Thermoelectric effects of structural defects in scandium nitride nanostructures

Presented by:
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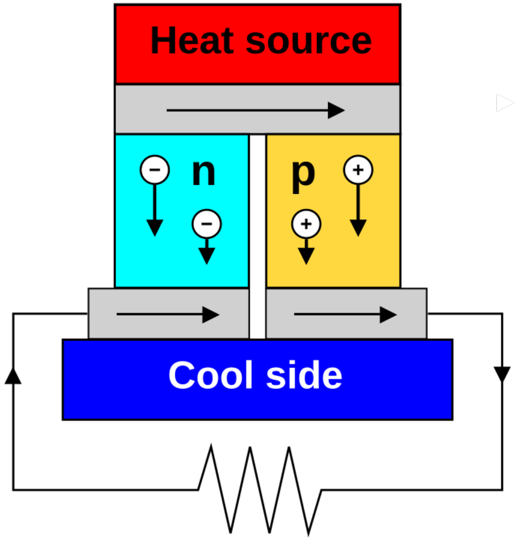
Why we want to study thermoelectricity?

With current technologies, it is estimated that 72% of the total energy converted from primary sources is not transformed into useful work, but is instead dissipated during transport or final use.

Primarily into waste heat.

Forman et al., *Renewable and Sustainable Energy Reviews* 57 (2016): 1568-1579.

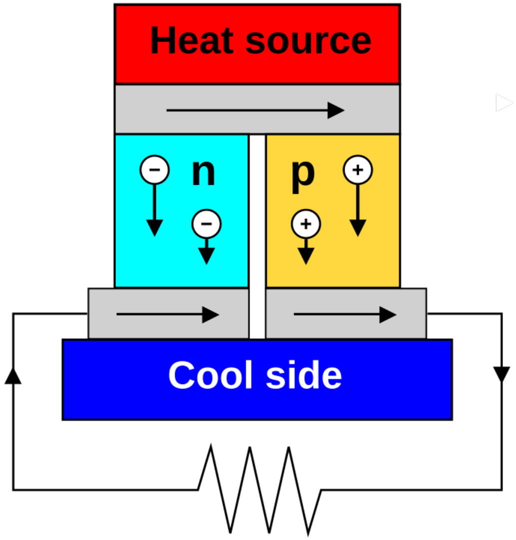


What is thermoelecticity?

It is the direct conversion between heat and electricity:

- Seebeck effect (generation of voltage from a temperature gradient)
- Peltier effect (heat absorption/release with electric current)
- Thomson effect (thermoelectric currents)

Thermoelectric figure of merit



$$ZT = \frac{S^2 \sigma T}{\kappa}$$

Good thermoelectric materials:

High Seebeck coefficient

High electrical conductivity

Low thermal conductivity

For technological applications — waste heat recovery — the following benchmarks are typically considered:

- ZT ≥ 1 is the minimum threshold for a marginally useful application.
- ZT ≥ 2 is a desirable target for significant energy recovery.
- ZT ≥ 3 would be excellent and competitive with conventional conversion technologies.

Material	Max ZT (~)	Thermal Stability	Toxicity	Microelectronics Compatibility	Notes
Bi_2Te_3	1.0–1.2	Low	Toxic	Poor	Best at low temperatures, very expensive
PbTe	1.5–2.2	Medium	Toxic	Poor	High efficiency, not environmentally friendly, very expensive
SnSe	Up to 2.6	Low–Medium	Non-toxic	Difficult	Fragile, hard to fabricate, very expensive
ScN	0.4–1.0 (theoretical)	**High**	Non-toxic	**Excellent**	Stable, CMOS-compatible, **cheap**

- Efficiency is NOT the only parameter to consider: the chosen material must be inexpensive, suitable for the intended application, easy to process, and non-toxic.

$$ZT = \frac{\boxed{S^2}\sigma T}{\kappa}$$

- Early TMNs—with the known exception of CrN—exhibit Seebeck coefficients in their BULK FORM, up to high temperatures (< 1000 K), on the order of magnitude: −1 to −10 μV/K.

- → The perspective on TMNs in thermoelectricity became realistic with the discovery of remarkable Seebeck coefficients in ScN THIN FILMS (Kerdsongpanya et al. 2011): −156 μV/K at 840 K (Burmistrova et al. 2013).

- NANOSTRUCTURING and GROWTH METHOD are key factors

- S. Kerdsongpanya et al., Appl. Phys. Lett. 99, 232113 (2011).
- P. V. Burmistrova et al., J. Appl. Phys. 113, 153704 (2013).

$$ZT = \frac{S^2 \sigma T}{\enclose{circle}{\kappa}}$$

The main drawback

- High lattice thermal conductivity.

  Reported values until year 2022:
  between 10 and 12 W/(mK) at room temperature
  [Saha et al. 2018].

- This is the main reason why the good Seebeck coefficients and high electron mobilities achieved so far are still insufficient for high ZT.

- B. Saha et al., Phys. Rev. B 97, 085301 (2018).

$$ZT = \frac{S^2 \enclose{circle}{\sigma} T}{\kappa}$$

- Also the electron mobility of ScN is strongly dependent on the growth method and experimental conditions.

