EPSRC Thermoelectric Network UK Meeting, Feb. 2017

Electronic transport simulations for TE power factor in nanostructures

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General description of our group’s work

Theoretical investigations of:

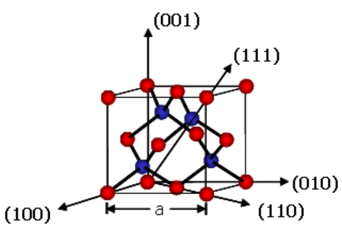
- **electronic**
- **thermal**
- **thermoelectric properties**

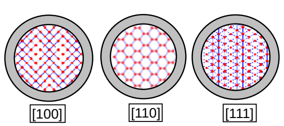
in nanoscale materials and devices

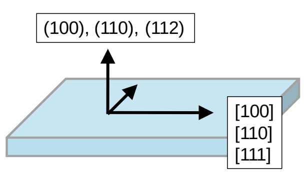
Approach - Tools

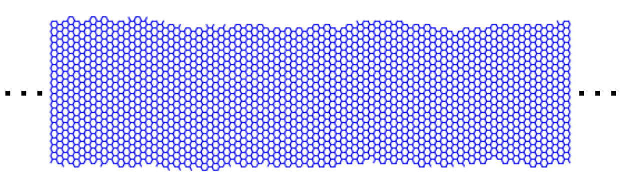
Electronic structure (atomistic to continuum)

1) Tight-binding ($sp^3d^5s^*$)
2) Valence Force Fields
3) Force Constants
4) Effective mass approx.
5) Etc…





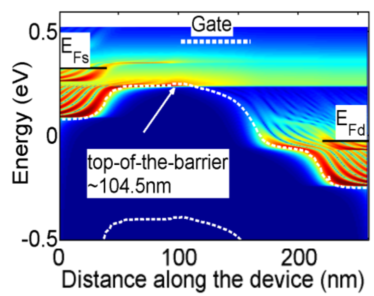


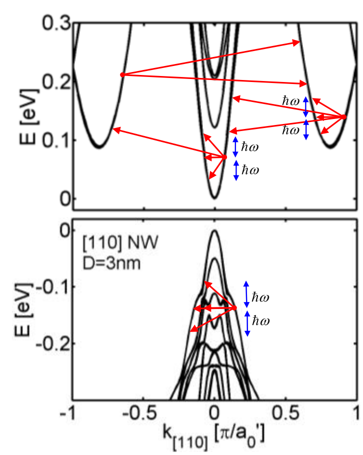


graphene nanoribbon

Transport (ballistic to diffusive)

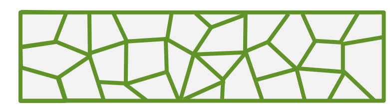
1) Quantum mechanical (NEGF)
2) Semiclassical – L. Boltzmann
3) Monte Carlo
4) Landauer formalism

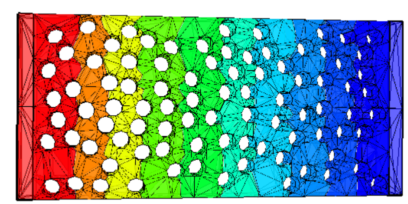


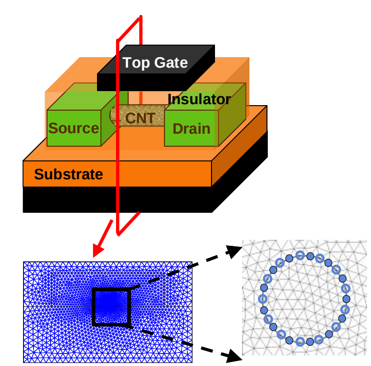


Geometries (1D-3D, non-uniform)

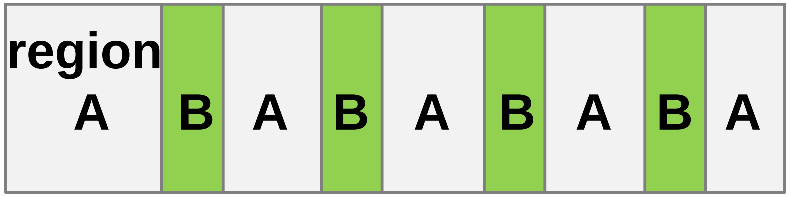
1) 3D geometry solvers
2) Nanocrystallines
3) Nanomeshes
4) Low-dimensional



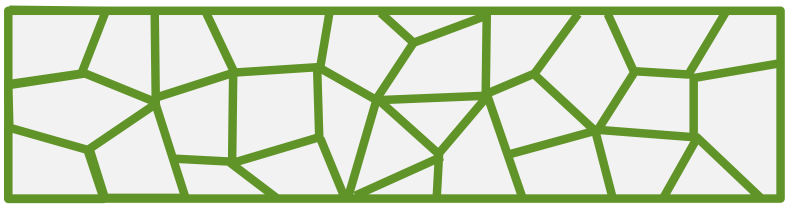




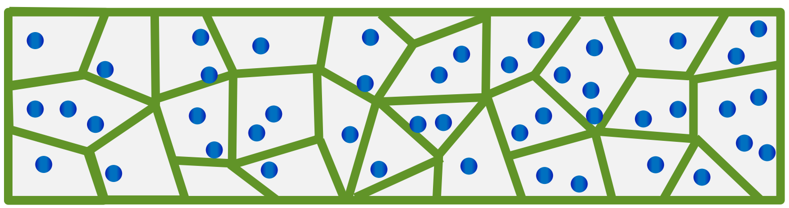
Motivation - Very high thermoelectric power factors



