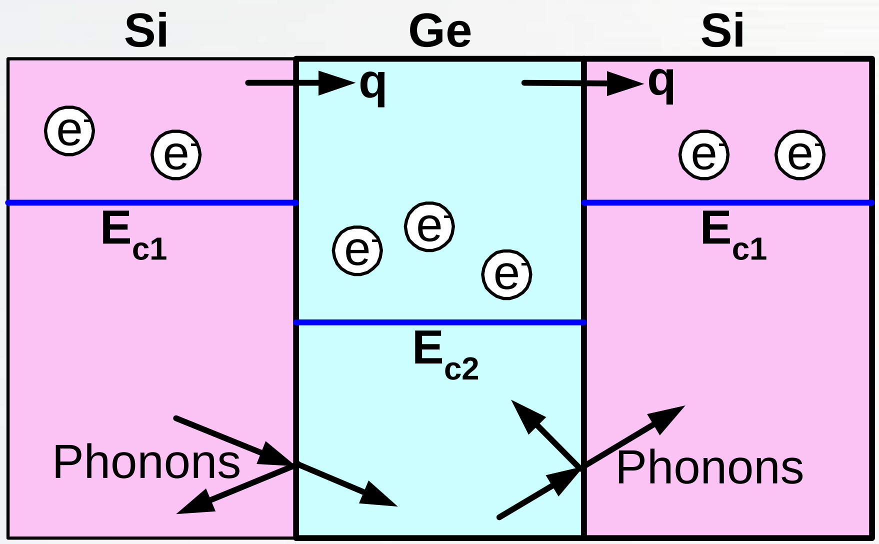
# Coupled Quantum-Scattering Modeling of the Thermoelectric Properties of Si/Ge/Si Quantum Well Superlattices

Anuradha Bulusu
Advisor: Prof. D. G. Walker
Interdisciplinary Program in Material Science
Vanderbilt University, Nashville, TN

