Electronic transport simulations for nanostructured TE materials

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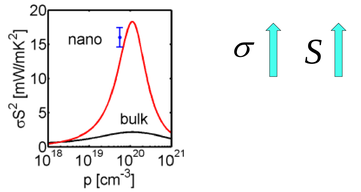
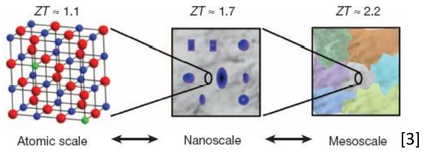
1 Motivation

- Nanostructures have shown large improvements in power factor[1][2]



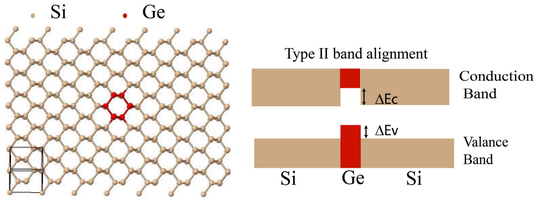
$\sigma \uparrow \quad S \uparrow$

Very high PF:
2-phase materials: 15 mW/K²m⁻¹
3-phase materials: 22 mW/K²m⁻¹
(~7x compared to bulk Si)



2 Methods – bands

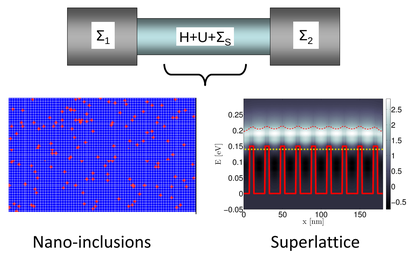
- DFT



- Ab-initio, many-body quantum approach
- Barrier shape and dimensions depend on lattice growth direction, strain etc.
- Calculated band structure then used extracted parameters in continuum codes

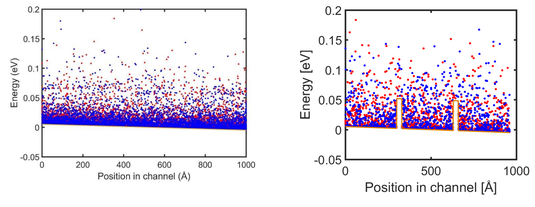
2 Methods – transport

- NEGF

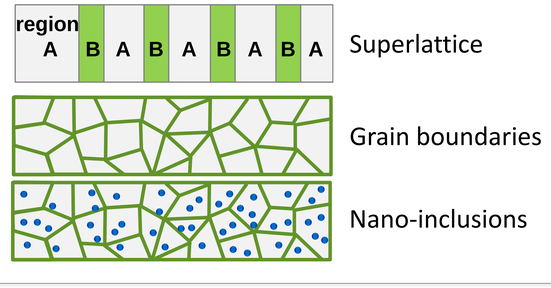


- Fully quantum mechanical approach[4]
- Can include scattering
- Captures exact geometry and disorder
- But, computationally expensive

- Monte Carlo

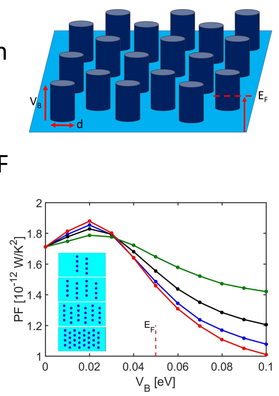


- Semi-classical method[5]
- Electrons distributed in the channel and allowed to disperse
- Scattering mechanisms and potential in the channel considered

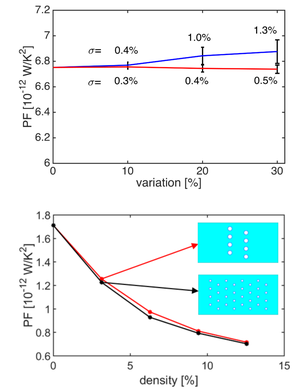


3 Results

- NEGF simulations of 2D channels with nanoinclusions
- Only small improvements in PF possible (unlike in superlattices)
- With correct band offset, PF is independent of NI density

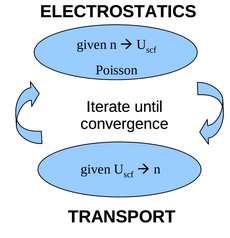


- Limited impact from random variations
- NEGF simulations of 2D channels with voids
- PF independent of geometry
- Dependent only on void density

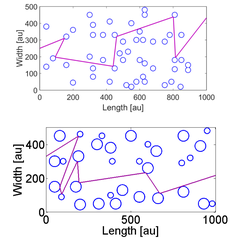


4 Further work

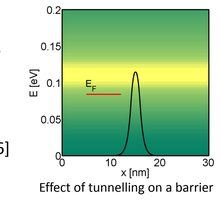
- Self-consistent Poisson
  - Obtain the actual potential profile from specific doping distributions



- 2D Monte Carlo



- Quantum tunnelling
  - Provide a probability for electrons seeing the barrier in MC[6]



Effect of tunnelling on a barrier

5 Conclusion

- Nanostructures have the potential to improve thermoelectric performance.
- Such materials can be modelled using a variety of simulation methods.
- We aim to provide guidance on the design of future nanoscale thermoelectric devices.

References:

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