Superlattices

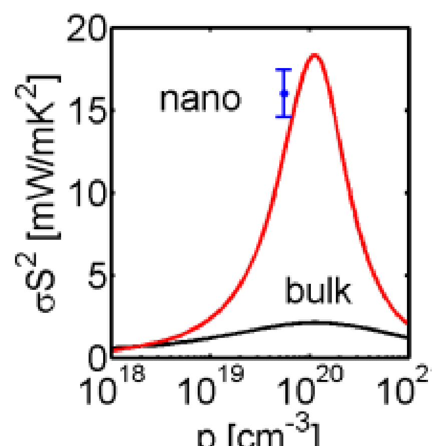


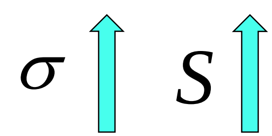
Nanocrystalline materials



Multi-phase nanocomposites

<u>Very high PF:</u>
2-phase materials: 15 mW/K^{2}m^{-1}
3-phase materials: 22 mW/K^{2}m^{-1}
(~7x compared to bulk Si)





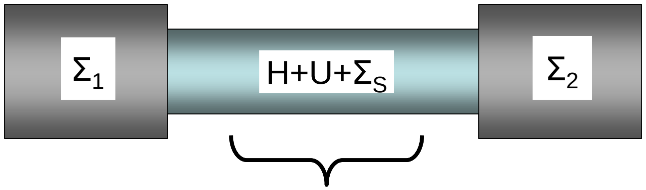
Simultaneous improvement in σ and S

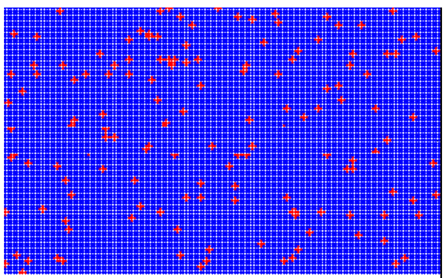
Neophytou *et* al., Nanotechnology 2013,
Lorenzi *et* al, J. Electronic Materials 2014

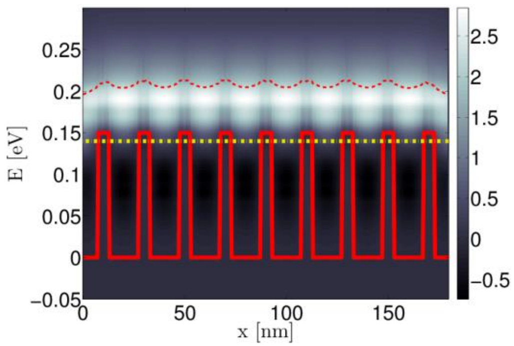
Outline

- Non-Equilibrium Green's Function (NEGF):
  - Method
  - Example 1: Influence of variations in SLs
  - Example 2: Filtering in 1D vs 2D
  - Example 3: Nanocomposites
- Monte Carlo semiclassical simulator development:
  - Method
  - Self-consistency
  - Scaling to large geometries
  - Inclusion of quantum effects
- Conclusions

Non-Equilibrium Green's Function (NEGF)







nano-inclusions

superlattices

- Very powerful approach
- Can include scattering (decoherence)
- Can be computationally very expensive
- Captures the exact geometry and disorder

- Device Green's function:

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

- Transmission:

$$T(E) = Trace(\Gamma_1 G \Gamma_2 G^+)$$

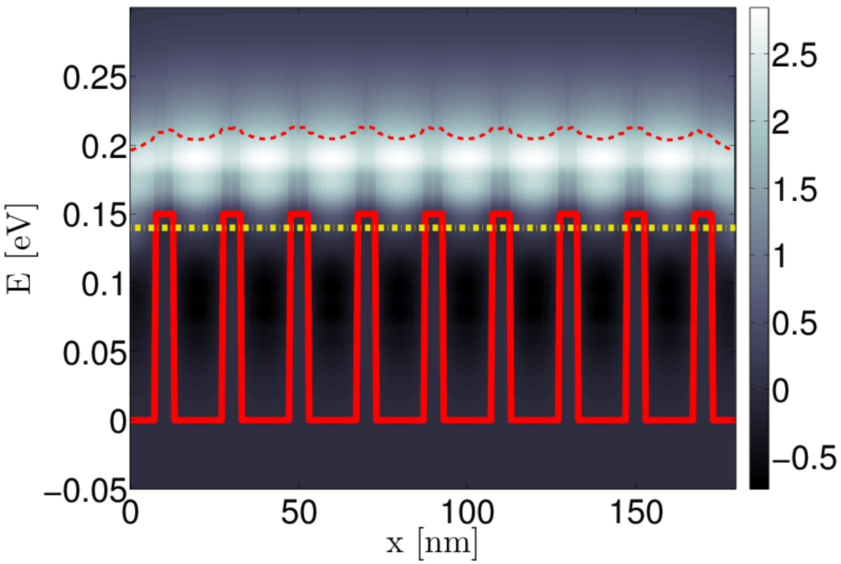
- TE coefficients:

