Nanostructured semiconductors as thermoelectrics

- **thermoelectric figure-of-merit** *ZT* describes maximum efficiency attainable by a thermoelectric converter

$$ZT = \frac{\sigma S^2}{\kappa_{\rm el} + \kappa_{\rm ph}} T$$

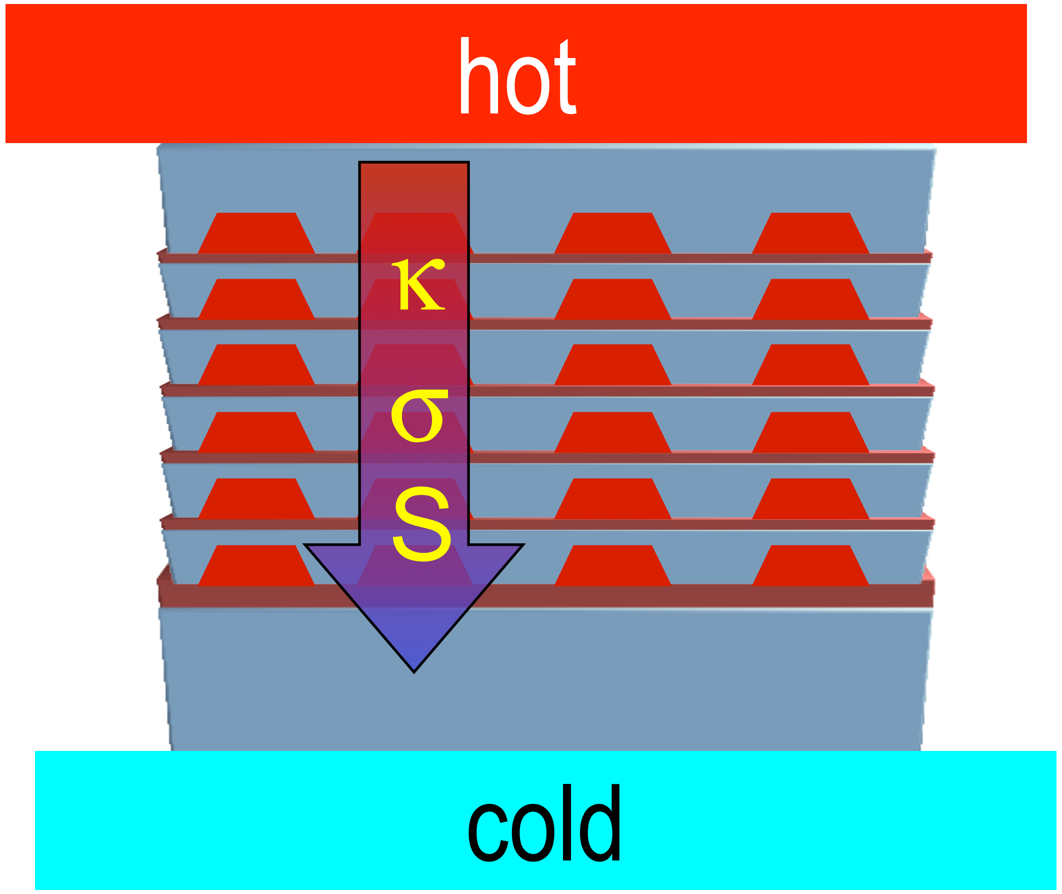
  - σ electrical conductivity
  - S Seebeck coefficient (thermo power)
  - $\kappa_{el/ph}$ electronic / phononic contribution to thermal conductivity

- Heterostructures enable small κ_{ph} due to phonon reflection at interfaces

- electric transport should be iso-entropic, i.e. should proceed in narrow isolated bands

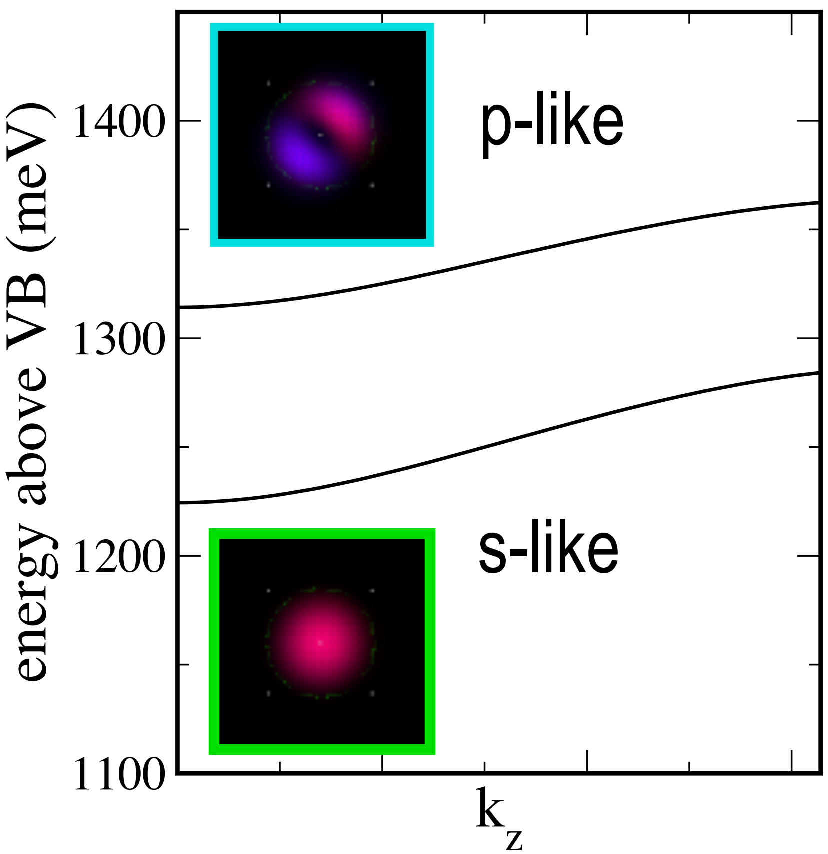
  [Mahan & Sofo, PNAS **93**, 7436 (1996)]