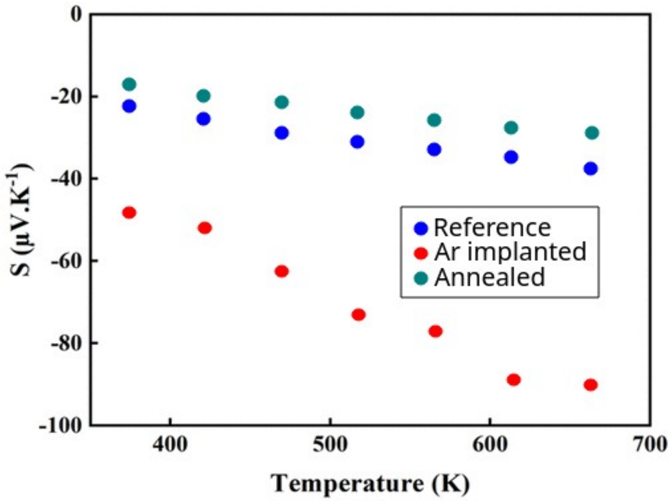
  Reported values:

  from less than 10 cm^2/(Vs) [Moustakas et al. 1996]
  to 284 cm^2/(Vs) [Oshima et al. 2014]

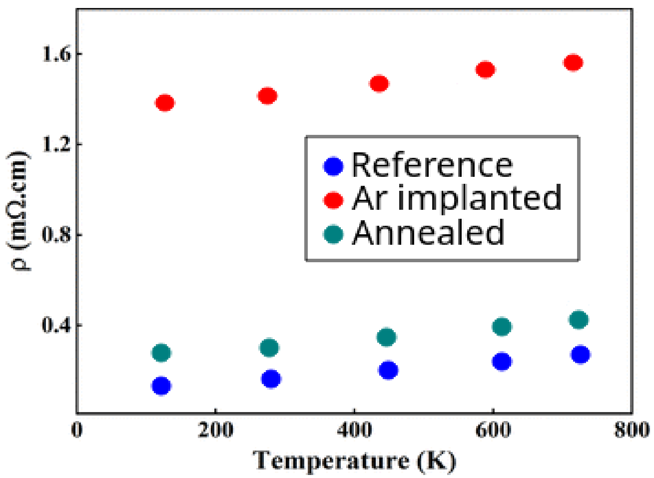
- NANOSTRUCTURING and GROWTH METHOD are key factors

- T. Moustakas et al., Proc. Electrochem. Soc. 96, 197 (1996).
- Y. Oshima et al., J. Appl. Phys. 115 (2014).

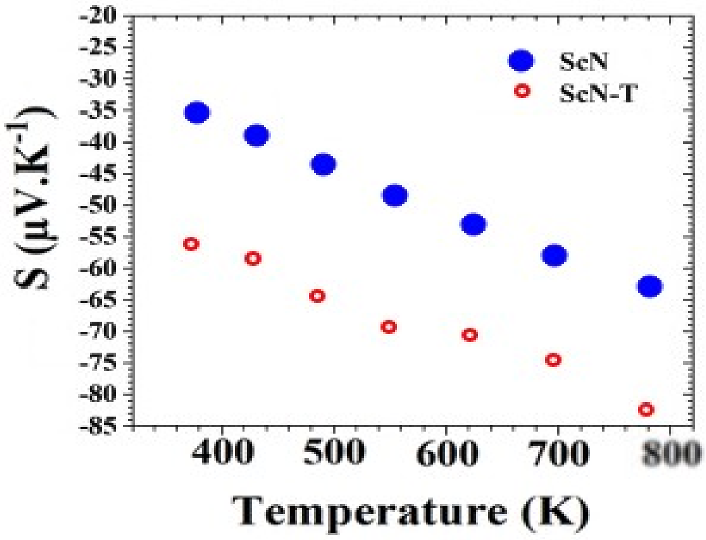
Seebeck coefficient

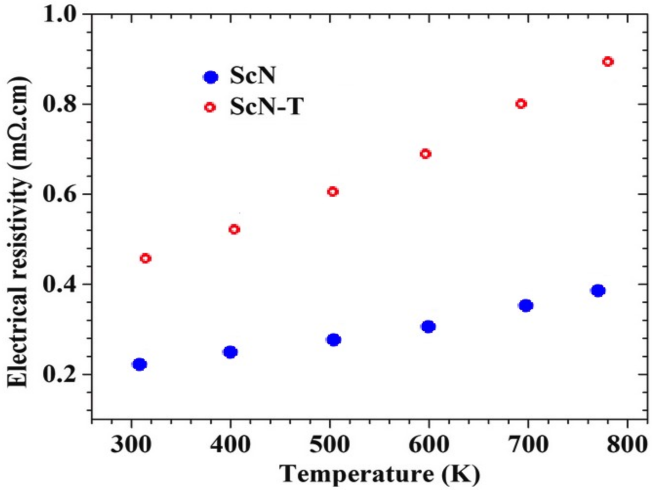


Electrical resistivity



- R. Burcea et al., ACS Appl. Energy Mater. 5, 11025 (2022).

