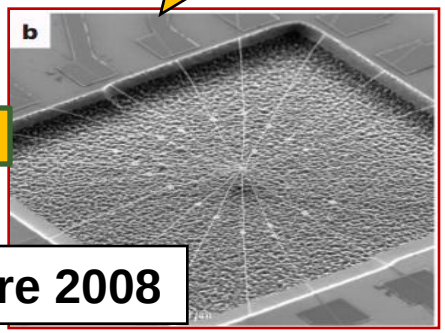
# Atomistic modeling of thermoelectric power factor in Si Nanowires -- Abhijeet Paul & Gerhard Klimeck

**Objective:** Atomistic effects on Themo-electric Power-Factor (PF) design in **ultra-scaled SiNWs**.

**ZT ~1.0 @ T=200K**




**Boukai et. al. Nature 2008**

## Approach:

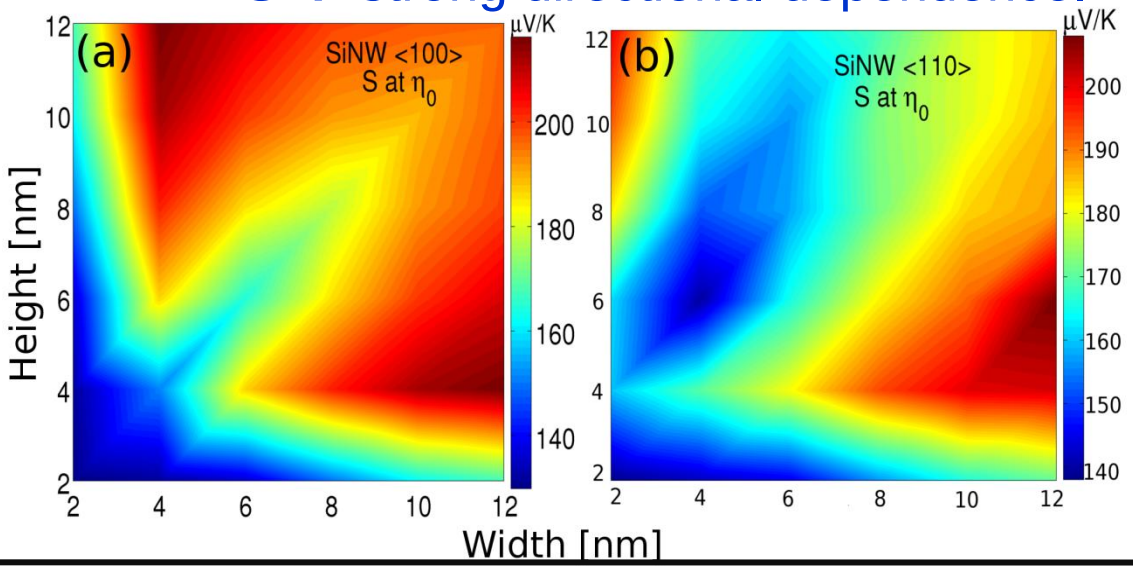
**E(k)** → Atomistic $sp^3d^5s^*$ basis includes
- Crystal symmetry
- Valley coupling.

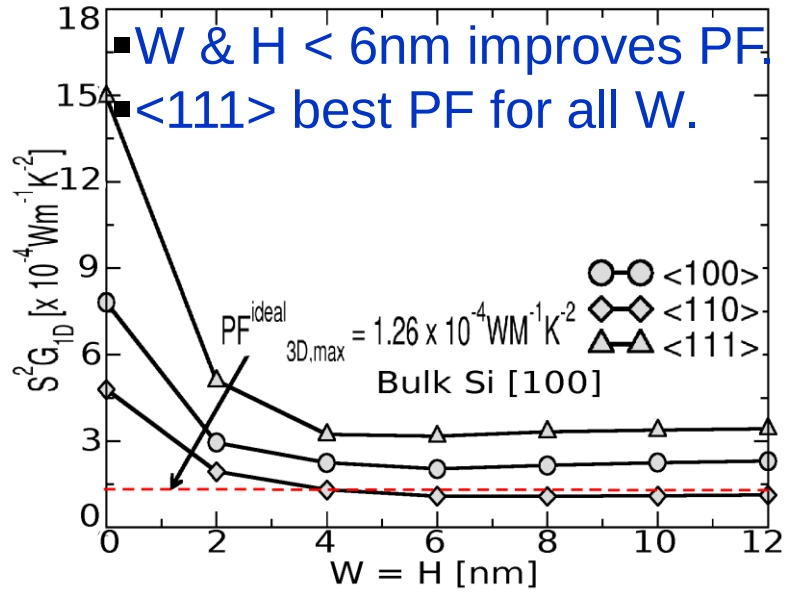
**Seebeck (S) and Conductance (G)** →
- Landauer's Method.

$$PF = S^2G$$

**Consider [100], [110], [111] SiNWs.**

## Results : S → strong directional dependence.




 Impact: IEEE SNW, 2010 doi: 10.1109/SNW.2010.5562583