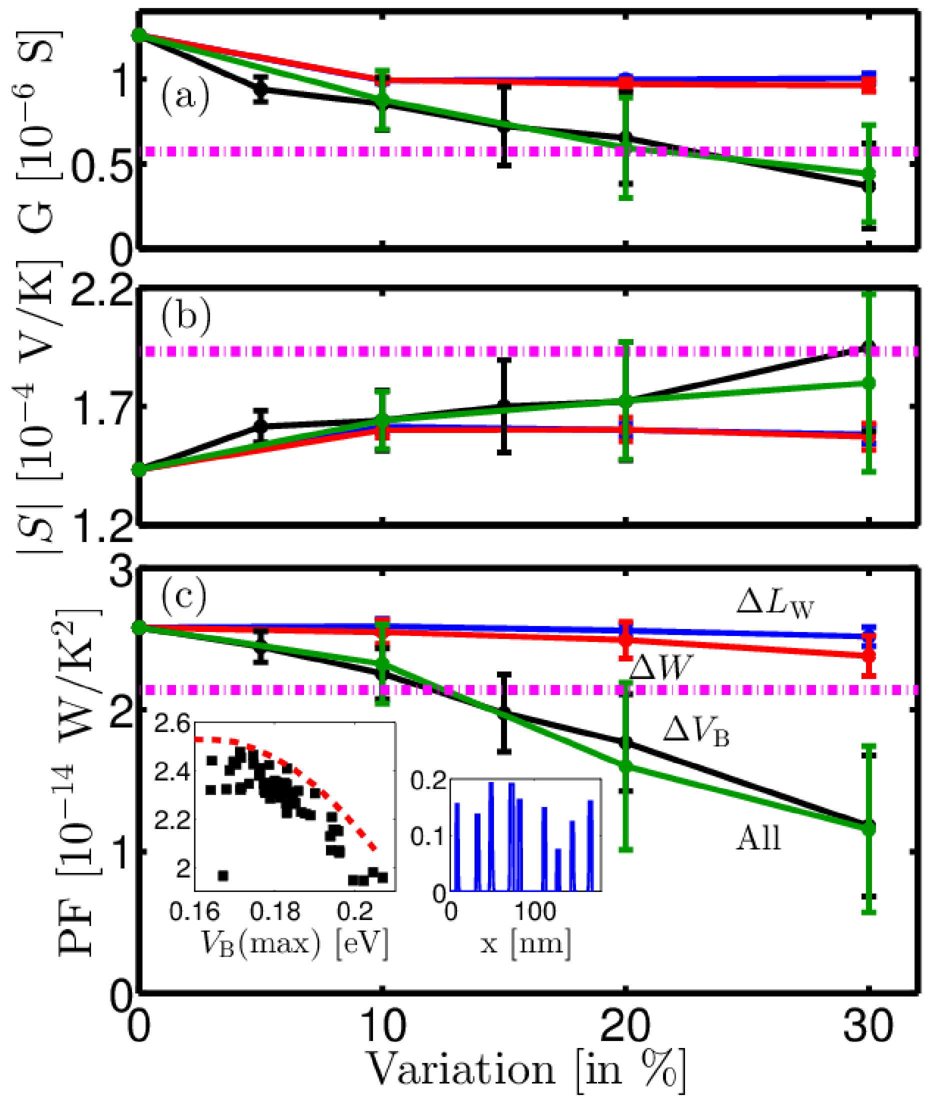
$$I^{(j)} = \int_{-\infty}^{+\infty} \left(\frac{E - E_F}{k_B T} \right)^j T(E) \left(-\frac{\partial f}{\partial E} \right) dE$$