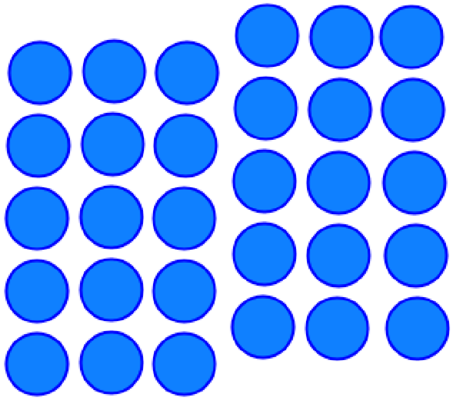




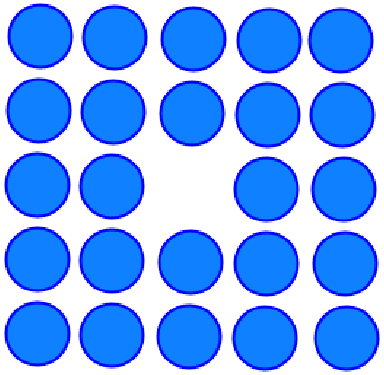
- J. More-Chevalier et al., Appl. Surf. Sci. Adv. 25, 100674 (2025).

What happens in these samples?

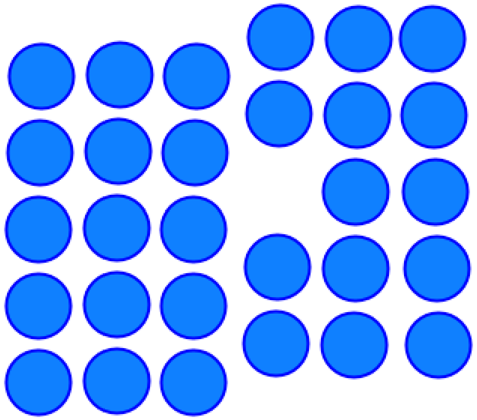
Geometrical considerations:



Glide-type defects



Point defects



Or a combination of both

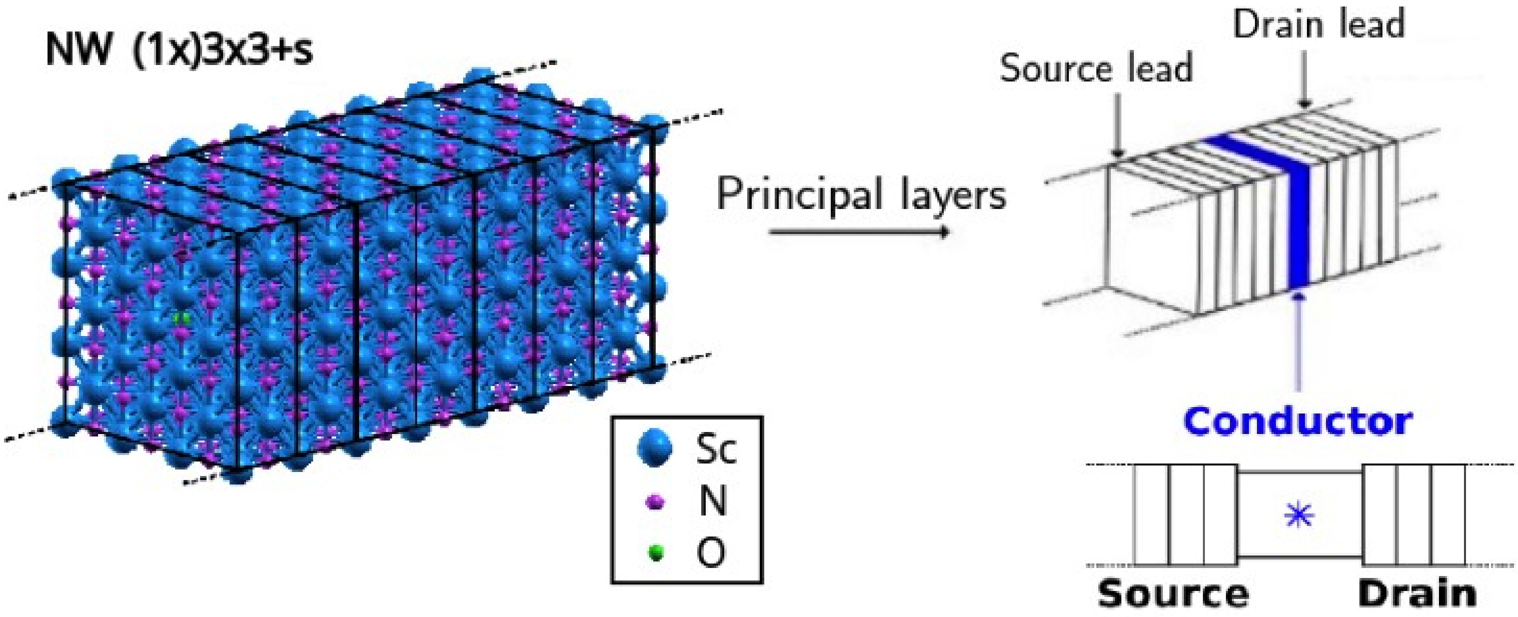
Thermodynamical considerations:

- There is only one possible symmetry of glide-type defects (rocksalt structure).
- Given experimental conditions, the energetically more favorable point defects are:

