

Annex B: Overview available functions

The zip file contains the sample script ([main_densityVsTemperature_lean.m](#) or [main_densityVsTemperature_lean.py](#)) and useful functions.

In **MATLAB** and **GNU Octave**, all needed functions are stored separately, one file per function. Their filename exactly corresponds to their function_name, e.g., `AssignSemiconductor.m` contains the code necessary for the function `AssignSemiconductor`.

In Python, all the functions are bundled in a module `semiconductor_functions.py`.

Choose the semiconductor		
AssignSemiconductor		

Construct a density of states		
InitializeEnergyAndDOS		
InitializeDOSAdministration		
AddConductionBandToDOS AddValenceBandToDOS	AddGaussToDOS	AddLevelToDOS
Obtain electron density (occupation)		
GetDensityInBand	GetDensityInGauss	GetDensityInLevel
FIntegrationForBands	FDIntegrandGauss	
FermiDirac		

Evaluate charge neutrality		
chargeNeutralityIntrinsic		
chargeNeutrality		

Additionally required functions, service functions		
DensityOfBandStates	FindRootNestedIntervals	SetPlotProperties
AddContributionToDOS	GaussDOS	GetFullDOS