# Abstract

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Over the last six decades there has been a trend for miniaturization of electronic devices, and especially integrated circuits (1) by cramming as many electronic components as possible in a defined space. The benefits of this trend are the improvement of portability and efficiency, as well as the reduction of the cost of silicon-based devices. Nevertheless, the miniaturization of silicon-based devices has reached its physical limit (2), making the discovery of new materials necessary.

In my research towards the investigation of alternative materials that can substitute silicon, I focused on on a new class of quasi-1D structures. These structures are made of extreme nanowires (ENWs) of crystalline materials with a cross sections of up to 3 atoms wide, encapsulated inside carbon nanotubes (CNTs). The material that I studies as a CNT-filling was silver selenide ($Ag_2Se$). Such quasi-1D structures can be used as conducting wires in nano-circuits, and are promising candidates that can be used as nano-phase-change materials in memory devices.

I my talk I will give an overview of the theoretical work I did, on $Ag_2Se$ ENWs encapsulated inside CNTs. I will describe the computational tools that I utilized for the discovery of the $Ag_2Se$ geometries, namely *Ab Initio Random Structure Searching (AIRSS)* (3) method, *MATerials and Atomistic Database Of Relaxations (MATADOR)* (4) database, and the DFT code CASTEP(5).

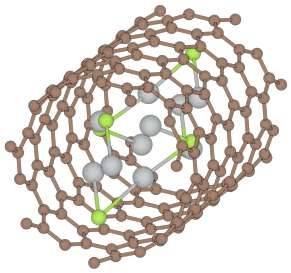

Figure 1: $Ag_2Se$ ENW inside CNT.

## References

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