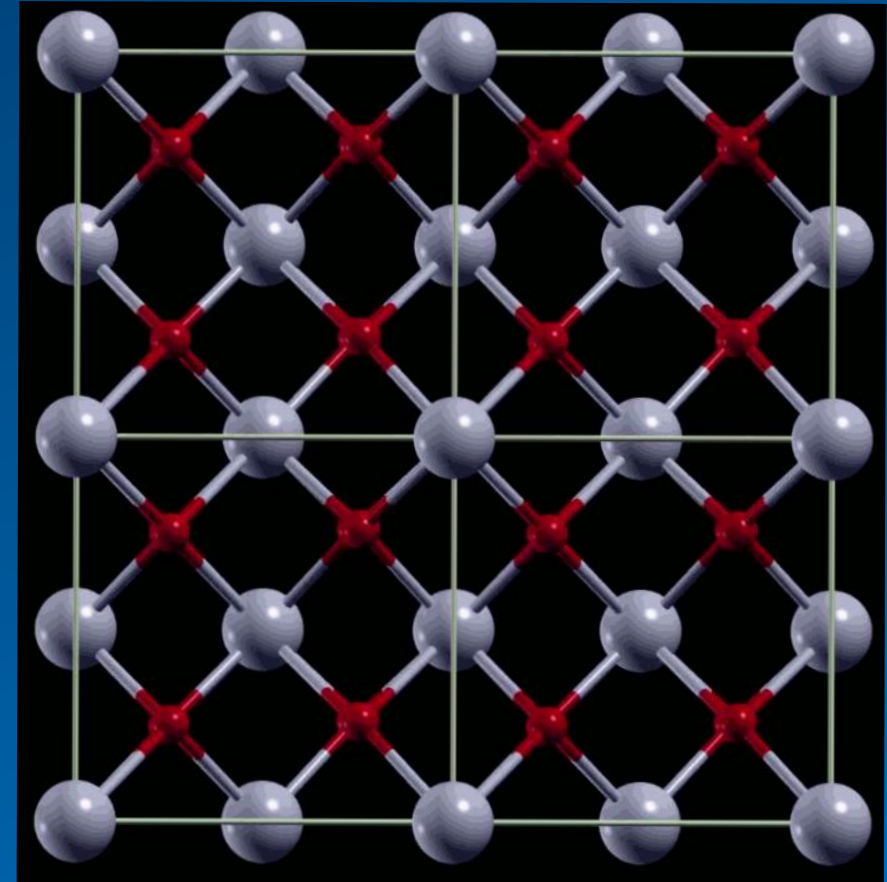


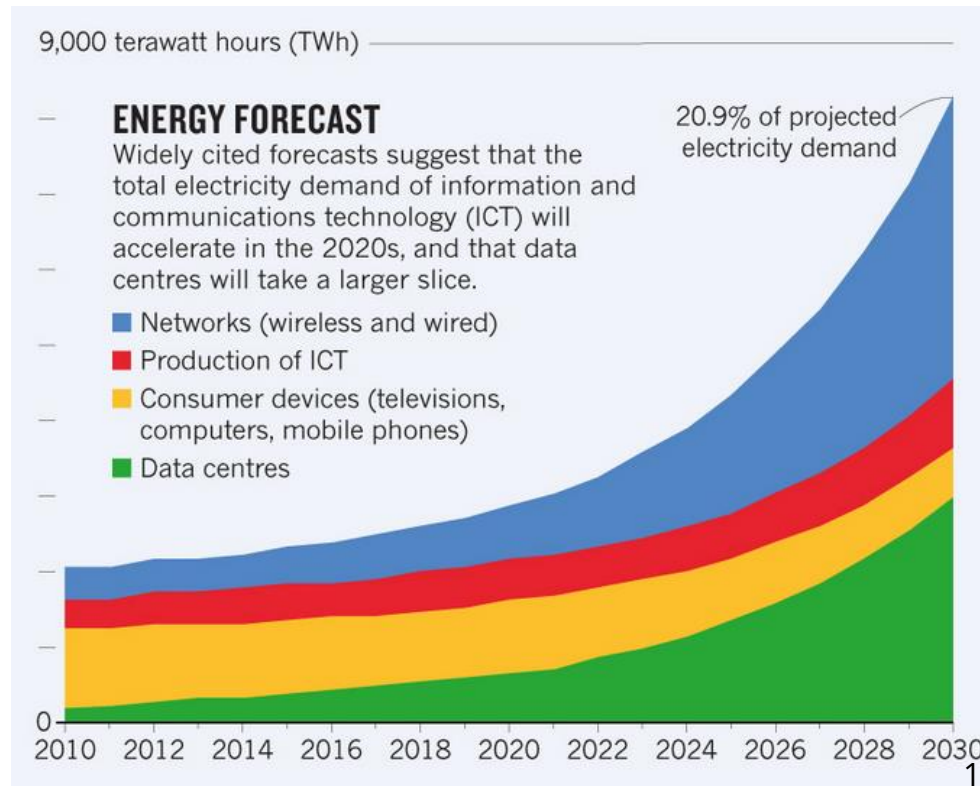
Faculty of electrical and computer engineering