- Substitution of a nitrogen atom with an oxygen atom

- Substitution of a nitrogen atom with a vacancy

Computational model



Computational model

DFT: Quantum ESPRESSO 7.3.1 (NVHPC CUDA build)
Transport: WanT code

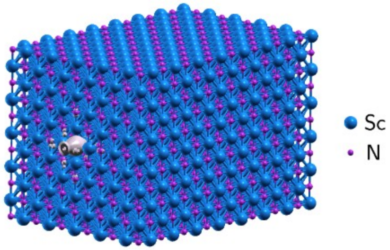
Workflow:
→ Structural relaxation (GPU)
→ Self-consistent SCF (CPU)

→ Electronic transport (CPU)

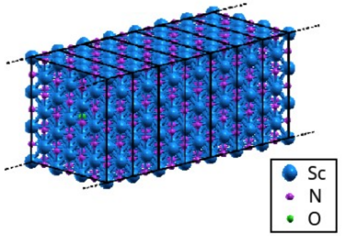
- P. Giannozzi et al., J. Phys.: Condens. Matter 21, 395502 (2009).
- P. Giannozzi et al., J. Phys.: Condens. Matter 29, 465901 (2017).
- WanT code by A. Ferretti et al., http://www.wannier-transport.org

Computational model

Structural relaxations



PBE functional
PAW pseudopotential
Ecutwfc = 40.0 Ry
Ecutrho = 320.0 Ry



1x5x5

200 atoms

350 k-points

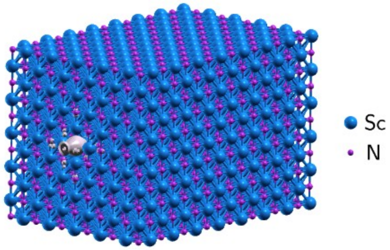
3x3x3

216 atoms

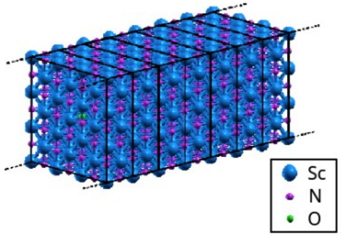
343 k-points

Computational model

Self-consistent SCF



PBE functional
PAW pseudopotential
Ecutwfc = 50.0 Ry
Ecutrho = 400.0 Ry



1x5x5 (+s)

242 atoms

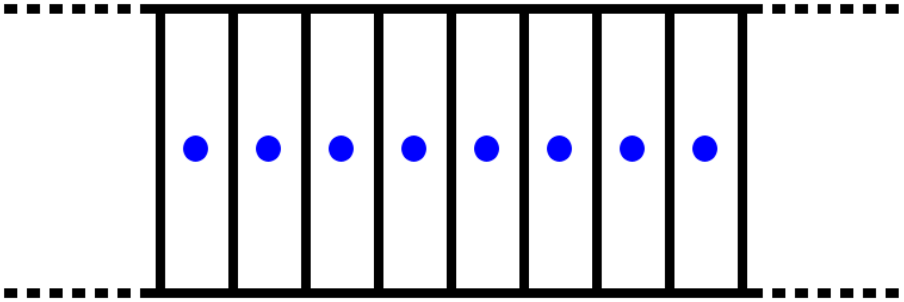
7 k-points

3x3x3 (+s)