# Motivation



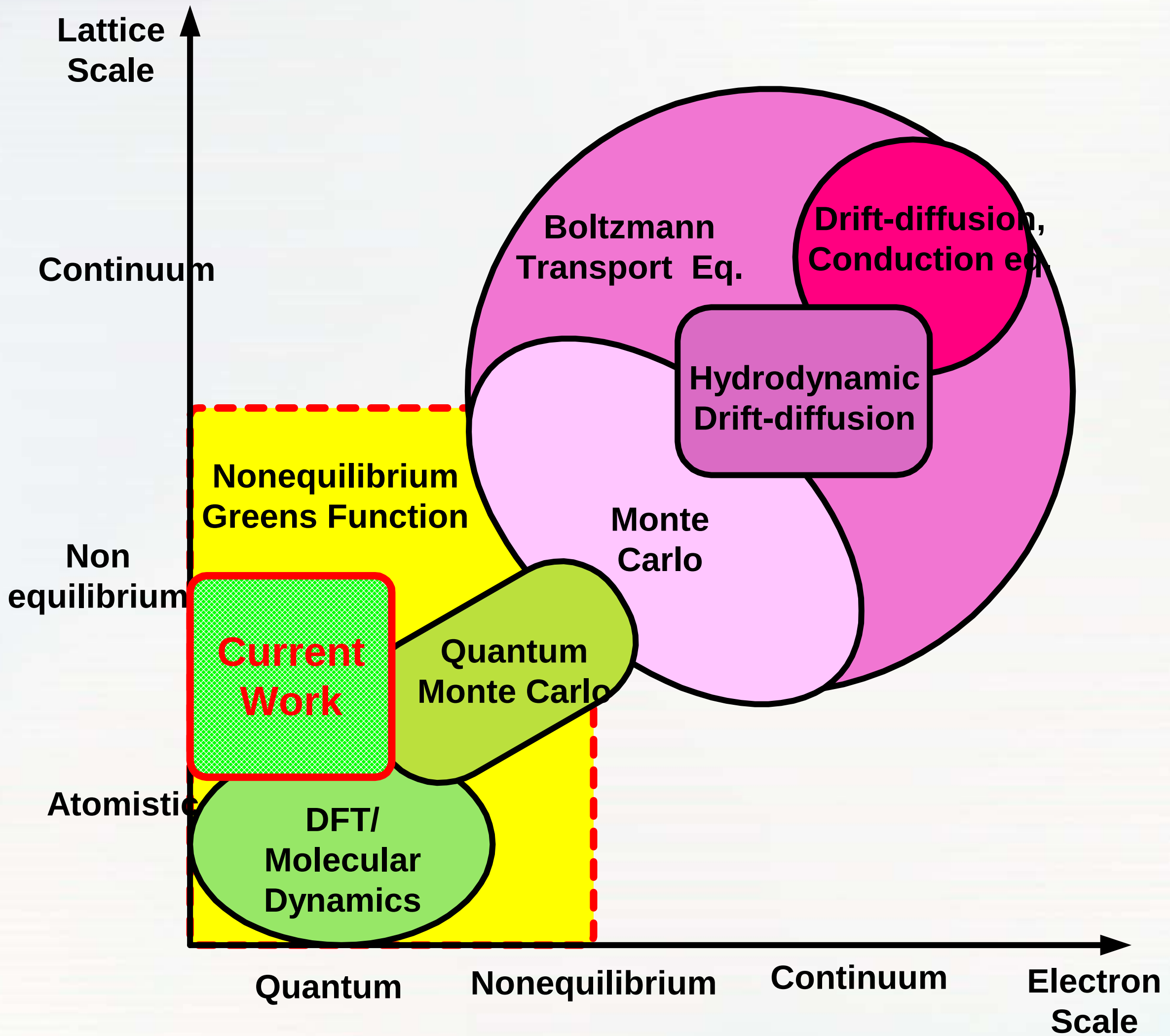

$$ZT = \frac{S^2 \sigma T}{\kappa}$$

- Quantum well superlattices proposed to improve thermoelectric figure of merit *ZT*.
- Phonon interface scattering and phonon confinement contribute to low $\kappa$.
- Most models assume electrical conductivity to not change significantly with confinement.

# Objective

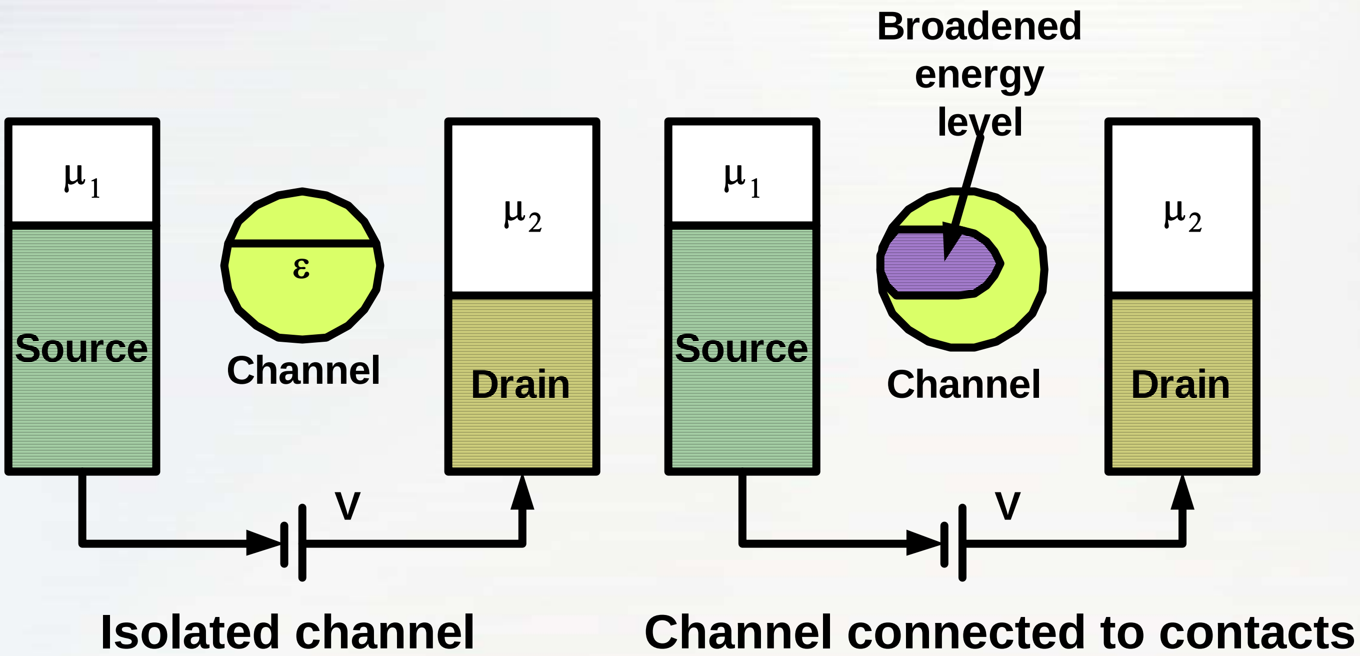
- NEGF (Nonequilibrium Green's Function)
  - Coupled quantum and scattering modeling in nanodevices.
- Study Nanoscale Effects
  - Effect of reduced dimensionality on
    - Seebeck coefficient of the device.
    - Electrical conductivity.
    - Device performance i.e. Power factor $S^2\sigma$.

