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Relative Stabilities of Silicon Nanowires of Different Orientations[1] ALEXANDER TCHERNATINSKY, CHRIS LEAHY, DMITRY MIGAS, MING YU, CHACRAM JAYANTHI, SHI-YU WU, University of Louisville — This work presents a theoretical study of equilibrium structures of silicon nanowires oriented along <001>, <110>, and <111> directions with a particular attention to relative stabilities of these wires with respect to their diameters and their shapes. The diameters of nanowires considered in this work ranges from a few nm to 10 nm. Because of the size of the system, we employ a semi-empirical Hamiltonian that: (i) captures electron screening and many-body effects via self-consistent (SC) and environment-dependent (ED) terms, and (ii) is built on the framework of the linear combination of atomic orbitals (LCAO). Initial configurations of wires were chosen carefully to minimize the number of dangling bonds. The reliability of the SCED-LCAO method was first established by comparing the results obtained from this method to ab-initio method for small-diameter silicon nanowires. To allow the relaxation of large-diameter wires up to 10 nm, a linear scaling algorithm is implemented within the SCED-LCAO molecular dynamics. Energetic considerations show that silicon nanowires oriented along the ¡011¿ direction are most stable in the diameter range from 3 to 10 nm and this result is in agreement with a recent experiment (C. M. Lieber et al., Nano Lett, 4, 433, 2004).

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