Abstract Submitted
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**All-electron and pseudo-potential studies of structural and electronic properties of Si chains and nanowires**[1] JUN LI, ARTHUR FREEMAN, Northwestern University, ANDREW WILLIAMSON, JEFFREY GROSSMAN, GIULIA GALLI, Lawrence Livermore National Laboratory — Recent experiments[2] invoke Si nanowires as promising materials for nanoscale electronic and optical devices. We carried out electronic structure calculations of silicon chains and nanowires, by using both the full-potential linearized augmented plane wave (FLAPW) method[3] and the pseudopotential plane wave method. We studied two sets of H-terminated one nanometer silicon wires, one oriented along (001) and the other along(111); both show direct band gaps, with the (111) oriented wires showing a smaller gap (∼2.1 eV) than (001) (∼2.5 eV). This trend differs from that reported in the literature [4], but it is the same in both our all-electron and well converged pseudopotential calculations. We also found that structural relaxations induce different effects on the band structure of differently oriented wires; the band gap change is nearly 0.2 eV between the ideal and relaxed models for (001) while it is negligible for (111) wires.

[1]Supported by DARPA PROM
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[3]E.Wimmer, H.Krakauer, M.Weinert, AJ Freeman, PRB 24, 864 (1981)
[4]F. Buda, et.al., PRL 69, 1272 (1992); A. M. Saitta, et.al., PRB 53, 1446 (1996)

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