# Device Models



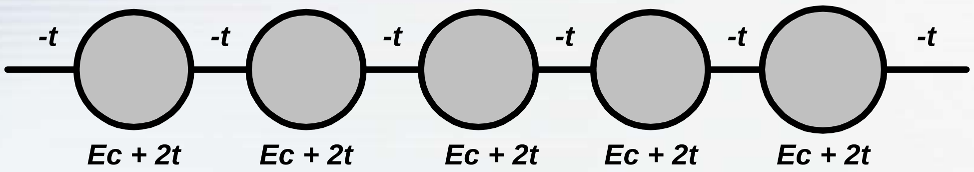

NEGF: Non-Equilibrium Green's function

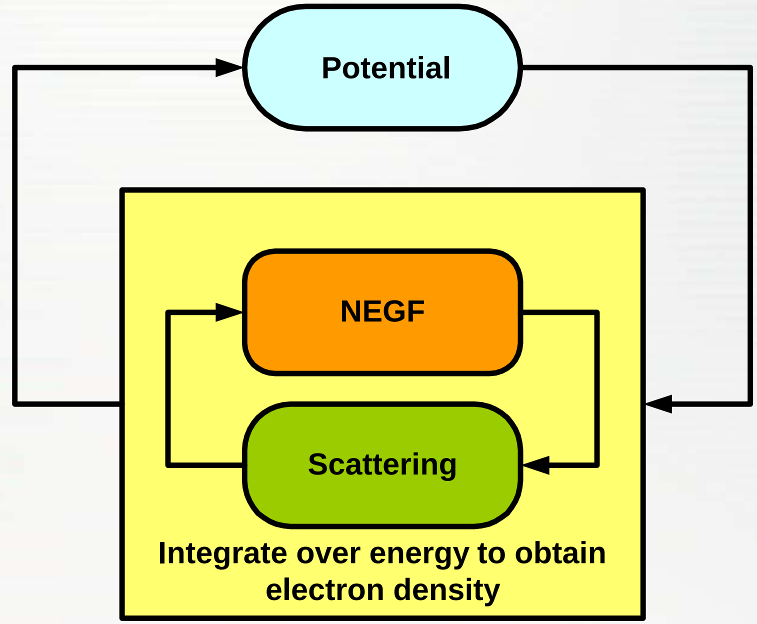
# Nonequilibrium Green's Function Method




- Broadening of energy density of states near source and drain contacts leads to current flow.
- NEGF method does not require a statistical distribution of carriers within the device.
- Can be used to solve extreme nonequilibrium problems.

# Numerical Scheme



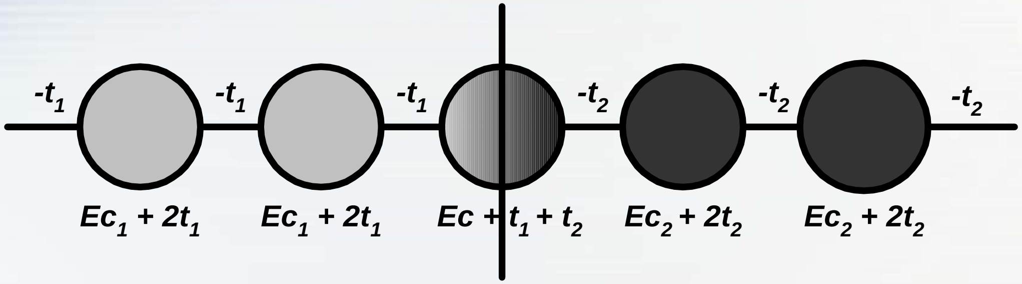




Hamiltonian $$[H] = \begin{bmatrix} Ec+2t & -t & \\ -t & Ec+2t & -t \\ & -t & Ec+2t \end{bmatrix}$$

$$t = \frac{\hbar^2}{2m^* a^2} \qquad L = a(N-1)$$

- Standard control volume approach used to model films and wires.
- Grid spacing $\boldsymbol{a}$ chosen so that value of $\boldsymbol{t}$ > energy range of integration to ensure grid independence.
- Green's function $G(E) = \left[\left(E - i0^+\right) I - H - \Sigma_1 - \Sigma_2 - \Sigma_s\right]^{-1}$
- Opportunities to improve computational efficiency: Parallelization of energy integration loop, adaptive mesh integration.

# Numerical Scheme Contd.




$$[H] = \begin{bmatrix} Ec_1 + 2t_1 & -t_1 & \\ -t_1 & Ec + t_1 + t_2 & -t_2 \\ & -t_2 & Ec_2 + 2t_2 \end{bmatrix}$$

- Spatially varying effective mass at the interface.
- Effective mass at interface is harmonic mean of the two masses.
- Interface lies on node to ensure Hamiltonian is Hermitian.