$$G = \left(\frac{2q^2}{h} \right) I^{(0)} \qquad [1/\Omega]$$

$$S = \left(-\frac{k_B}{q} \right) \frac{I^{(1)}}{I^{(0)}} \qquad [V/K]$$

Example 1a: Variation study in superlattices

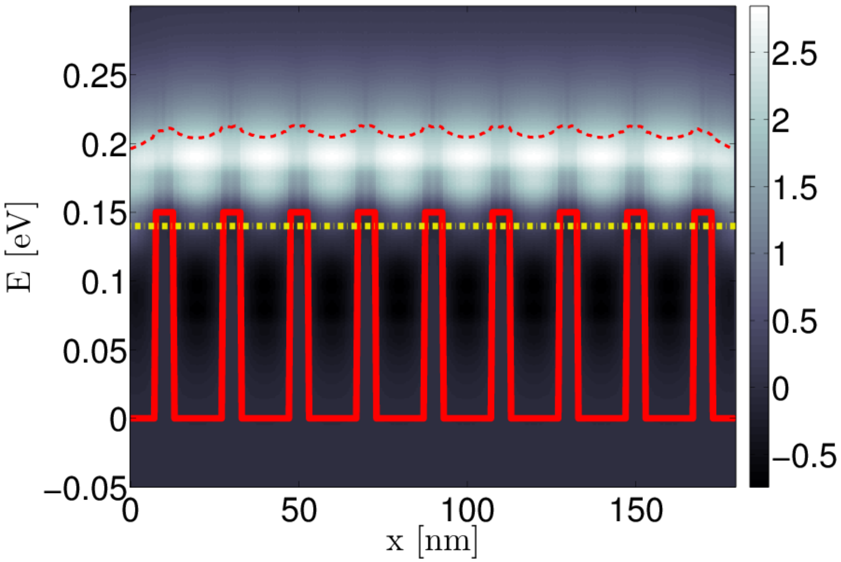


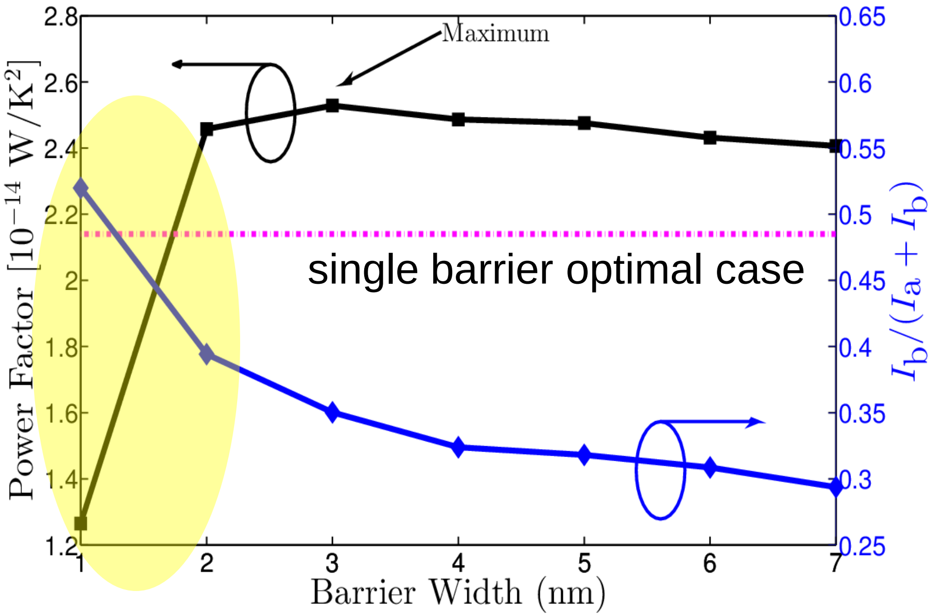


(1) *Variation in V_B reduces PF*

(2) Variations in wells size, barrier width do not affect the PF

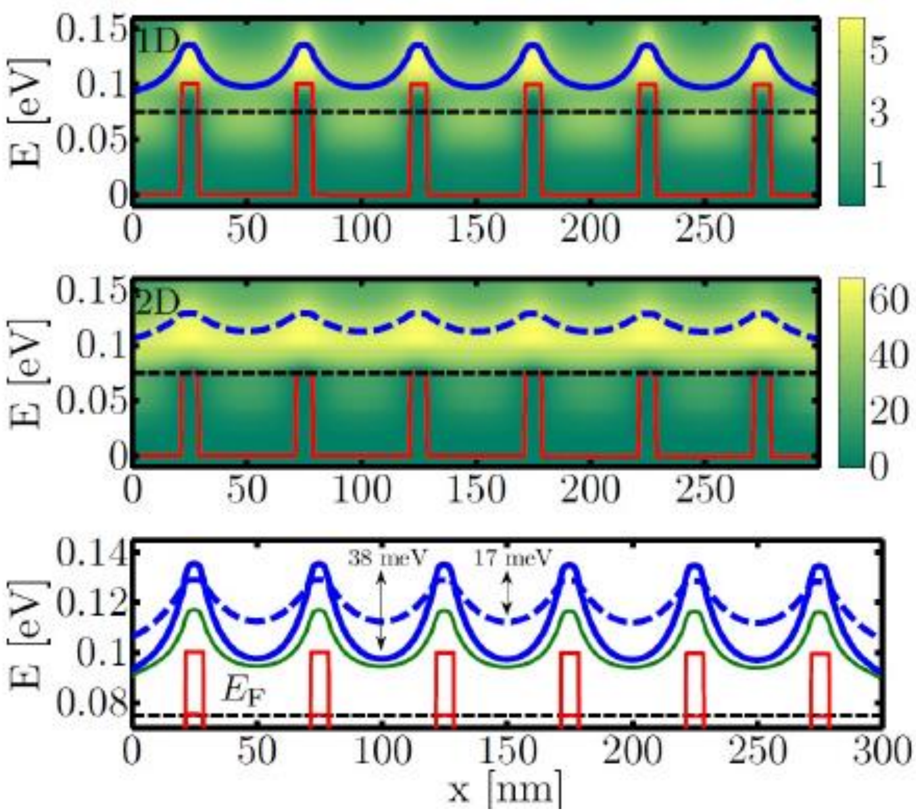
Example 1: Detrimental effect of tunneling





