DustEM User's Guide

April 24, 2023

`DustEM` is a numerical tool in fortran 95 jointly developed by IAS and IRAP to compute the extinction, the emission and the polarization properties of interstellar dust grains heated by photons. The dust emission is calculated in the optically thin limit (no radiative transfer) and the default spectral range is 40 to 10^8 nm. The code has been designed so that dust properties can easily be changed and mixed and to allow for the inclusion of new grain physics (Compiègne et al. 2011). The grain temperature distribution dP/dT is derived with the formalism of Désert et al. (1986), assuming that the grain cooling is continuous. To describe the long wavelength emission of dust, the initial algorithm has been revised to cover the low temperature part of dP/dT. The current stable version of `DustEM` is available at

> `https://www.ias.u-psud.fr/DUSTEM`.

The fortran files are in `/src`, data files in `/oprop`, `/hcap`, `/data` and output files are in `/out`. All data files have headers (where each line begins with #) that document their content. Python routines useful to generate or visualize `DustEM` files can be found in `/py` (see section 4).

After describing how to set up `DustEM`, we detail below the way to control `DustEM` as well as the files it needs or produces.

Contents

1   Getting started

After downloading the tar ball from the `DustEM` website:

1. Unpack the archive:

   `tar xvzf dustem.tar.gz`

   This will generate the `/dustem` directory which should contain the following subdirectories: `/data`, `/hcap`, `/oprop`, `/out`, `/pro`, and `/src`.

2. In `/src` edit the file `DM_constants.f90` to define the string `data_path` as the absolute path to the `/dustem` directory you just created. If you are running `DustEM` coupled to the Meudon PDR code, you must also define the string `dir_PDR` as the absolute path to `/dustem/out`.

3. Edit `Makefile` and set up the standard commands corresponding to your fortran compiler (`gfortran`, `g95` and `ifc` have been tested), *e.g.*

   `FC = gfortran`
   `FFLAGS = -O2 -fno-second-underscore`

4. Type `make` to compile, possibly preceded by `make clean`, if a former attempt went wrong. A successful compilation will end with `That's it !`. The executable is called `dustem`.

5. Running command is `./src/dustem`. This runs the model of Compiègne et al. (2011) and should take a few seconds CPU on current computers.

6. After running `DustEM`, you can check your run by using `show_dustem.py` in `/py`.

2   Input files

The main input file for `DustEM` is `GRAIN.DAT` and must be located in the directory `/data`. This file contains the main parameters and keywords that define a dust model. Each dust *population* is defined by its grain *type* noted `tt` and its size distribution as set in `GRAIN.DAT`. For a given type, `DustEM` requires the files `/oprop/Q_tt.DAT` and `/hcap/C_tt.DAT` containing the optical properties and heat capacities of grain of type `tt`, respectively. These files are described in section 2.5. DustEM can handle an arbitrary number of dust populations. In general, a grain type has a well defined composition (bulk material), structure (porosity, mass density) and shape (spherical or spheroidal). All these properties are taken into account while generating the grain data. These aspects and others are discussed in the THEMIS website (`https://www.ias.u-psud.fr/themis/index.html`).

2.1   Defining a dust model

Within `DustEM`, a dust model is defined by the control input file `GRAIN.DAT`. We show below a typical example of this file (as in Compiègne et al. (2011)).

```
# DUSTEM: definition of grain populations
#
# run keywords
# G0 scaling factor for radiation field
# grain type, nsize, population keywords, Mdust/MH, rho, amin, amax, alpha/a0 [, at, ac, gamma (ED)] [, au, zeta, eta
(CV)]
# cgs units
#
 sdist / run_name
 1.00
 PAH0_MC10        10 logn-chrg-zm    7.80E-04 2.24E+00 3.50E-08 1.20E-07  6.40E-08   1.00E-01
 PAH1_MC10        10 logn-chrg-zm    7.80E-04 2.24E+00 3.50E-08 1.20E-07  6.40E-08   1.00E-01
 amCBEx           15 logn            1.65E-04 1.81E+00 6.00E-08 2.00E-06  2.00E-07   3.50E-01
 amCBEx           25 plaw-ed         1.45E-03 1.81E+00 4.00E-07 2.00E-04 -2.80E+00  1.50E-05 1.50E-05 2.00E+00
 aSil             25 plaw-ed         7.80E-03 3.50E+00 4.00E-07 2.00E-04 -3.40E+00  2.00E-05 2.00E-05 2.00E+00
```