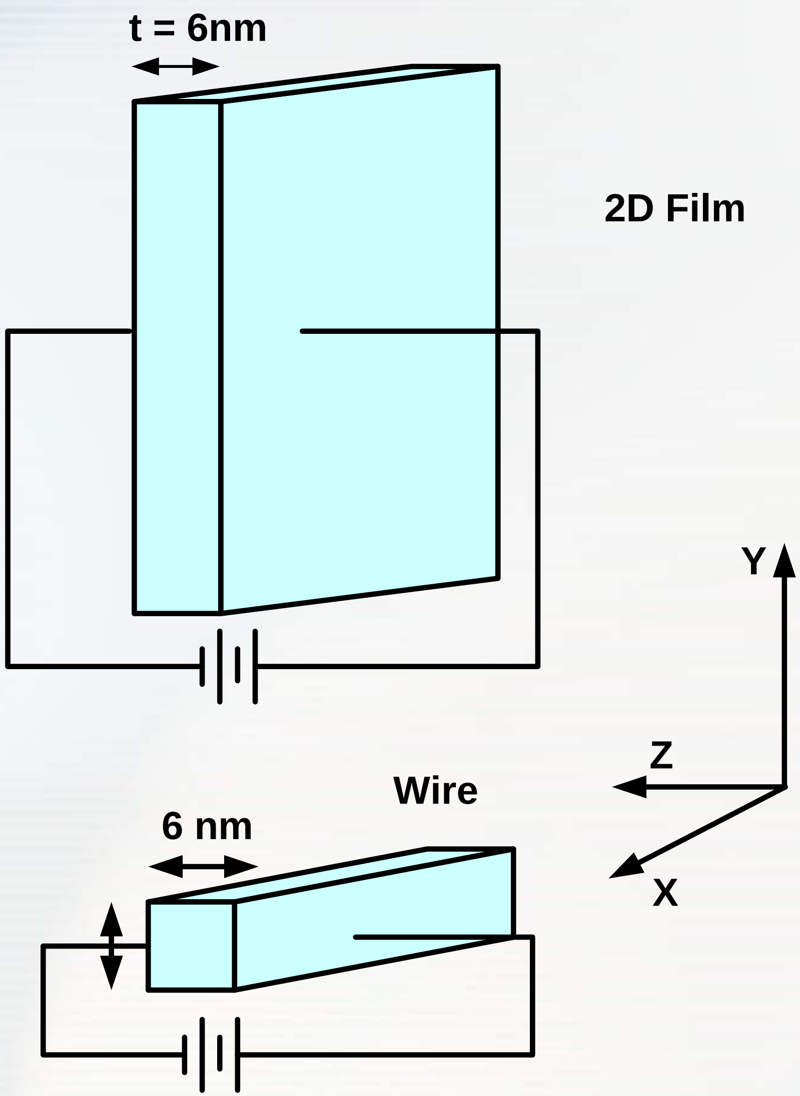
## Poisson's equation

$$\nabla^2 \{U\} = U_0 \left(n(r) - n_0\right) \qquad U_0 = -\frac{q^2}{\varepsilon_0 \varepsilon_r a}$$

Value of grid spacing ***a*** must be chosen so that $U_0 \approx k_B T$.

Anderson mixing used to accelerate convergence.

# Modeling Confinement Effects




Source and drain Fermi functions have to take into account the effect of infinite boundaries in x, y directions for film and along the x axis for the wire.

