First-principles Informed Analysis of Thermal and Electrothermal Transport

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Objectives

- New thermoelectric materials and structures are being developed toward higher ZT.
- Device level performance, however, can be significantly lower than that predicted from atomic models.
- A TE device simulation must capture correctly all the physics in a full 3D device.

LanTraP 2.0

Overview

1. Bandstructure calculations (DFT)
2. DOS & DOM
3. Device-level simulation
4. Circuit-level simulation

TE material analysis

DC performance

Status and Plans

Summary:
- Capability for full, numerical simulation of realistic 3D TE devices is ready.
- Physics-based SPICE model produces essentially identical results.
- Sentaurus informed by first principles + SPICE informed by Sentaurus provide the tools needed.

Plan:
- Benchmark with experimental device performance
- Coupling to characterization techniques