Quantum tunneling is detrimental to S and to the PF

Example 2: Filtering in 1D vs 2D



1D Superlattice

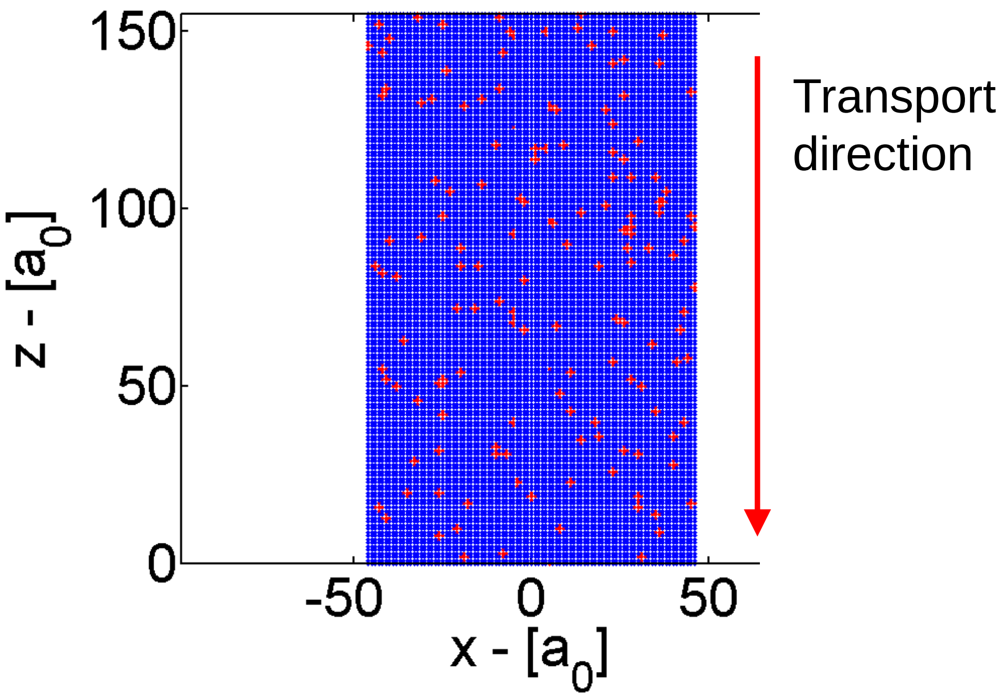
2D Superlattice

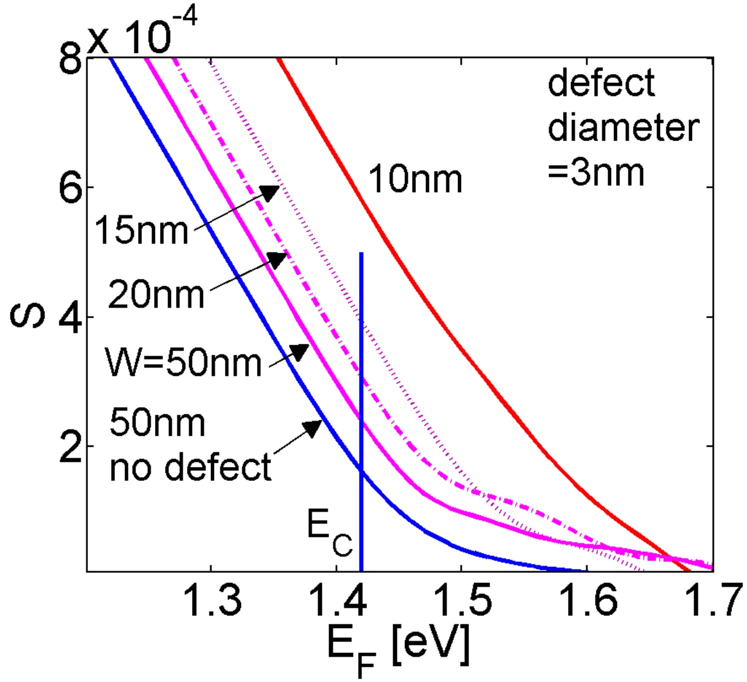
(1) Variation in energy of current is larger in 1D

(2) 1D Utilizes S of barriers and σ of wells better

(3) 1D Utilizes energy filtering more effectively

Example 3: Nanocomposites – increase in *S*





Red spots: nano-inclusions
(here they are barriers of Vb=0.3eV)
Blue region: channel

(1) Nano-inclusions improve *S*
(2) As the domain size decreases, the increase in *S* is larger

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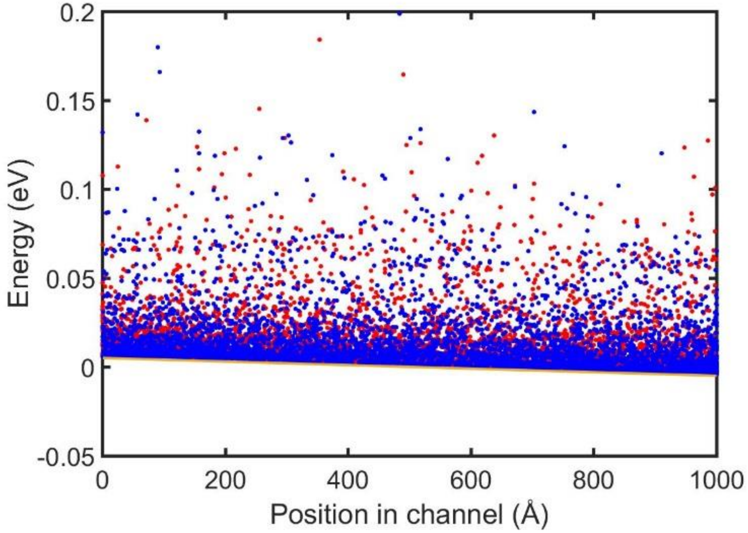
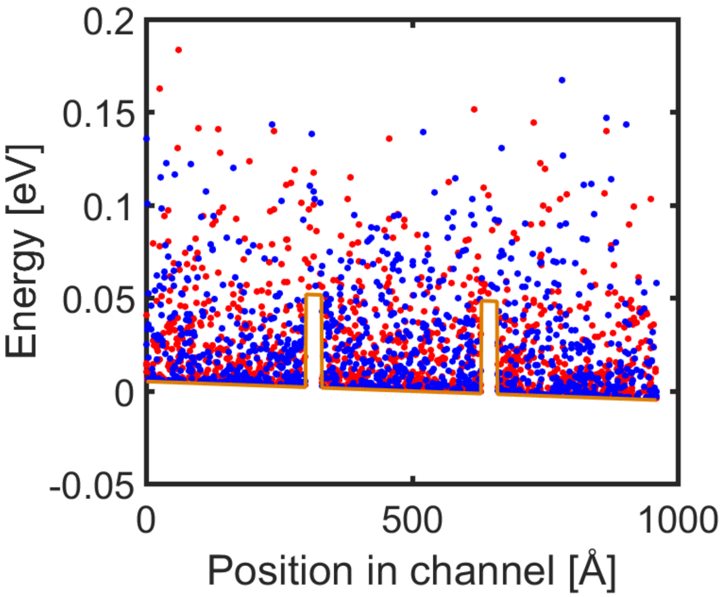
Monte Carlo method





Uniform channel

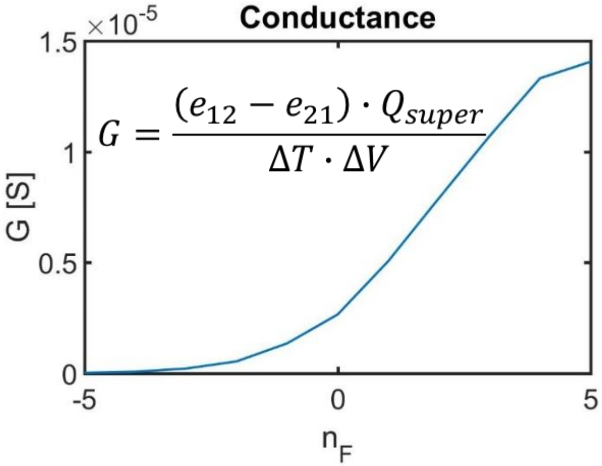
Superlattice

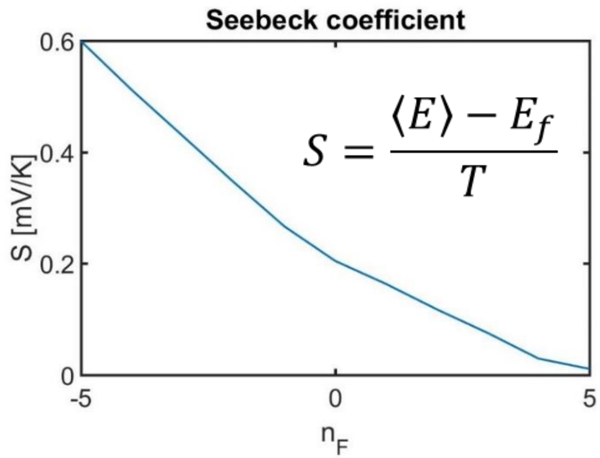
- Electrons distributed in the channel according to the Fermi distribution and the Density of States