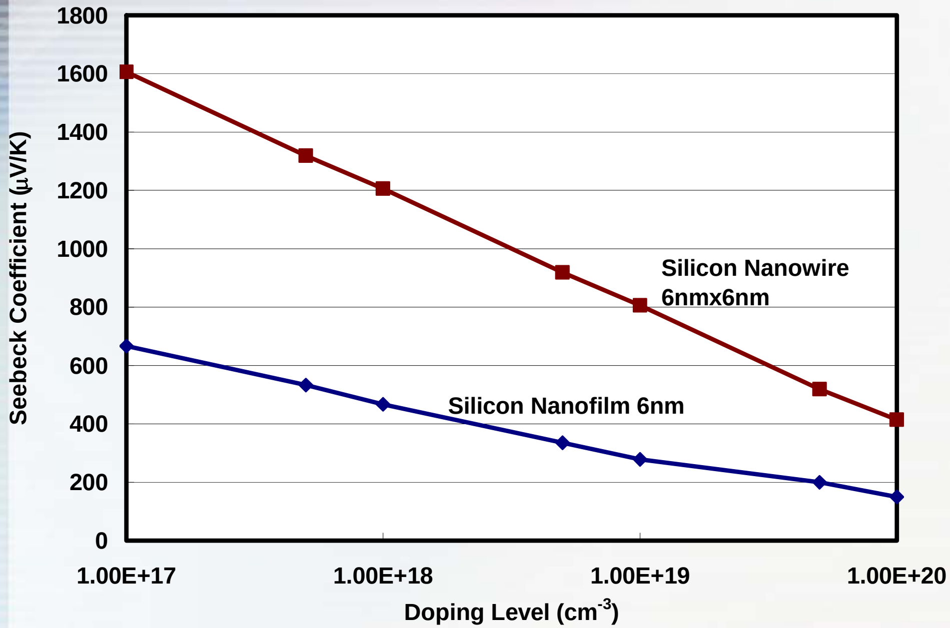
$$f_{2D}(E_n)$$

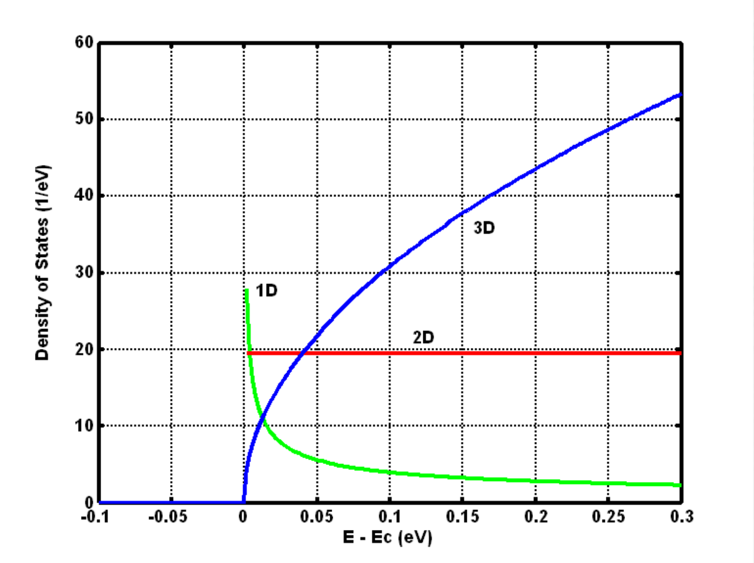
$$E_n = \int_0^\infty \frac{\hbar^2 k_x^2}{2m^*} + \int_0^\infty \frac{\hbar^2 k_y^2}{2m^*} + \frac{\hbar^2}{2m^*}\left(\frac{n\pi}{L_z}\right)^2$$

$$f_{1D}\left(E_n\right)$$

$$E_n = \int_0^\infty \frac{\hbar^2 k_x^2}{2m^*} + \frac{\hbar^2}{2m^*}\left(\frac{n\pi}{L_y}\right)^2 + \frac{\hbar^2}{2m^*}\left(\frac{n\pi}{L_z}\right)^2$$

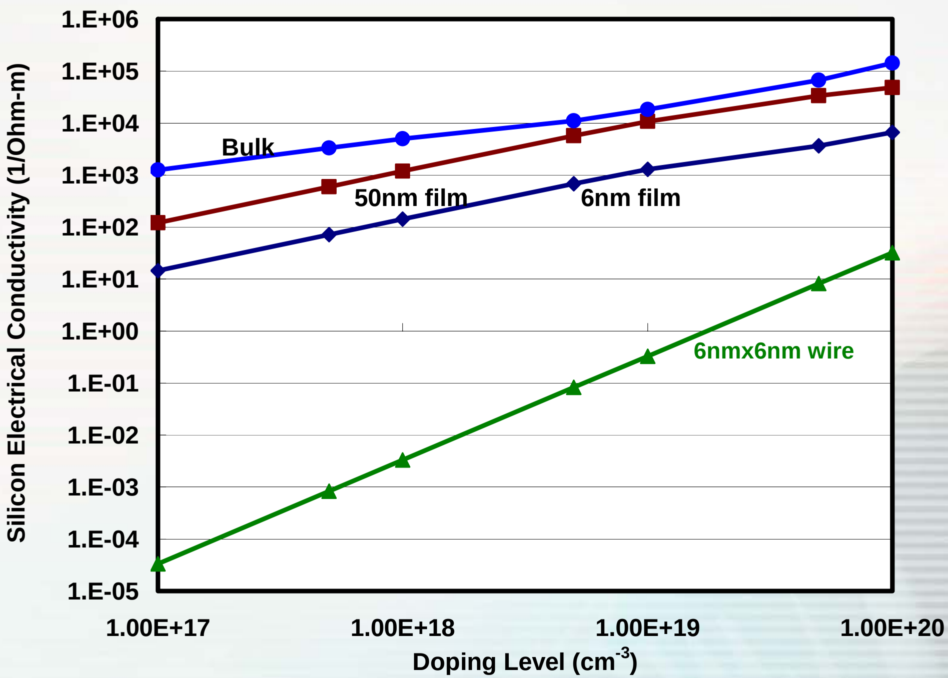
# Nanoscale Effects on Thermoelectric Properties



