Plasma Parameter Calculator

This web tool calculates many parameters for electron-ion plasmas from one to five ion species. In this document example usage is given as well the formulary for the calculations.

Input

The required inputs for the calculator are,

- first, the number of species in the system,
- then the types of ions, given by the charge and mass of each ion type,
- and finally the total density and the temperature of the system.

In addition if the system has more than one species, the concentration of each species must be given. And *optionally* for simulation cell information a total number of ions in the simulation may be given.

Examples

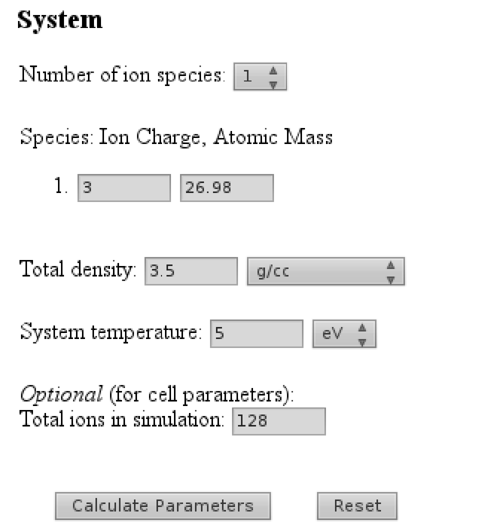
In the examples to the right the input usage can be seen.

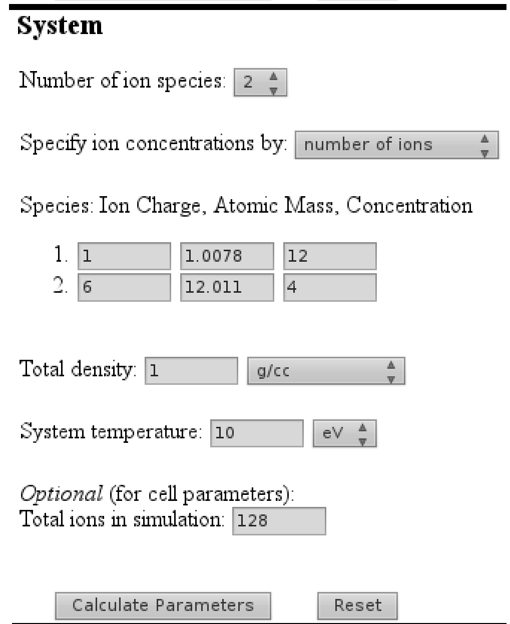
Top Here a single species is considered. In this case aluminum with only 3 valence electrons is to be calculated, fully ionized aluminum by contrast would have an input ion charge of 13.

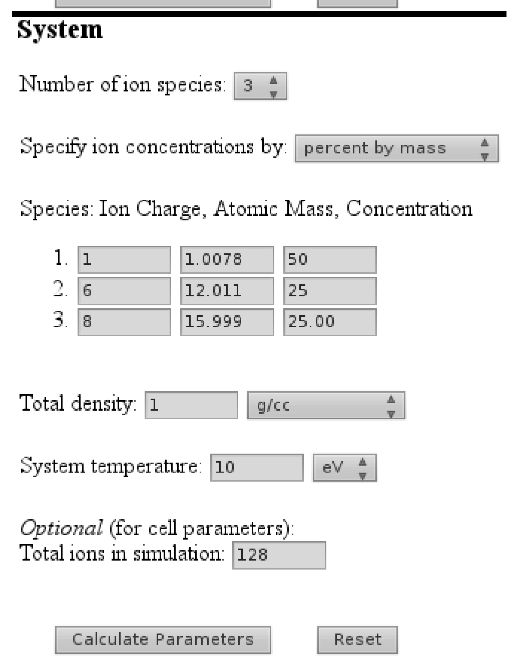
Middle Next is a binary mixture, and a concentration must now be given. Shown here the mixture is given by the relative number of ions, that is 12 hydrogen atoms to 4 carbon atoms. Note a fractional number of ions can be used also.

