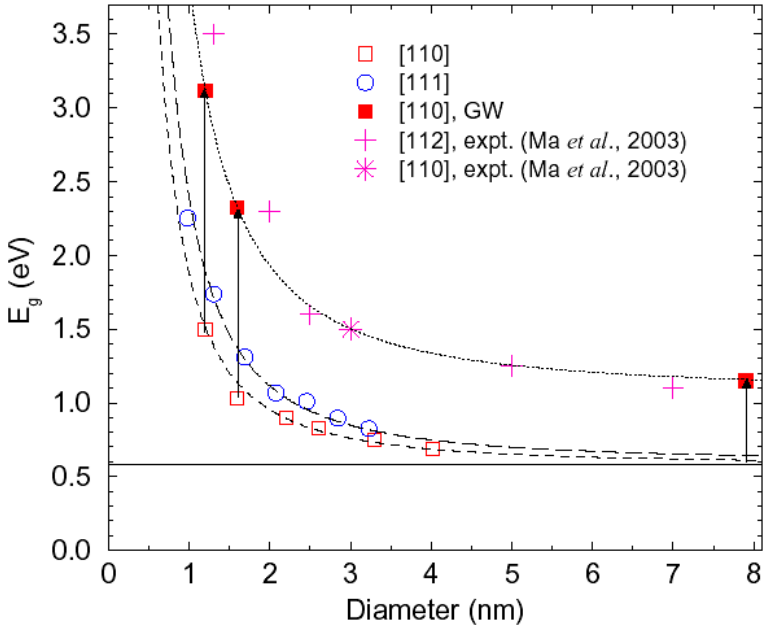
ITR: Modeling and Simulations of Quantum Phenomena in Semiconductor Structures of Reduced Dimensions

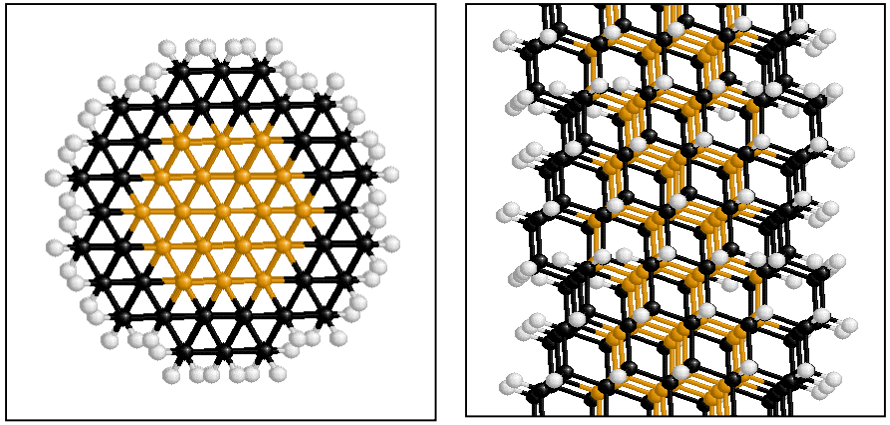
Mei-Yin Chou and Uzi Landman (Georgia Tech), Cyrus Umrigar (Cornell University), Xiao-Qian Wang (Clark Atlanta University); DMR-0205328

We are conducting a comprehensive simulation of the electrical, optical, structural, and transport properties of various nanowires, with the focus on their size dependence. The goal is to make use of the computational capabilities provided by today's information technology to perform theoretical modeling of materials that may play a key role in the hardware development for tomorrow's information technology. Issues being examined include stability and growth, electronic structure, vibrational modes, conductance, and nanocontacts.

Direct gap as a function of diameter



Core-Shell Nanowire Heterostrctures



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Education and Outreach

- Train students (undergraduate and graduate) and postdocs in computational techniques for materials simulations
- Involve undergraduate students in materials research through the existing REU program at Georgia Tech
- Partnership between Georgia Tech and Clark Atlanta University (a Historically Black University): regular exchange visits of faculty and students; joint seminars; joint courses; joint workshops
- Information Technology Research Seminars
- Special course “Physics of Small Systems” taught by Landman (2003-2004)

- Minority students in the project (from left to right)

  Anthony Cochran (Clark Atlanta)
  Carmen Robinson (Clark Atlanta)
  Alexis Nduwimana (Georgia Tech)
  Damian Cupid (Clark Atlanta)

- Mini-workshop on Quantum Approximate Methods for Novel Materials (Clark Atlanta University, October 2003); all participants are minority students