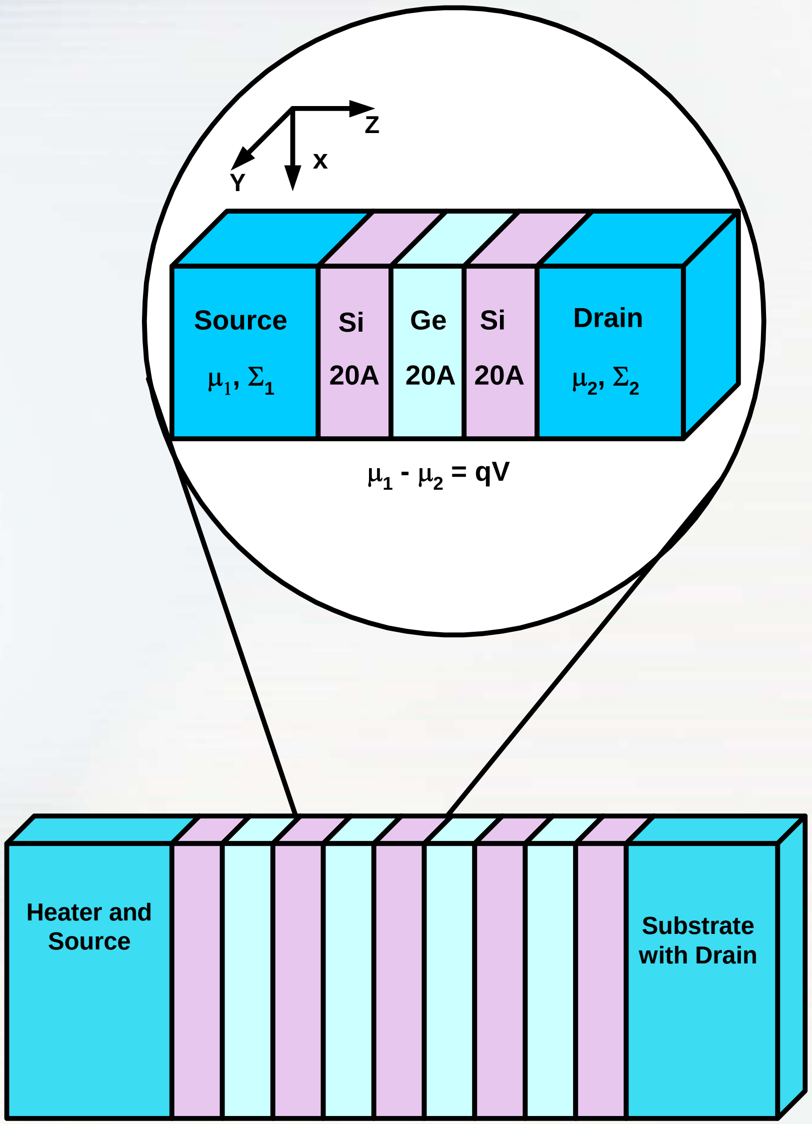



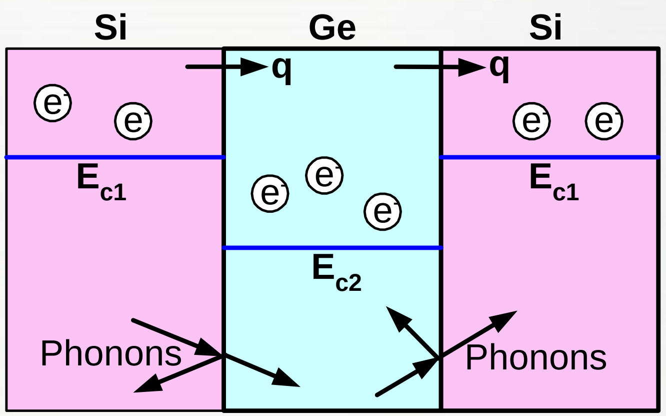

Reduced dimensionality of the nanowire compared to the nanofilm results in

- Higher Seebeck coefficient of the wire.
- Decreased electrical conductivity of wire due to size quantization.



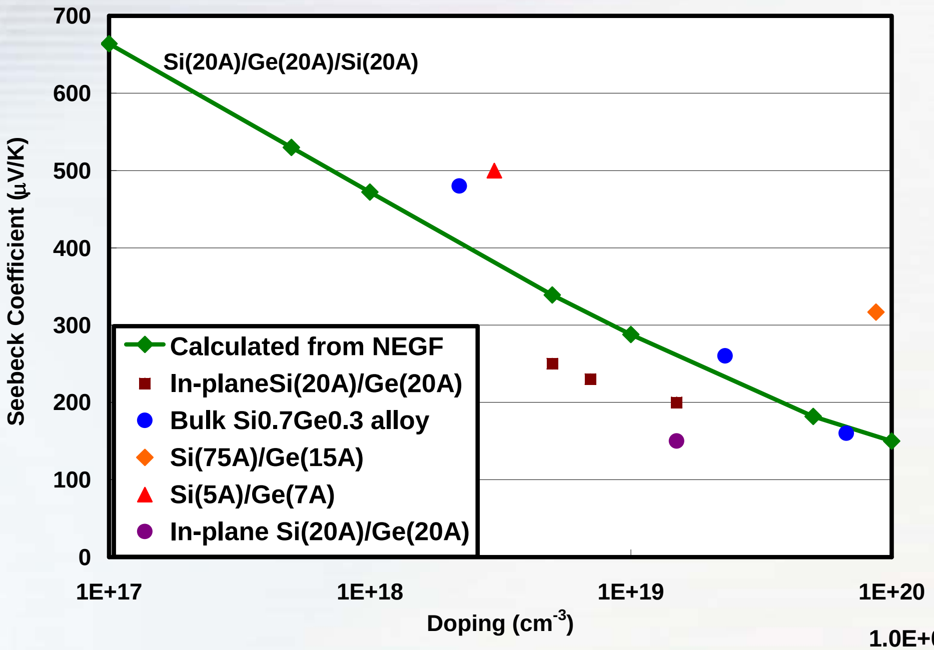
# Si/Ge/Si Quantum Well Superlattice Film




NEGF used to model and study electron-phonon scattering and confinement effects on a single period of Si/Ge/Si superlattice film.