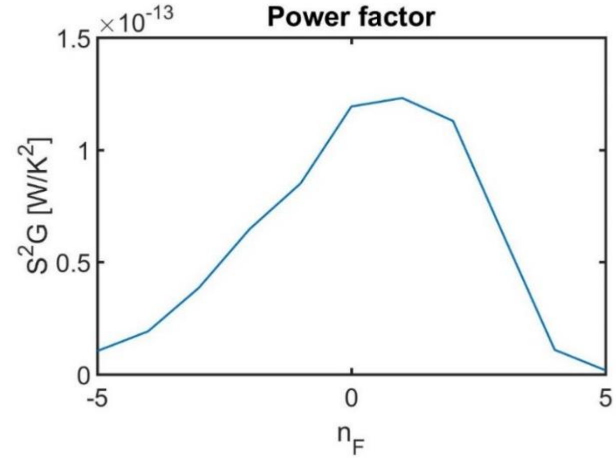
- Allowed to disperse under the influence of the potential

- Scattering by acoustic and optical phonons, ionized impurities, etc.

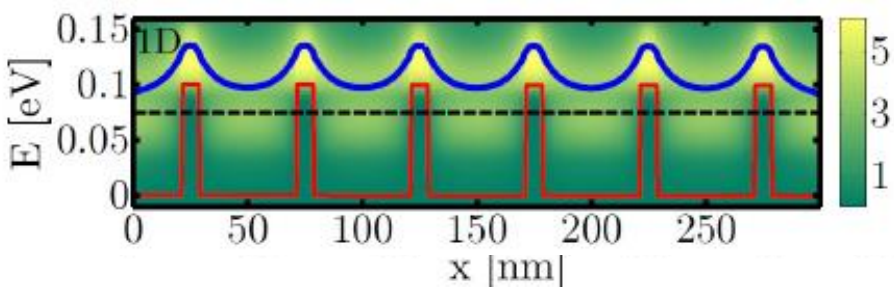
Thermoelectric coefficients from MC



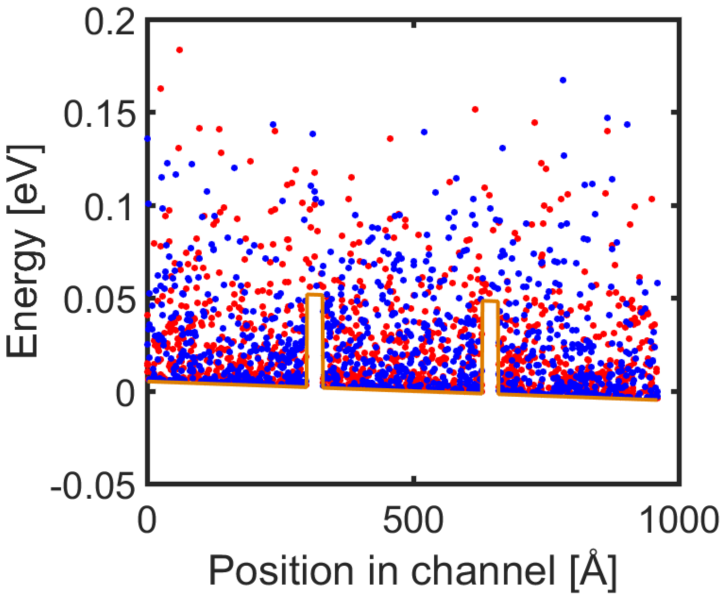


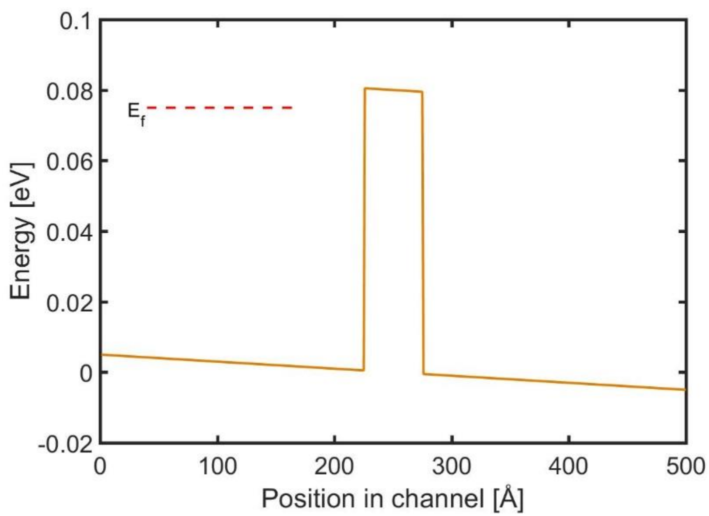


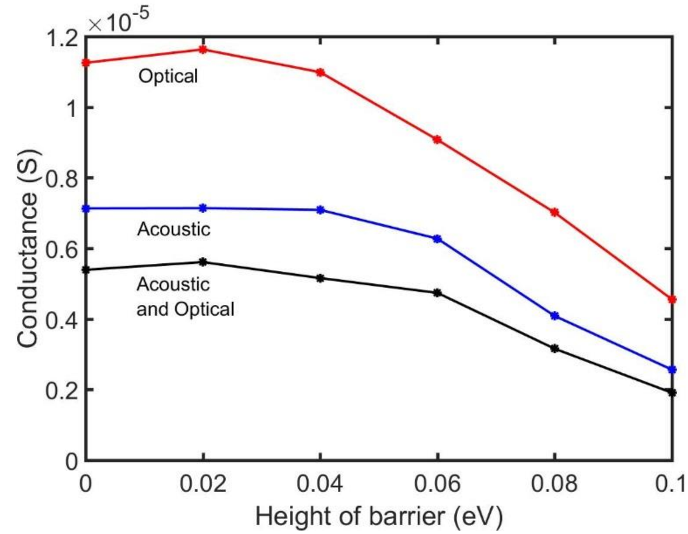
1. Calculate the average energy of the current