Mechanism of Antiferroelectricity in polycrystalline ZrO_2

13.11.2024 Richard Ganser

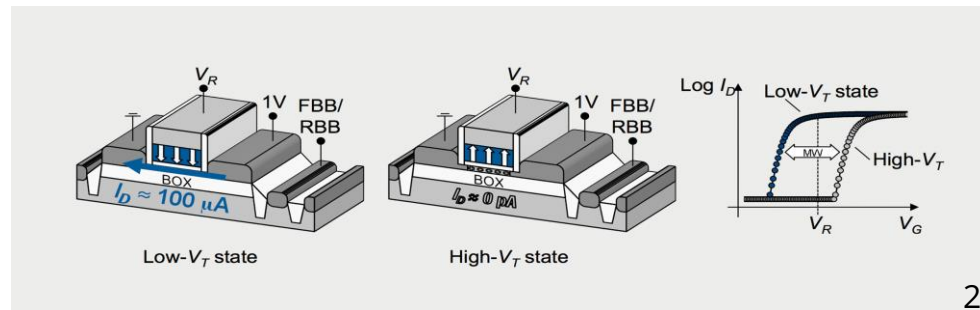


Motivation

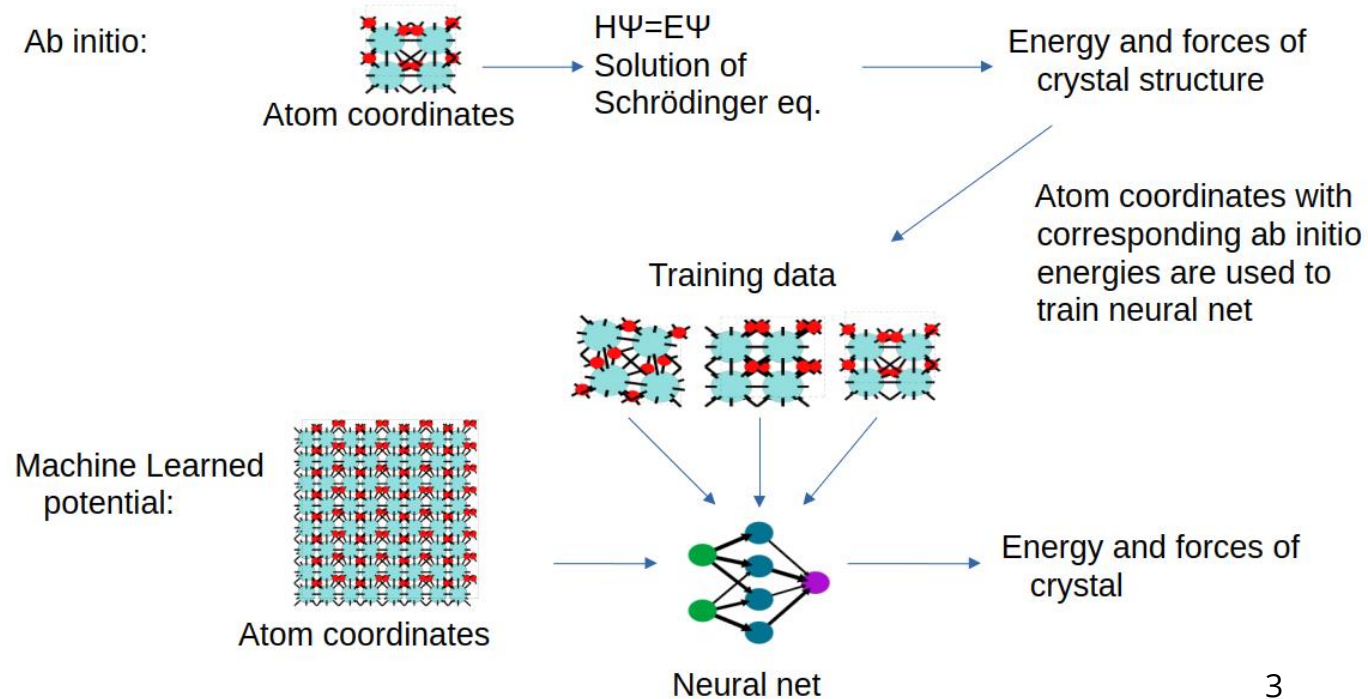


Energy consumption of servers and AI cluster is exponentially rising partly due to Gate-Drain Current

