at about 1.2 nm diameter, which is consistent with recent experimental reports of nanowires with diameters of about 3 nm.

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Date submitted: 30 Nov 2005

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