2. $S = \frac{-I_{\Delta T} \cdot \Delta V}{I_{\Delta V} \cdot \Delta T}$ for arbitrary ΔV and ΔT
3. $S = \frac{-\Delta V}{\Delta T}$ for $I_{\Delta T} = I_{\Delta V}$



Simulations of superlattices in MC

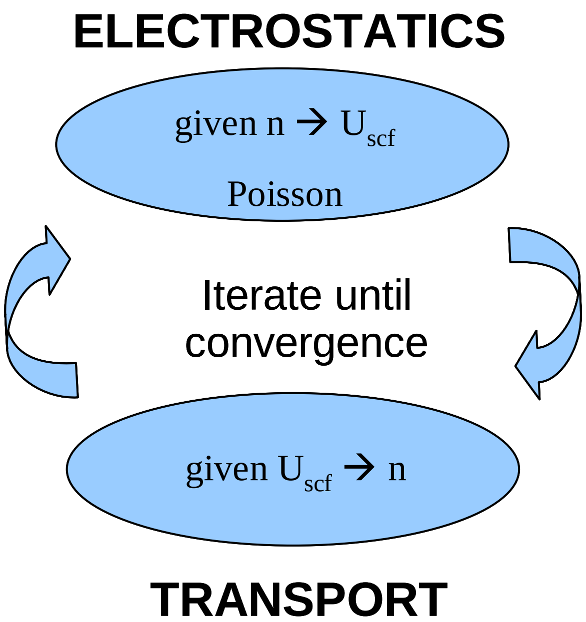


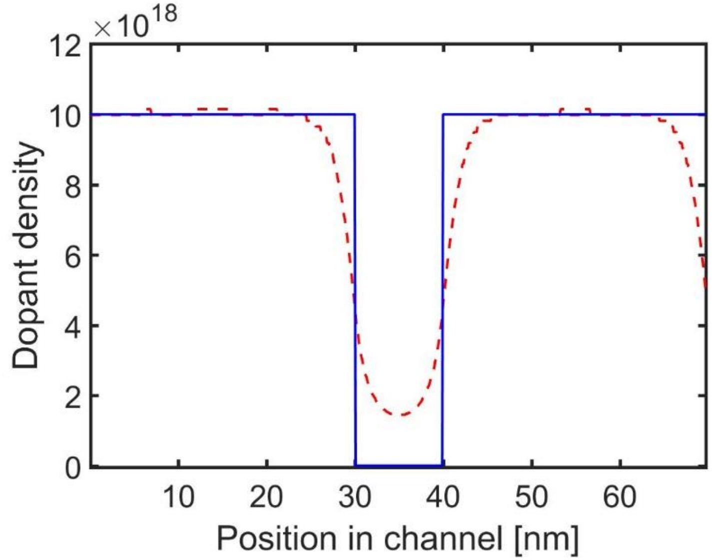


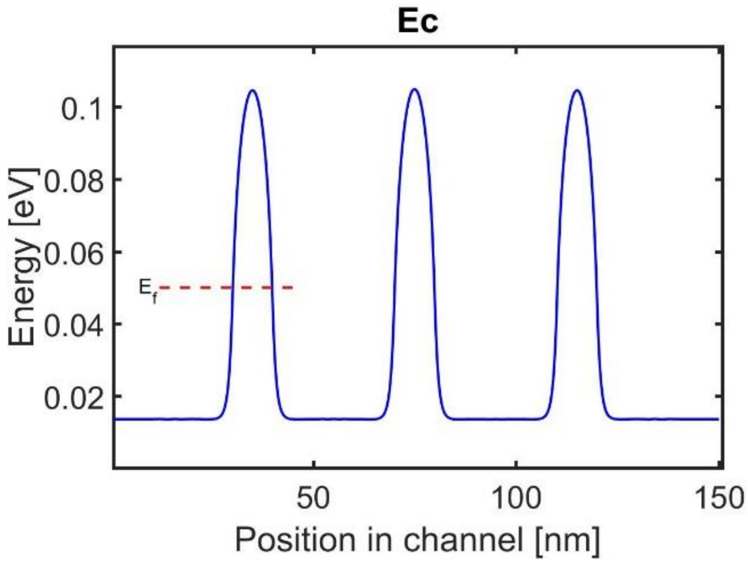


- Include all relevant scattering parameters (next Ionised Impurities)