- Ferroelectric Gates could retain polarization without applied Gate-Voltage
- HfO_2 and ZrO_2 promising candidates due to successful usage as high-k materials
- Partial polarization could achieve synoptic behaviour



Simulation Challenge



Simulation Issue:

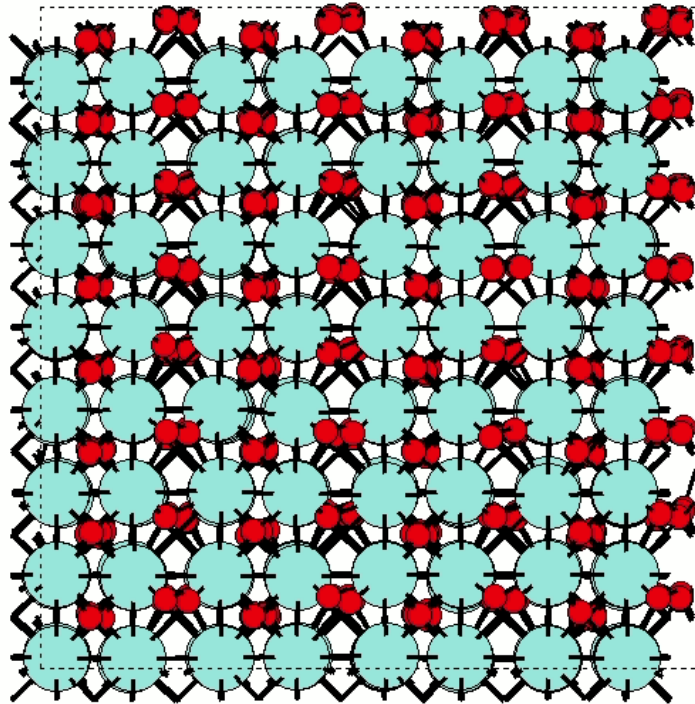
The stabilization mechanisms of the dielectric and ferroelectric phases are not accessible by density functional theory (DFT)

⇒ Training of machine learned potential for large scale molecular dynamics

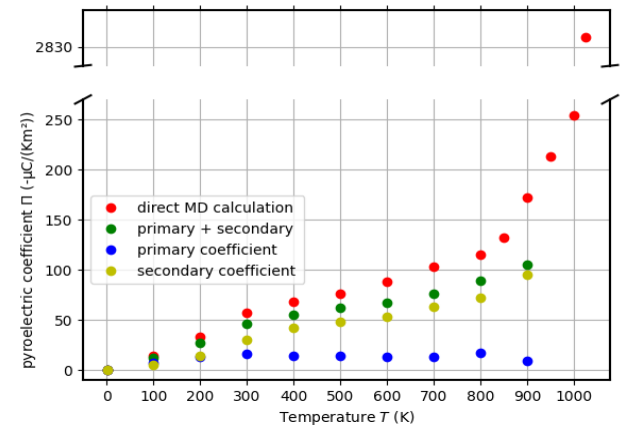
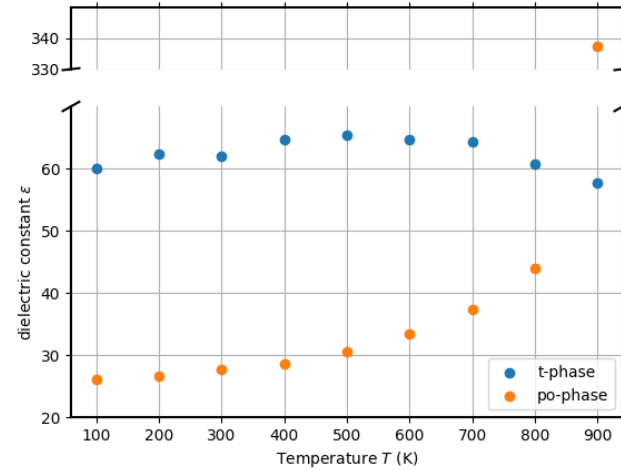
3

3) <https://journals.aps.org/prapplied/abstract/10.1103/PhysRevApplied.18.054066>