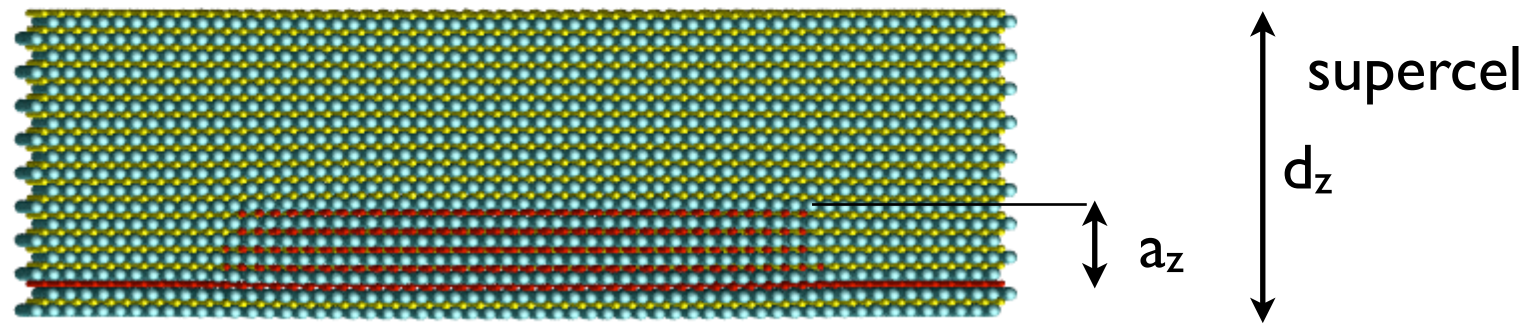
  ⇒ miniband transport



Prediction for a stack of InAs/GaAs quantum dots

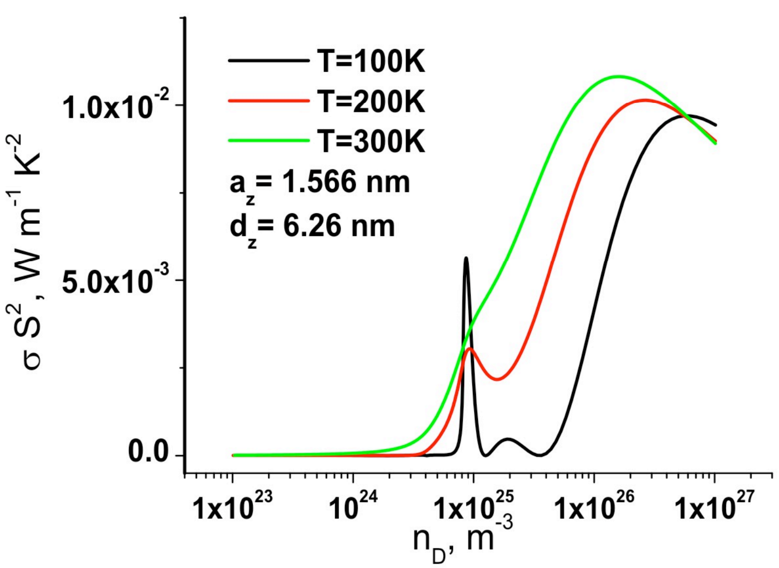
- atomistic description of strain and tight-binding wavefunctions
- QD energy levels are broadened to minibands due to tunneling

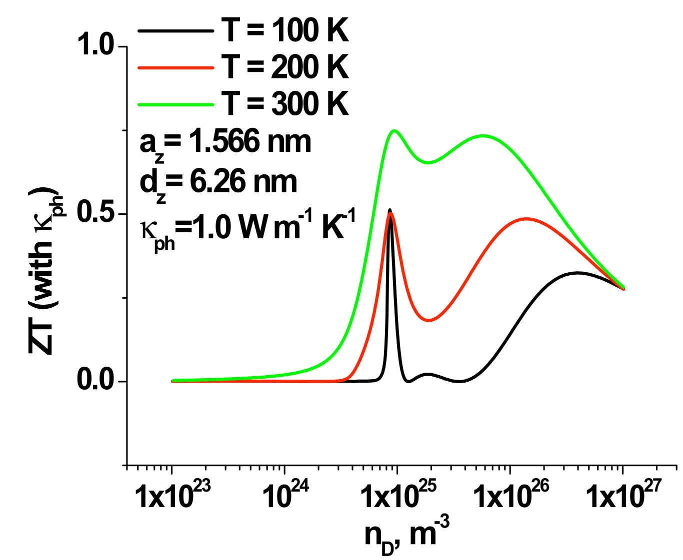




- Boltzmann transport equation in minibands & host
- doping concentration n_D, allows us to tune the Fermi energy into a miniband

A QD stack exemplifies a system whose efficiency as a thermoelectric converter is controlled by its architecture on the nanoscale.





V. M. Fomin and P. Kratzer, Phys. Rev. B **82**, 045318 (2010)