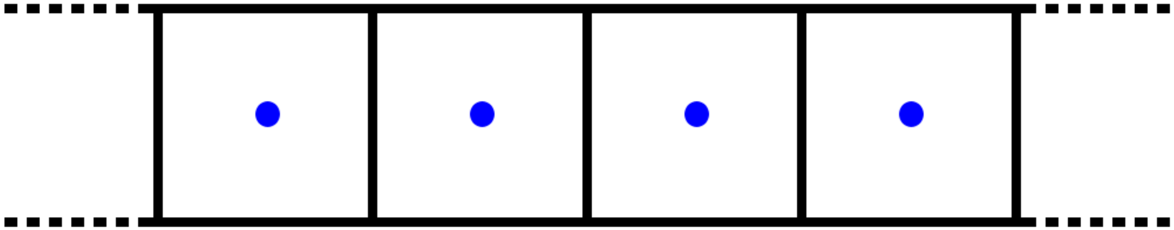
294 atoms

5 k-points

Computational model



1x5x5



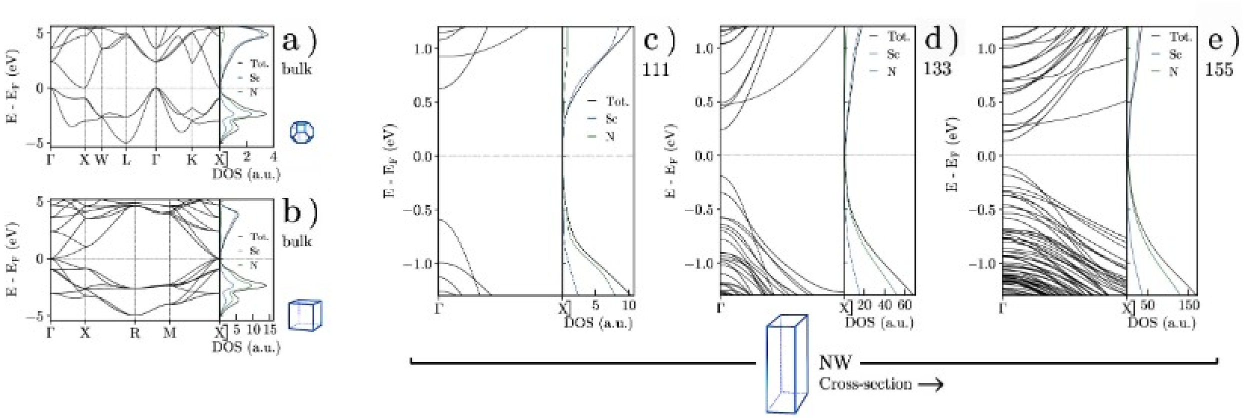
3x3x3

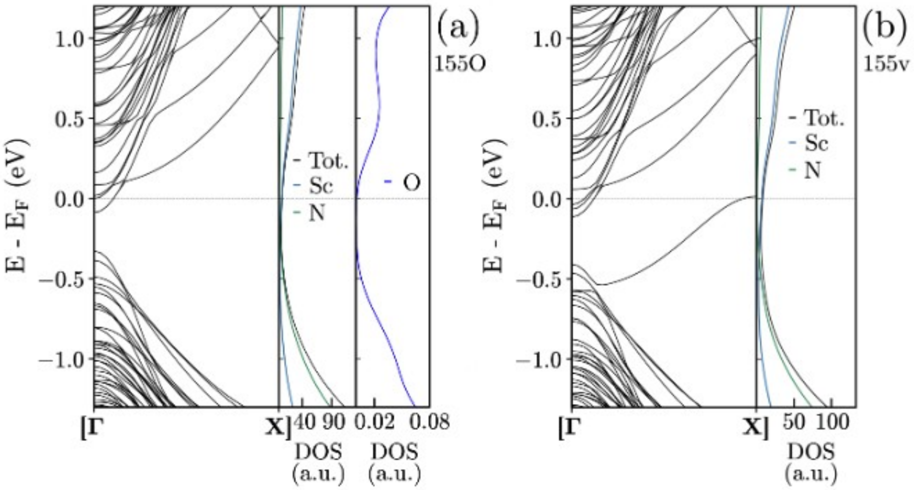
Hybrid Parallelism: MPI + OpenMP

1 MPI rank → 1 GPU

Example: 5 nodes × 8 MPI ranks per node = 40 MPI ranks
4 OpenMP threads per rank → 160 CPU threads total feeding 40 GPUs

```
ml impi/2019.9.304-iccifort-2020.4.304

ml ifort/2019.1.144-GCC-8.2.0-2.31.1

ml QuantumESPRESSO/7.3.1-NVHPC-24.3-CUDA-12.3.0

# OpenMP

export OMP_NUM_THREADS=4

export OMP_PROC_BIND=spread

export OMP_PLACES=threads

# UCX settings

export UCX_TLS=rc,cuda_copy,cuda_ipc

# Run

mpirun -n 40 pw.x < input.in > output.out
```

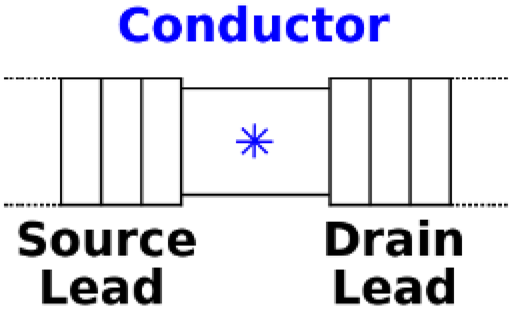




- L. Cigarini, U.D. Wdowik, D. Legut, arXiv:2509.14762 (2025).

The Landauer model of transport

- Links microscopic transport to measurable macroscopic properties



- Electronic conduction is viewed as quantum-mechanical transmission of electrons through a quantum channel

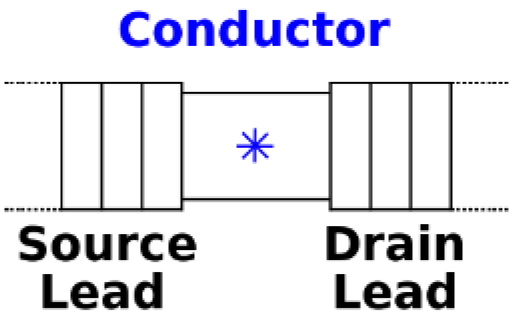
$$I = \frac{2e}{h} \int T(E) \left[f_L(E) - f_R(E) \right] dE$$

$$L_0 = \int_{-\infty}^{\infty} \mathcal{T}(E) \left(-\frac{\partial f(E)}{\partial E} \right) dE$$

$$L_1 = \int_{-\infty}^{\infty} (E - \mu) \mathcal{T}(E) \left(-\frac{\partial f(E)}{\partial E} \right) dE$$

