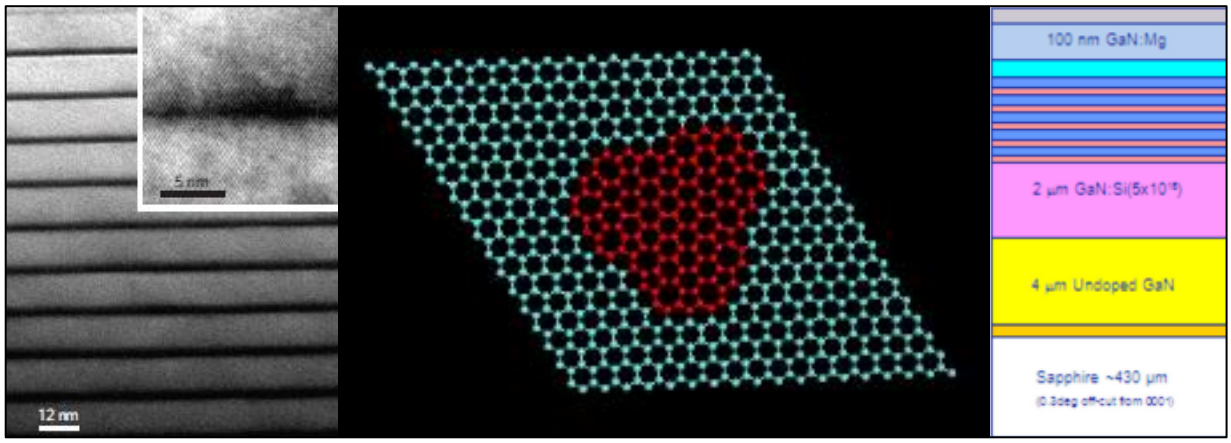
Access provider – CEA-Liten

Energy Harvesting / Micro-Power Management - Access description

Access to materials' thermal conductivity modelling: ab initio prediction of thermal conductivity for bulk solid compounds, superlattices and nanostructures.



Technical offering

- ab initio prediction of thermal conductivity for bulk solid compounds
- modelling of thermal transport in compounds with point defects
- ab initio modelling of thermal transport in superlattices and nanostructures
- ab initio modelling of ballistic transport effects in power electronic devices
- expertise in shengBTE and almaBTE simulations
- Dimensioning of harvester

Main equipment

- 1500 core supercomputer cluster
- Home-made harvester dimensioning tool

Typical applications

Development of new thermoelectric materials. Modelling of ballistic heat transport effects in power electronics, such as HEMTs or LED's. Theoretical understanding of experimental thermal conductivity measurements in complex materials. Design of harvester (definition of junction's number, width, length, junctions spacing, etc.).

Case study

For newly synthesized bulk materials and superlattices: ENABLES can make ab initio calculations of thermal conductivity, even in the absence of measurements. For materials with point defects: it can theoretically calculate thermal conductivity versus temperature, as a function of point defect concentration.

Responsible

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