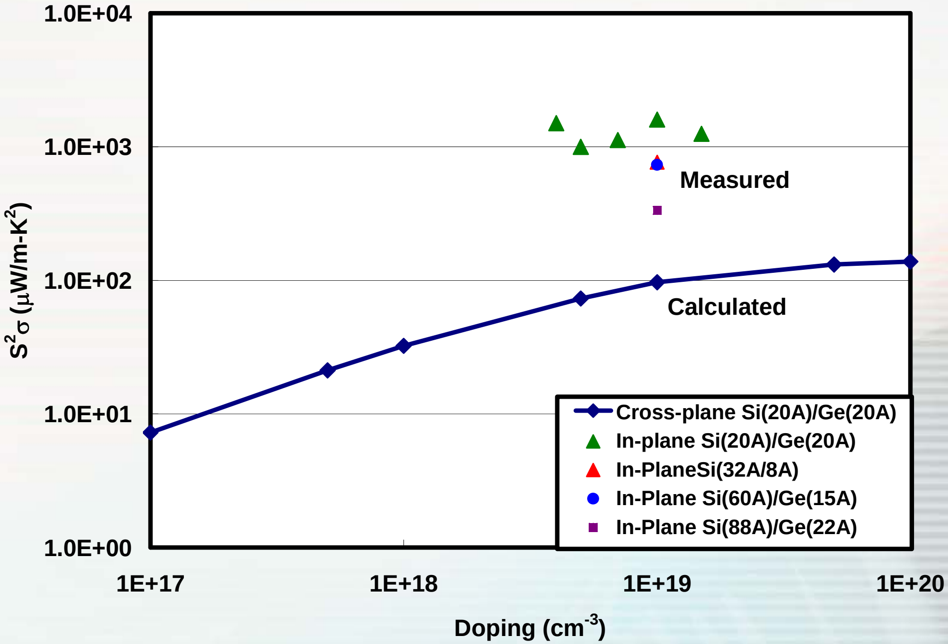
# Thermoelectric Properties of Quantum Well



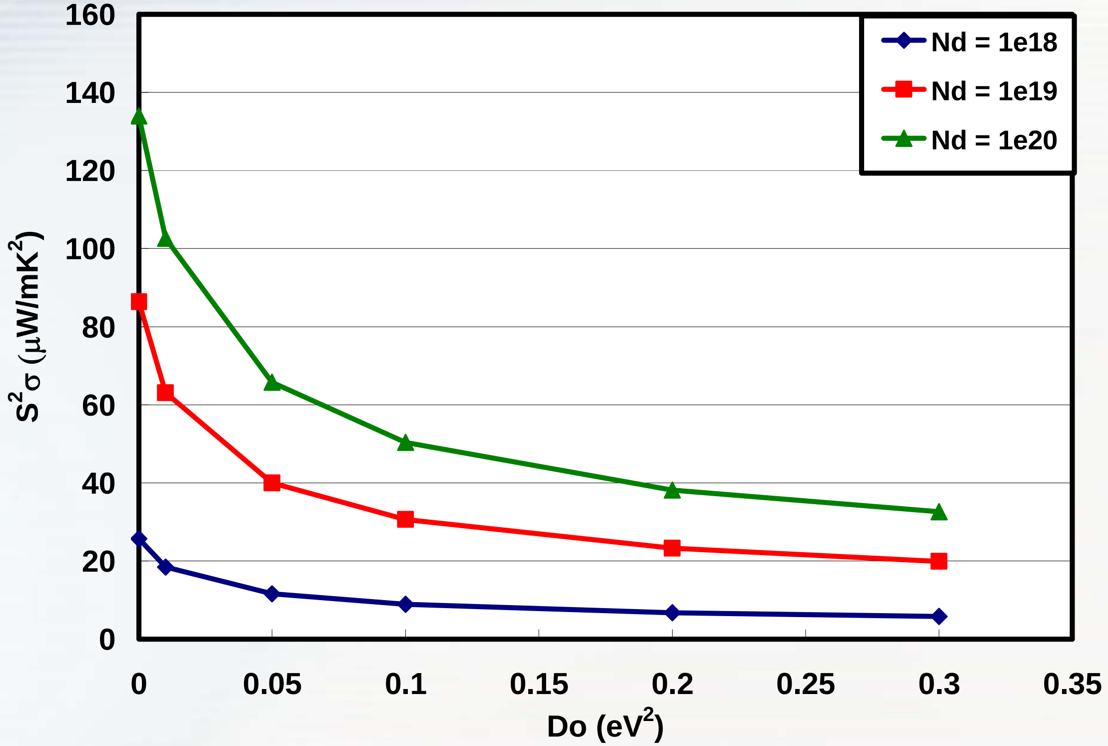

NEGF successfully predicts Seebeck coefficient of Si/Ge/Si quantum well structure.

NEGF calculations performed on single layer of Si/Ge/Si superlattice layer.

Experiments usually carried out on 1200 layers of superlattices on strained substrate.



# Scattering Effects on Power Factor of Superlattice




Near-elastic, phase-breaking, electron-phonon scattering.

Scattering introduces resistance to current flow through momentum redistribution of electrons.

- Scattering and confinement effects dominate over doping effects to decrease electrical conductivity.
- Decrease in electrical conductivity dominates over increase in Seebeck coefficient to reduce net power factor.