$$S = -\frac{1}{eT} \frac{L_1}{L_0}$$

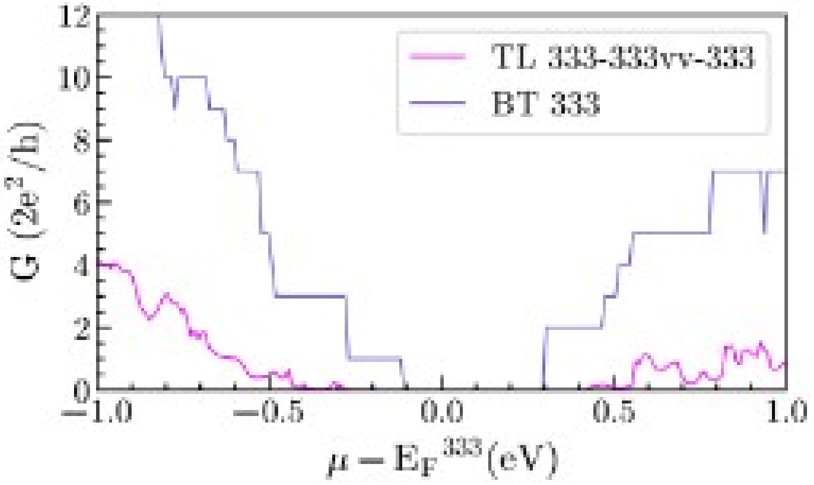
The Landauer model of transport



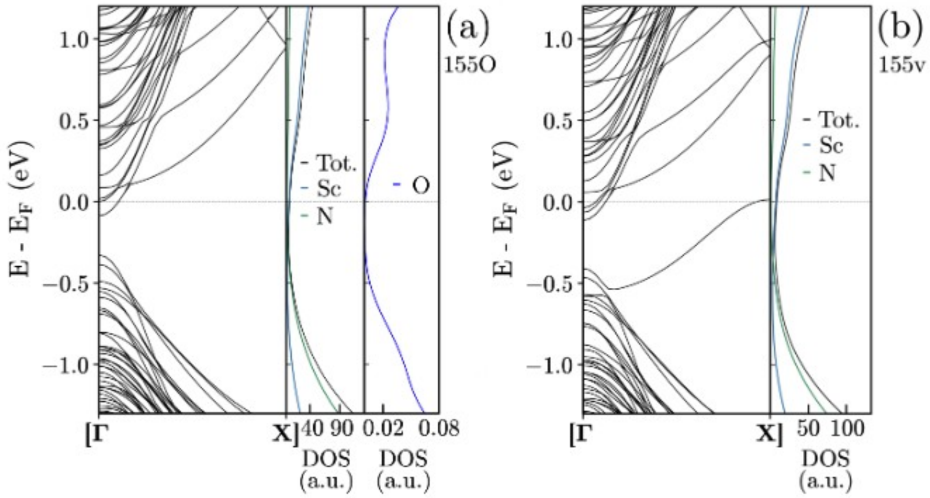
Conductor

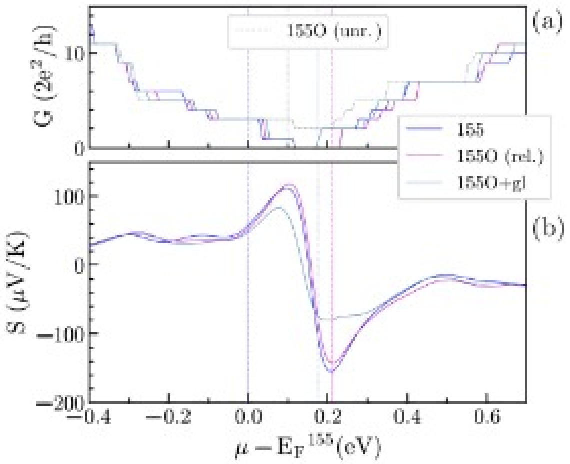
Source Lead

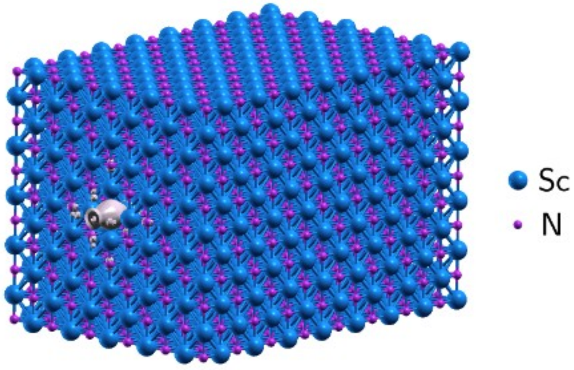
Drain Lead

