

Objective: Application of Modified VFF for phonon modeling in free-standing Si nanowires.

High I_{ON}
SOI finFETs

High ZT
Thermoelectricity

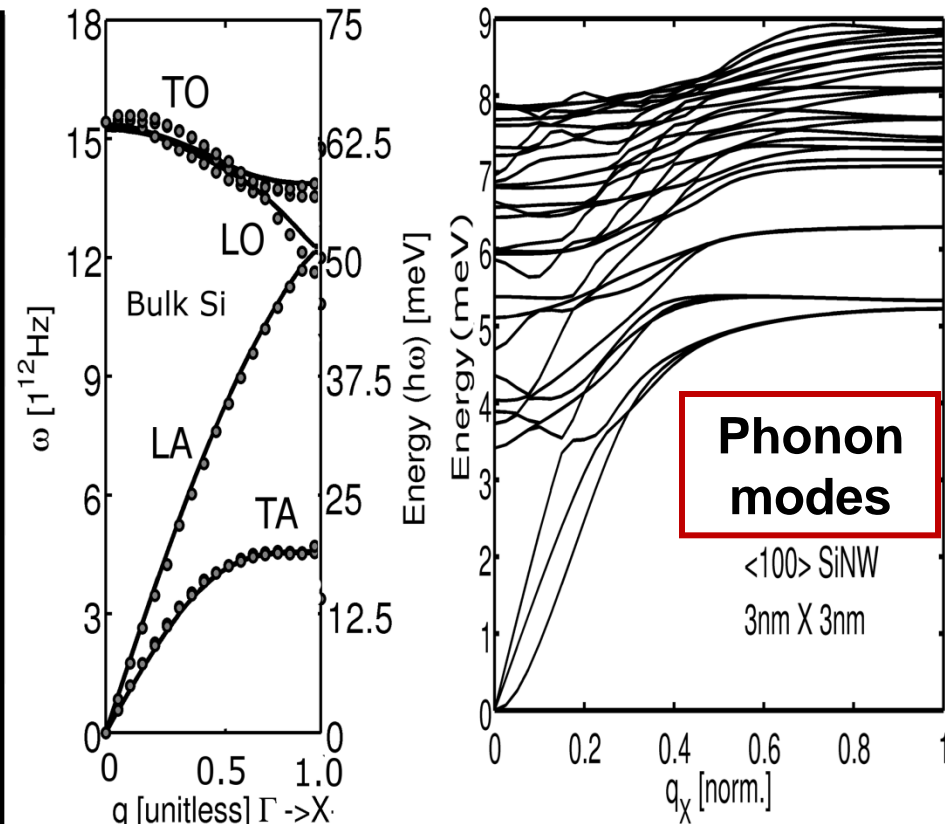
Approach: Modified VFF \rightarrow potential energy (U) \rightarrow Dynamical matrix + boundary conditions \rightarrow Phonons.

$$U_{MVFF} = U_{bb} + U_{bs} + U_{bb-bb} + U_{bb-bs} + U_{bs-bs}$$

bb = bond-bending

bs = bond stretching

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Results:

1. Bulk and wire modes very different.
2. New modes of vibration in SiNW..
3. $V_{sound} (NW) < V_{sound} (bulk)$.
4. Thermal conductance inc. with wire cross-section.