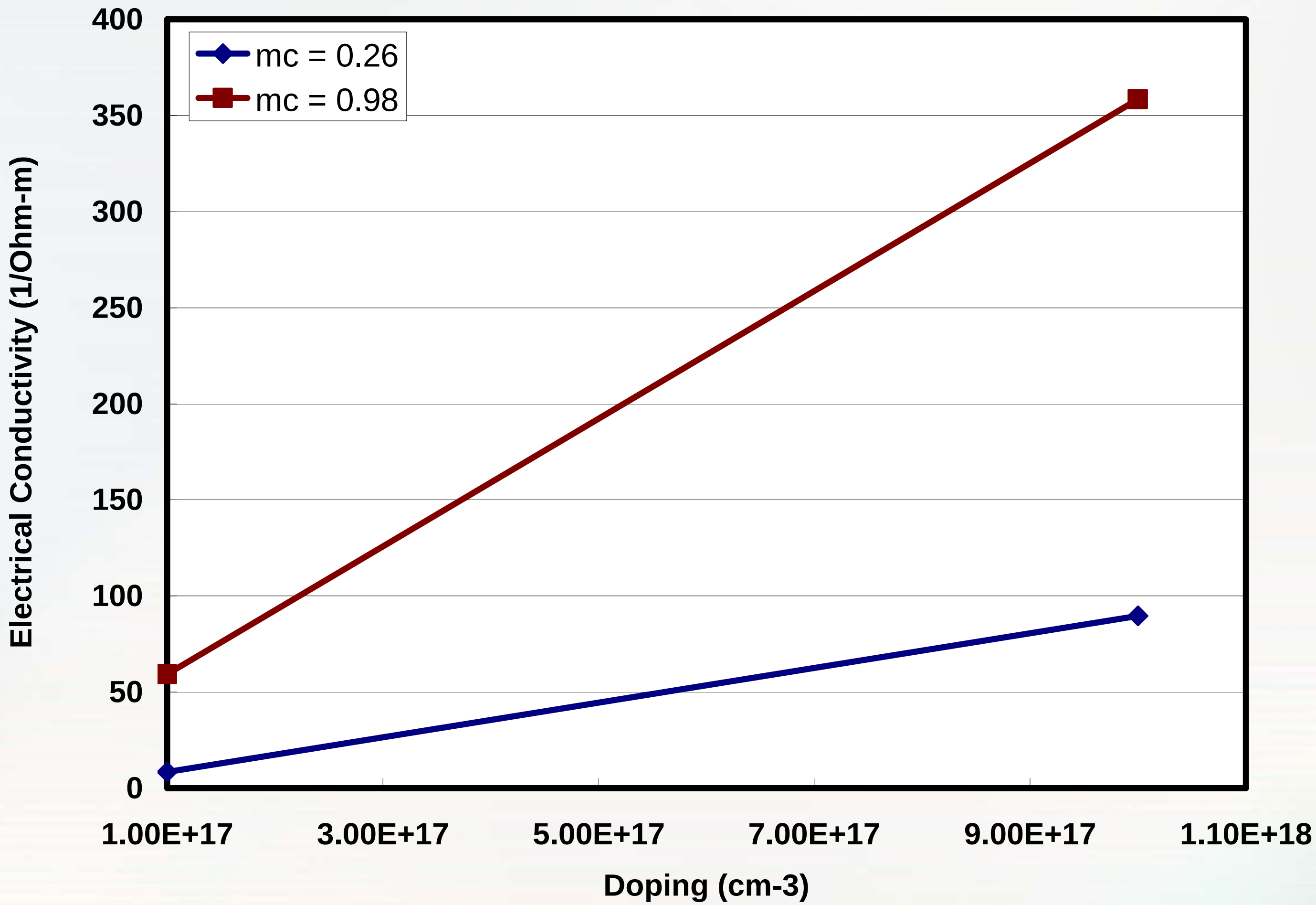
# Conclusions

- NEGF successfully couples quantum confinement effects with scattering effects.
- Confinement of electrons decreases electrical conductivity and increases Seebeck coefficient in films and wires.
- Incoherent electron-phonon scattering introduces resistance to electron transport.
- 28% to 77% decrease in power factor with scattering due to increased electrical resistance.
- Optimal film width has to be chosen when designing thermoelectric structures with electron confinement.

# Acknowledgements

- Prof. Supriyo Datta, Dept. of Electrical and Computing Engineering, Purdue University, West Lafayette, IN.
- Vanderbilt Discovery Grant, VINSE Fellowship and NSF.

# Electrical Conductivity of Silicon Thin Films with Varying Effective Mass



# Non-Equilibrium Green's Function Formalism

Modified wave equation with self-energy terms

$$\left(H + U + \Sigma_1 + \Sigma_2 + \Sigma_s\right)\psi_\alpha(\vec{r}) = \varepsilon_\alpha \psi_\alpha(\vec{r})$$

Green's function

$$G(E) = \left[\left(E - i0^+\right)I - H - \Sigma_1 - \Sigma_2 - \Sigma_s\right]^{-1}$$

Spectral function

$$\frac{A(E)}{2\pi} = D(E) = i\left(G(E) - G^+(E)\right)$$

Device Current

$$I_i = f\left(A_i, G^n\right)$$

where $G^n$ is the density matrix.