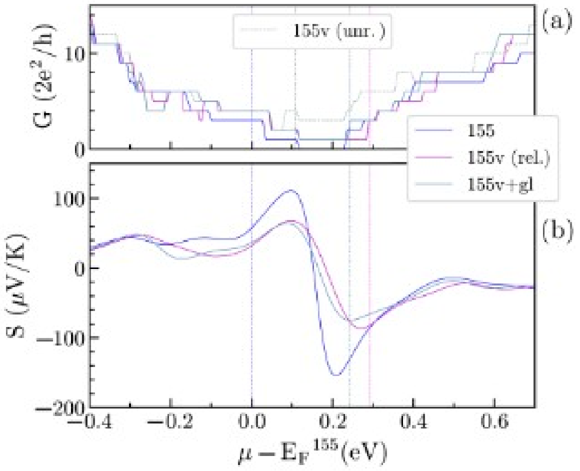


1x5x5 Models



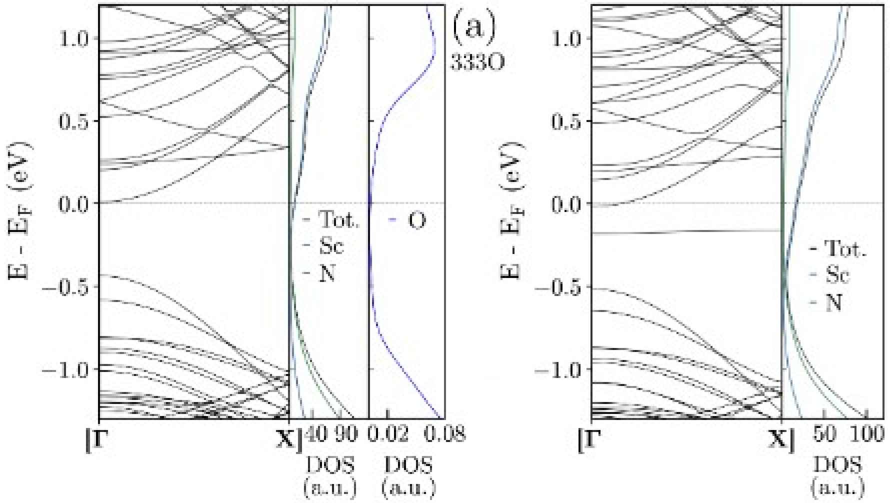


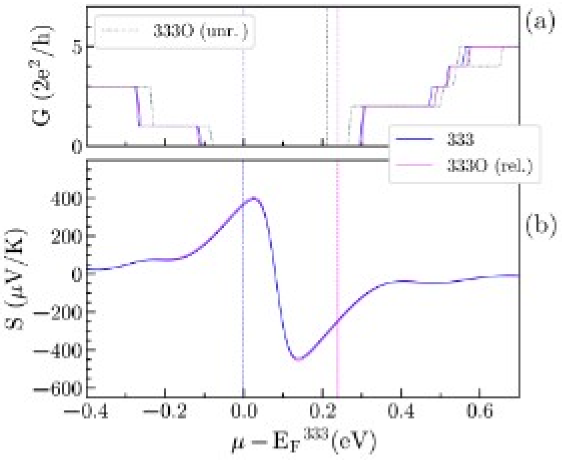


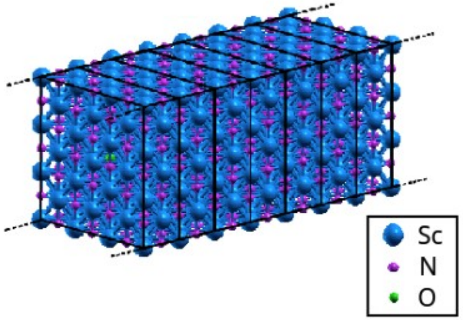


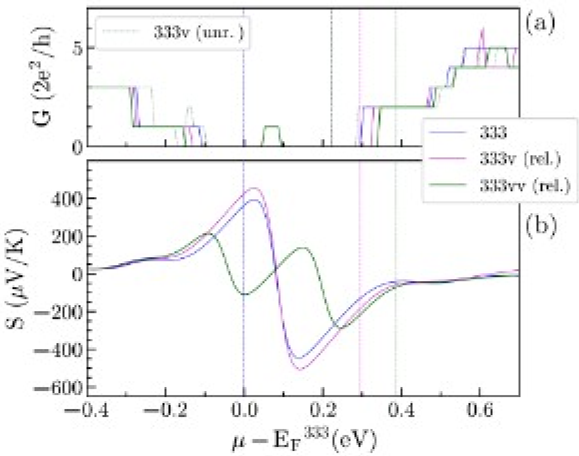
- L. Cigarini, U.D. Wdowik, D. Legut, arXiv:2509.14762 (2025).

