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

PI: Mei-Yin Chou (Georgia Tech)
Co-PI’s: Uzi Landman (Georgia Tech)
Cyrus Umrigar (Cornell University)
Xiao-Qian Wang (Clark Atlanta University)

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Group IV, III-V, II-VI, and oxides

2 nm < diameter < 50 nm

Doping, cross-wire p-n junctions, light-emitting diodes, logic gates

Nanosized photodetectors, and biological/chemical sensors
Project Summary

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• A comprehensive study of the electronic, optical, structural, and transport properties of various semiconductor nanowires.
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• A comprehensive study of the electronic, optical, structural, and transport properties of various semiconductor nanowires.

• 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.
Physical Issues

• **Stability and growth**

  a. Catalyst assisted vapor-liquid-solid growth: size-dependent orientation

  b. Thermal evaporation synthesis of nanobelts of semiconducting oxides: rectangular cross sections, atomically flat surfaces, unique orientation
Physical Issues

• Stability and Growth

• **Electronic Structure: band gaps, excitons, and optical properties**

Electrons and holes are confined in two out of three dimensions.

- Gap dependent on the diameter AND orientation of the wire
- Excitons with larger binding energies and oscillator strengths
- Quantization effect in collective electronic excitations (plasmons)
Physical Issues

• Stability and Growth

• Electronic Structure: band gaps, excitons, and optical properties

• “Phonons” in Nanostructures

  Thermal properties important for heat conduction and power dissipation

  Confinement effect → broadening and shift of peaks

    → acoustic phonon dispersion and group velocity modified

    → phonon distribution modified by boundary scattering

  Size and shape dependence
Physical Issues

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• **Device Simulations (conductance, contacts, etc.)**

  Conductance spectra exhibit size-dependent oscillations due to interference resonance from scattering with the contacts
Si (yellow)  H (dark blue)  Al (light blue)

Computational Methods

- **First-principles molecular dynamics simulations within density functional theory with pseudopotentials and plane waves**

  Stability, growth, energetics, electronic wave functions, vibrational modes, *etc.*

- **Quantum Monte Carlo methods (variational, VMC and diffusion, DMC)**

  Energy gap, excitation energies, algorithm development (linear scaling with nonorthogonal Wannier functions, calculation of optical transition strength using DMC to obtain the imaginary-time correlation function)

- **Many-body perturbation theory**

  GW quasiparticle energies, optical excitations including exciton effects (Bethe-Salpeter equation, evaluate the Coulomb scattering matrix in real space using Wannier functions)
• First-principles calculation of conductance

Recursion-transfer-matrix method to solve the coupled differential equation involving reflected and transmitted waves (Hirose and Tsukada) and eigenchannel analysis for the transmission (Brandbyge et al.)

The Green’s function method and the self-consistent Lippmann-Schwinger equation with scattering boundary condition (Lang et al.)
Educational and Outreach Activities

- Students (undergraduate and graduate) and postdocs well trained in computational techniques
- Involve undergraduate students in the project through existing REU program at Georgia Tech
- Strengthen partnership between Georgia Tech and Clark Atlanta University (a predominantly minority institution)
  Co-advising Ph.D. students; regular exchange visits of faculty and students
  A special monthly seminar series on applications of information technology to be held alternately at Georgia Tech and Clark Atlanta (potential speakers: PI’s of other ITR grants)
  A new course on computational approaches to scientific and engineering problems to be taught at both Georgia Tech and Clark Atlanta University
  Workshop, with hands-on sessions, to train students to use our codes