Include self-consistent electrostatics

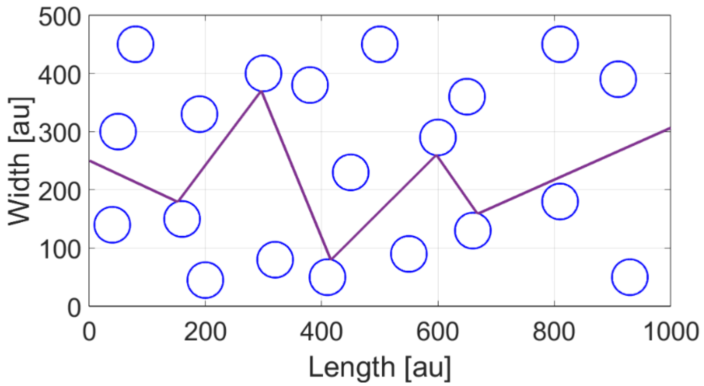


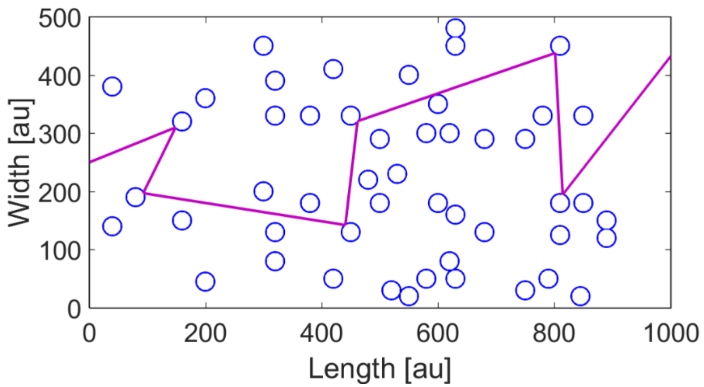


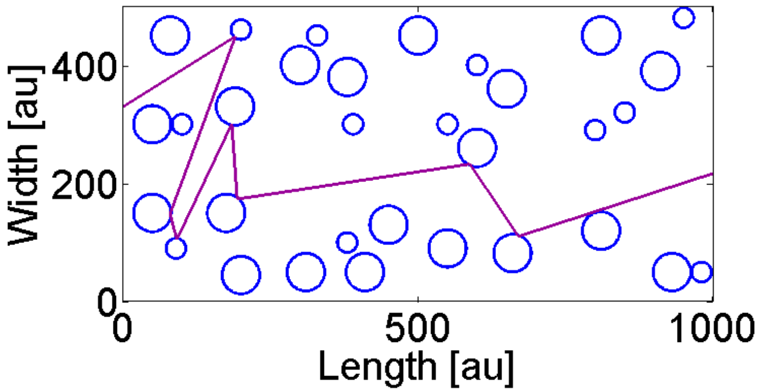


- Obtain the actual potential profile for specific doping distributions

Extension to 2D

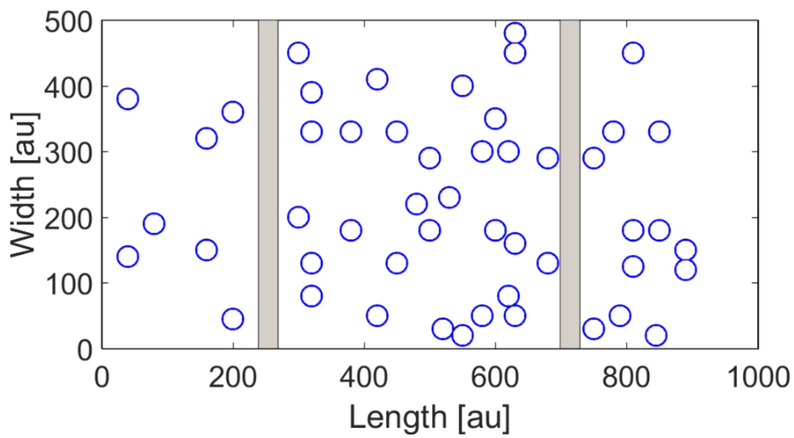


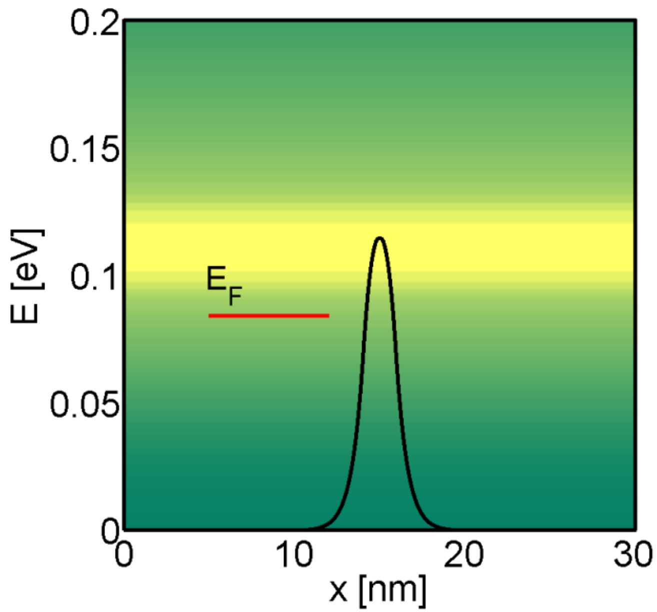




- Extend to larger geometries, where NEGF cannot reach
- Envision 100nm x 1000nm domains
- Nano-inclusions of various sizes
- Extend to nano-inclusions, grain boundaries dislocations, etc.
- *Electron AND phonon transport*

Incorporate quantum tunneling





Effect of tunnelling through a barrier

- Incorporate quantum tunneling
- Basic idea:
  - Solve 1D NEGF for simplified cases
  - Provide a probalitity of going through the barrier when an electron reaches a barrier in MC

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Conclusions

- Techniques for electronic transport in nanocomposites

- Quantum mechanical (NEGF)
- Semiclassical Monte Carlo

- Extend to large geometries
- Perform realistic simulations
- Incorporate all important transport effects

Acknowledgements:

Mischa Thesberg, Hans Kosina (TU Vienna group),
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FFG FWF SEVENTH FRAMEWORK PROGRAMME HORIZON 2020 erc

ERC StG: NANOthermMA