3x3x3 Models



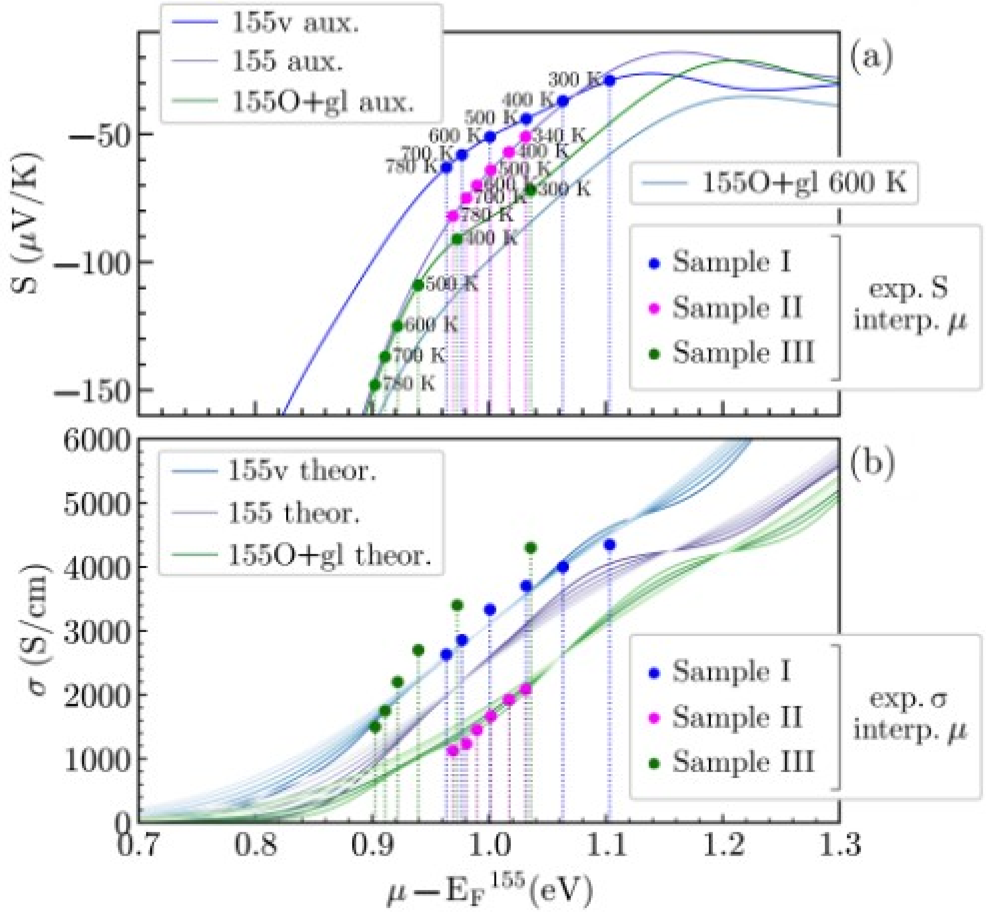






- L. Cigarini, U.D. Wdowik, D. Legut, arXiv:2509.14762 (2025).

Comparison with experiments



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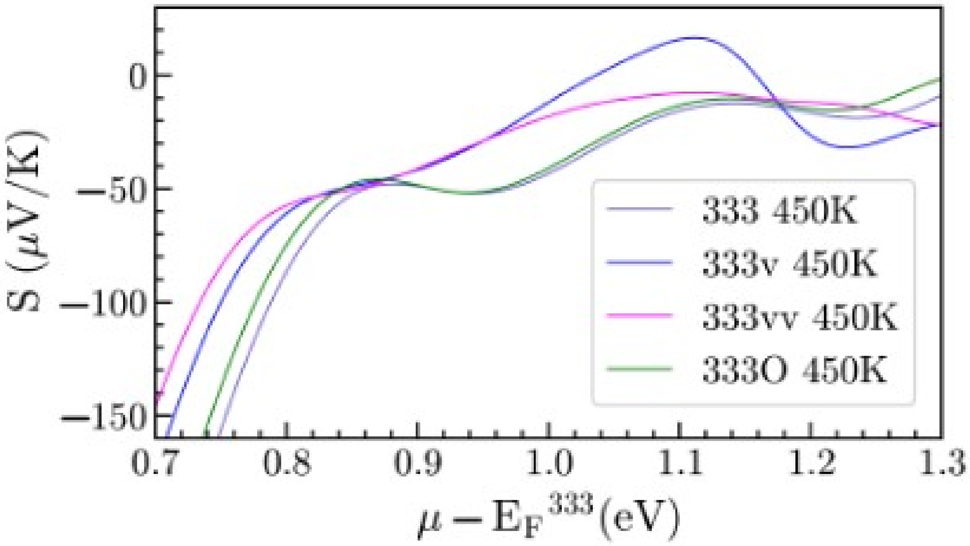
3x3x3 Models



- L. Cigarini, U.D. Wdowik, D. Legut, arXiv:2509.14762 (2025).

Discussion

- The first studies on the stability of nitrogen vacancy defects [L. Porte 1985] suggested that these defects are not energetically favorable and, therefore, were not expected to occur at all.
- However, more recent studies have shown clearly that nitrogen vacancies are instead particularly prevalent under scandium-rich growth conditions [Smith et al. 2001, Al-Brithen et al. 2002].
- These scandium-rich growth conditions are not easy to achieve using sputtering techniques. However, the demonstrated massive presence of nitrogen vacancy defects under these conditions points to the existence of complex stabilization mechanisms for nitrogen vacancies, which are not yet fully understood.

- L. Porte, J. Phys. C: Solid State Phys. 18, 6701 (1985).
- A. R. Smith et al., J. Appl. Phys. 90, 1809 – 1816 (2001).
- H. A. Al-Brithen et al., J. Cryst. Growth 242, 345 (2002).

Conclusions

- We performed a systematic analysis of the possible defects that may be present in a ScN nanostructure grown by magnetron sputtering under controlled conditions and that can have a decisive impact on determining the thermoelectric properties of this system.
- We found that the formation of structures characterized by the association of multiple contiguous nitrogen vacancy defects leads to a reduction in the absolute value of the Seebeck coefficient and an increase in electrical conductivity.
- We found that the formation of structures characterized by the association of a point defect—substitution of a nitrogen atom with an oxygen atom—and a glide-type defect leads to a reduction in the Seebeck coefficient.
- These theoretical results, combined with thermodynamic considerations on the possible formation mechanisms of such types of defects, open the possibility of formulating reasonable hypotheses to rationally explain recent experimental findings.

- L. Cigarini, U.D. Wdowik, D. Legut, arXiv:2509.14762 (2025).

Acknowledgements

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