Directory structure-:

a) **src**-: This directory contains the main source code for the project

    i. **main:** This directory contains the main scripts for creating graphene and cnt structures namely **create_graphenestruct.py** and **create_CNTstruct.py.**

    ii. **data**: This directory contains the script **database.py** which c contains class for database reading and writing. Currently it works for reading txt and dat files but can be easily extended for other file formats

    iii. **structures**: This directory contains classes in modules **graphene.py** and **cnt.py** for definitions of graphene and CNT structures as well as their constituent elements. These classes also contains member functions for geometrical transformations of these structures. These classes can be easily duplicated or inherited to describe similar structures.

    iv. **utils:** This directory contains utility functions for the project. It contains **config_reader.py** which can be used to read config files. It parses configuration as a python dict. Currently it works with dat and txt files but json and xml will be added.
It also contains **utils.py** which has utility functions for geometrical transformations.

    v. **test:** This is a directory for test code but tests will be added soon.

b) **config** - This directory contains dat files for configuring the structures of the two phase materials. All geometrical specifications and explicit fileneames i.e input - output dat files can be specified here. All filepaths should be relative to the topmost directory. No geometrical data is needed to be specified in the script.

c) **graphene and aerogel datfiles** - These directories are for specifying dat files for all structures.Can be changed but new path should be updated in the config file.

Running the script -:
This project is currently supported on python3 and only requires python numpy as an additional package.

Command for creating Graphene structure -:
python3 src/main/create_graphenestruct.py

Command for creating cnt structure-:
python3 src/main/create_CNTstruct.py

**These command should be run from the outer most directory of the project