Results for bulk ZrO_2

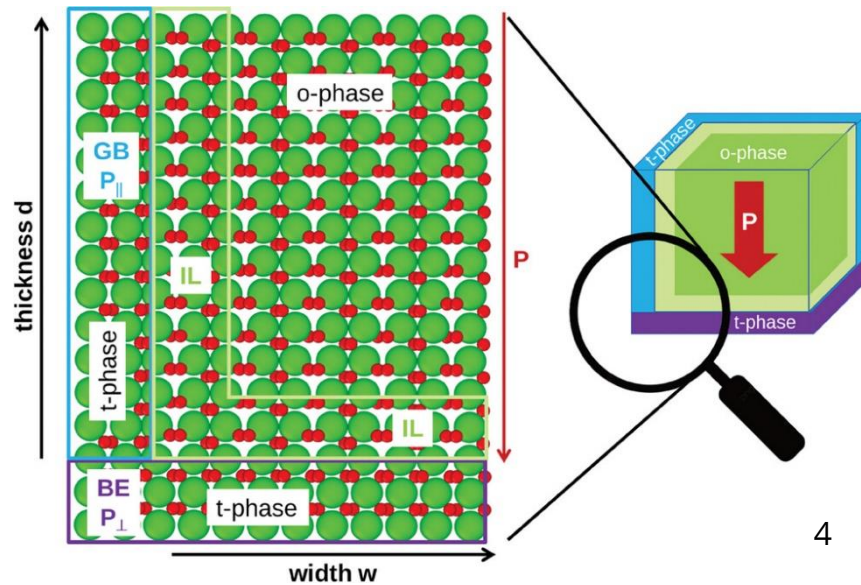


E-Field

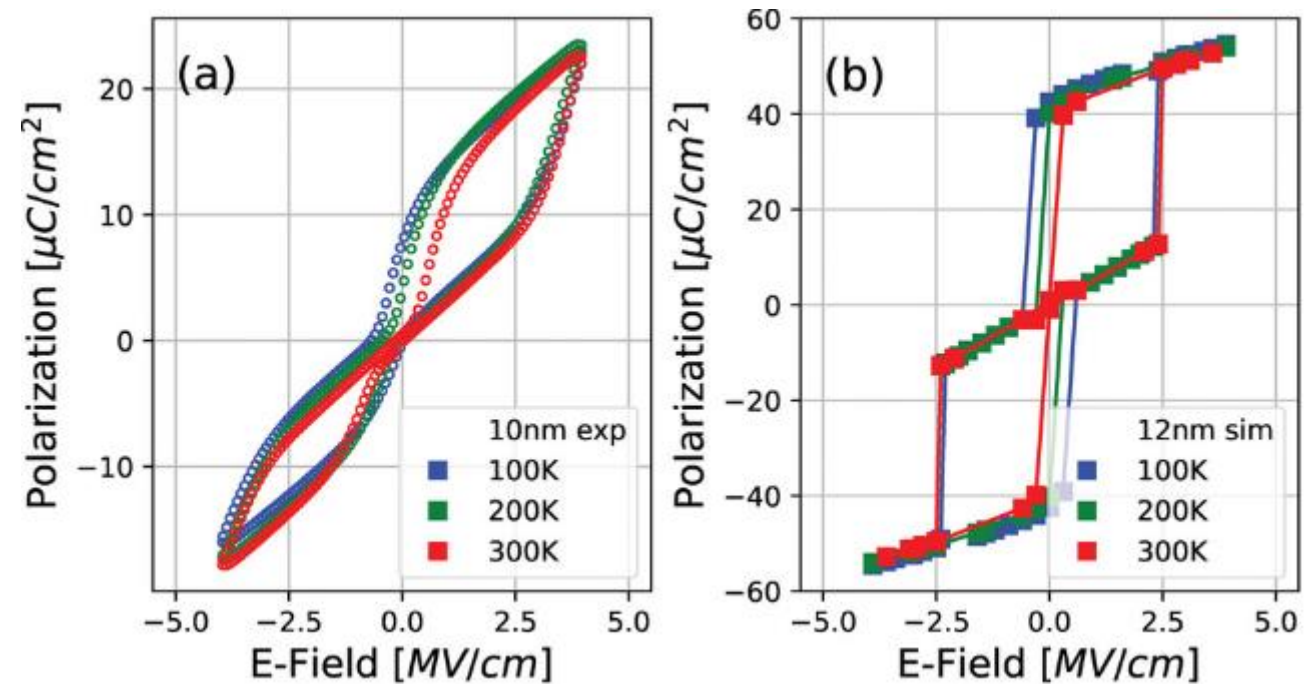


- Curie-Temperature
- Transition fields
- Piezo- and pyroelectric coefficients
- Dielectric constant
- Energy landscape
- Matching experimental results!

Antiferroelectricity



4



Attaching Interphase to the ferroelectric phase realizes Antiferroelectricity at room temperature!

Direct comparison with electrical and PFM measurements matches very well!

4) <https://onlinelibrary.wiley.com/doi/10.1002/adfm.202405513>

Questions?