An Ab Initio Study on Silicon and Germanium Nanotubes
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First principles calculations using hybrid density functional theory have been per-
formed to examine the electronic and geometric structure properties of single-walled
silicon (SWSiNT) and germanium (SWGeNT) nanotubes. Finite clusters $X_mH_n(X$
$=\text{Si or Ge})$ are used to model the nanotubes (e.g. the smallest SWSiNT is modeled
as $\text{Si}_{60}H_{12}$). Hydrogen termination is done to simulate the effect of longer tubes as
well as to take care of end effects. A pseudopotential basis set has been used for
the silicon atoms$^1$ and complete geometry optimizations of the structures has been
carried out using the Gaussian 03 suite of programs.$^2$ Computer simulations predict
that the existence and stability of the nanotubes are highly dependent on the ratio of
the $sp^2$ to $sp^3$ hybridization. Results will be presented on cohesive energies, HOMO-
LUMO gaps, and other electronic structure properties and their dependence on the
tube diameter. We will discuss the density of states (DOS) to explain the possible
metallic or semi-conducting character of the tubes. Detailed comparisons with pub-
lished data in the literature will also be presented. * Work supported, in part, by