

## Phononic band gaps in nanostructures

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**Abstract:** Phononic band gaps (PBG), frequency areas where the propagation of phonons is not allowed, are created in nanostructures consisting of atoms of different atomic mass. For example, in graphene when C atoms are substituted with Si or Ge atoms wide PBGs may be created. Similarly, in WS<sub>2</sub> monolayers, PBGs can be created by replacing W atoms with Mo or S atoms with Se. Those systems were studied with Density Functional Theory for small sizes. For bigger sizes nanoparticles, molecular dynamics simulations with empirical potentials were used. PBGs in the nanoscale may be used to make phononic interconnects where the information can be transmitted with phonons. They can be also used to control the thermal conductivity.