Bottom Lastly the ion mixture concentrations may also be given by mass percentage by molar percentage. If these methods are used the last species will be calculated so the total is 100%.

In all of these examples the total density is given in g/cm^3, and the temperature is given in eV, but other options are available. Also 128 total atoms are selected for total number of ions in the simulation unit cell, but this may be left blank if not desired.







Units and conversion factors

$$1 \text{ amu} = 1.66053892 \times 10^{-24} \text{ g} = 1822.8884\ m_e$$
$$1 \text{ Ang} = 10^{-8} \text{ cm} = 1.88972599 \text{ bohr}$$
$$1 \text{ Ha} = 27.211385 \text{ eV} = 27.211385\ k_B\,K$$
$$k_B = 8.617332 \times 10^{-5} \text{ eV/K}$$
$$a_B = 1 \text{ bohr}$$
$$1 \text{ s} = 10^{15} \text{ fs} = 4.134137 \times 10^{16}\ \hbar/\text{Ha}$$

Electron parameters

Electron density:

$$n_e = N_e/V =< Z > n$$

Wigner-Seitz radius:

$$a_e = (3/4\pi n_e)^{1/3}$$

Wigner-Seitz radius (dimensionless):

$$r_s = (3/4\pi n_e)^{1/3}/a_B$$

Fermi wave number:

$$k_F = (3\pi^2 n_e)^{1/3}$$

Fermi energy:

$$E_F = \hbar^2 k_F^2/2m_e$$

Fermi degeneracy (dimensionless):

$$\Theta = k_B T/E_F$$

Coulomb coupling (dimensionless):

$$\Gamma_e = e^2/a_e k_B T = 2(4/9\pi)^{2/3} r_s/\Theta$$

Relativistic parameter (dimensionless):

$$x_r = \hbar k_F/m_e c$$

Thermal de Broglie wavelength:

$$\lambda_{dB} = (2\pi\hbar^2/m_e k_B T)^{1/2}$$

Plasma frequency:

$$\omega_{pe} = (4\pi n_e e^2/m_e)^{1/2}$$

Thomas-Fermi screening length (at $\Theta = 0$):

$$\lambda_{TF}^{\Theta=0} = (\hbar^2\pi/4e^2 m_e k_F)^{1/2}$$

Debye length (TF screening for $\Theta \gg 1$):

$$\lambda_D = (k_B T/4\pi e^2 n_e)^{1/2}$$

Ion Parameters

Most quantities averaged over species.

Ion density:

$$n = n_{total} = \sum_i n_i = N_{total}/V$$

Ion averages:

$$\langle M \rangle = \sum_i M_i n_i/n$$

$$\langle Z^\alpha \rangle = \sum_i Z_i^\alpha n_i/n$$

Wigner-Seitz radius:

$$a = (3/4\pi n)^{1/3}$$

Wigner-Seitz radius (dimensionless):

$$R_s = (3/4\pi n)^{1/3}/a_B$$

Fermi wave number:

$$k_F = (6\pi^2 n)^{1/3}$$

Fermi energy:

$$E_F = \hbar^2 k_F^2/2\,\langle M \rangle$$

Fermi degeneracy (dimensionless):

$$\Theta = k_B T/E_F$$

Coulomb coupling (dimensionless):

$$\Gamma = e^2/a k_B T$$

Coulomb coupling effective:

$$\Gamma_{eff} = \left\langle Z^{5/3} \right\rangle \langle Z \rangle^{1/3}\,\Gamma$$

Relativistic parameter (dimensionless):

$$x_r = \hbar k_F/\langle M \rangle\, c$$

Thermal de Broglie wavelength:

$$\lambda_{dB} = (2\pi\hbar^2/\langle M \rangle\, k_B T)^{1/2}$$

Plasma frequency:

$$\omega_p = (4\pi n \langle Z \rangle^2 e^2/\langle M \rangle)^{1/2}$$