Appendix D: Reference of functions

Function	description	input	output
AssignSemiconductor	choose effective masses and bandgap according to a semiconductor	string with semiconductor composition	effective electron m^*_e and hole masses m^*_h, energies of conduction band minimum E_C and valence band maximum E_V (in eV)
InitializeEnergyAndDOS	creates an energy interval with desired resolution	E_C and E_V (in eV); maximal and minimal energy to be considered (in eV); number of bins in the energy interval	vector with discretized energy interval, empty vectors capable of storing DOS and occupation info with respect to energy interval
InitializeDOSAdministration	creates a data structure DOS_admin capable of holding information necessary to describe the nature of the states participating in the overall DOS	energy interval	DOS_admin
AddConductionBandToDOS	adds a conduction band to the DOS	DOS_admin, energy interval, m^*_e, E_C	DOS_admin
AddValenceBandToDOS	adds a valence band to the DOS	DOS_admin, energy interval, effective hole mass, energy of valence band maximum	DOS_admin
AddGaussToDOS	adds Gaussian-shaped DOS the DOS	DOS_admin, energy interval, total density, energy, width of Gaussian	DOS_admin
AddLevelToDOS	adds sharply defined level to the DOS	DOS_admin, energy interval, total density, energy	DOS_admin
AddContributionToDOS	service routine required by the former 4 routines to add DOS contributions to DOS_admin	DOS_admin, vector with size of energy interval, label (internal), type, position in energy interval (in eV), parameter, e.g., Gaussian width, density of states (in m^{-3})	DOS_admin
GetFullDOS	retrieves complete DOS information from DOS_admin and stores it a vector DOS of the size of the energy interval	DOS_admin	filled vector DOS
GetDensityInBand	provides electron density in a band	data set in DOS_admin, chemical potential, E_C, m^*_e, temperature	electron density
GetDensityInLevel	provides electron density in a sharply-defined level	chemical potential, E_v, m^*_h, temperature	electron density
GetDensityInGauss	provides electron density in a Gaussian-shaped DOS	chemical potential, temperature	electron density
FIntegrationForBands	performs an integration of the DOS*FermiDirac distribution in a band	chemical potential, temperature	occupation probability in the band
FDIntegrantGauss	performs an integration of the DOS*FermiDirac distribution in a Gauss-DOS	chemical potential, temperature	occupation probability in the Gauss DOS
GaussDOS	Gauss function	energy *E* (in eV) mean energy (in eV) width of Gaussian (in eV)	value of the Gauss function at energy *E*
FermiDirac	Fermi Dirac distribution function	chemical potential temperature	occupation probability
DensityOfBandStates	provides effective density of states for a band	effective mass temperature	density of states in m^{-3}
chargeNeutrality	yields the difference between negative and positive charges considering the properties of the total DOS	variable storing desired chemical potential, DOS_admin, E_v, E_c, m^*_h, m^*_e temperature	difference n-p of negative and positive charges
chargeNeutralityIntrinsic	yields the difference between negative and positive charges assuming an intrinsic	variable storing desired chemical potential, E_v, E_c, m^*_h, m^*_e temperature	difference n-p of negative and positive charges

	semiconductor with CB and VB	chemical potential temperature	
FindRootNestedIntervals	Finds at which argument x a function F(x) becomes zero	function handle referring to function F, energy interval, initial value for x, threshold for relative error below which search stops, number of maximum iterations	argument x fulfilling |F(x)| < threshold, relative error, number of iterations
SetPlotProperties	sets parameters for a unified and convenient appearance of plot figures	--	--