After some documentation lines (starting with #), the run keywords are given (`sdist` in the above example). After a / sign you can also give a run name that will be tagged to the output files, e.g., `SED_run_name.RES`. The next line gives a scaling factor for the intensity of the radiation field (here 1.00). The following lines define the dust populations. From left to right we have: grain type (e.g. `PAH0_MC10`), number of sizes (`nsize`), the population keywords, the dust-to-gas mass ratio ($Y_i = M_i/M_H$), the grain material specific mass density (ρ in g/cm^3), the minimum (a_{min}) and maximum (a_{max}) sizes in cm and other parameters for the size distribution. As seen in this example for `amCBEx`, several dust *populations* can make use of the the same grain *type*. Keywords are used to control the `DustEM` output. They can be written in uppercase or lowercase characters. The *run keywords* control the way `DustEM` is executed and the output files it produces. If multiple run keywords are used, they must be separated by blanks. The available run keywords are:

- **none:** if no run keyword required,

- **quiet:** sets the verbose mode off at runtime,

- **res_a:** writes output for each grain size (see section 3)

- **sdist:** for each grain size and type, writes the size distribution in the file `/out/SDIST.RES`,

- **zdistf:** for each grain size and type, writes the charge distribution and gas heating rates in the file `/out/ZDIST.RES`. If **zdist** is set only the mean and equilibrium charges are given.

- **tempf:** for each grain size and type, writes the temperature distribution in the file `/out/TEMP.RES`. If **temp** is set only the mean and equilibrium temperatures are given.

- **pdr:** writes a summary of `DustEM` output in `/out/DM_PDR.DAT`. To be set when `DustEM` is coupled with the Meudon PDR code (`http://pdr.obspm.fr/PDRcode.html`). Requires `G_tt.DAT` files in `/data` (see section 2.5).

The *population keywords* (e.g., `logn`, `plaw`) define the size distribution and the physical processes included in `DustEM` for each grain population. Population keywords can also be multiple, they are then separated by a dash. The population keywords defining the size distribution are described in section 2.3 and those defining the grain physics in section 2.4.

2.2   Template dust models

Several reference dust models are provided. The control input files for the following reference models are included in the current `DustEM` distribution:

- **GRAIN_DBP90.DAT:** for the model of Désert et al. (1990),

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- **GRAIN_DL01.DAT:** for the diffuse interstellar model of Li & Draine (2001),

- **GRAIN_WD01_RV5.5B.DAT:** for the model of molecular cloud of Weingartner & Draine (2001a) ($R_V = 5.5$, case B and $b_c = 3\,10^{-5}$).

- **GRAIN_DL07.DAT:** for the model of Draine & Li (2007) (see section A),

- **GRAIN_MC10.DAT:** for the model of Compiègne et al. (2011),

- **GRAIN_J13.DAT:** for the model of Jones et al. (2013) as updated in Köhler et al. (2014).

- **GRAIN_G17_ModelL.DAT:** with L = A, B, C and D for the models of Guillet et al. (2018).

To be used, these files must be renamed to `GRAIN.DAT` within `/data`.

2.3 The size distribution

When the population keyword `size` is not set, the size distribution is defined from the parameters in `GRAIN.DAT`. The size grid has `nsize` points and is defined over the interval $[a_{min}, a_{max}]$ with a constant logarithmic step. For each grain of mass density ρ, the radius a is defined as that of an equivalent sphere of same mass $m = \rho\, 4\pi a^3/3$. The shape of the size distribution dn/da (the number of grains with radius in the range $[a, a+da]$) is defined by the following population keywords and parameters:

- **logn:** defines a log-normal size distribution with $dn/d\log a \propto \exp(-\log^2(a/a_0)/2\sigma^2)$. The centroid a_0 (in cm) and then width σ are given after a_{max} in `GRAIN.DAT`.

- **plaw:** defines a power-law size distribution $dn/da \propto a^\alpha$. The index α is given after a_{max} in `GRAIN.DAT`.

- **ed:** applies an exponential decay to a power law size distribution multiplying dn/da by the function
$$D(a) = \begin{array}{ll} 1 & \text{for } a \leq a_t \\ \exp(-\,[(a-a_t)/a_c]^\gamma) & \text{for } a > a_t. \end{array} \tag{1}$$
The parameters a_t, a_c and γ are given in this order after α in `GRAIN.DAT`.

- **cv:** applies a curvature term to a power law size distribution multiplying dn/da by the function
$$C(a) = [\,1 + |\zeta|\,(a/a_u)^\eta\,]^{\text{sgn}(\zeta)} \tag{2}$$
If `ed` is set with `cv` the parameters a_u, ζ and η are given in this order after γ in `GRAIN.DAT`. Otherwise they are given after α.

The keywords `ed` and `cv` allow the user to define a size distribution similar to that of Weingartner & Draine (2001a).

Alternatively, the size distribution of a given grain population can be read from a file. When the population keyword `size` is set the size distribution and the size grid are read from the file `/data/SIZE_tt.DAT` which must have the following format (not including the #-lines):

Size distribution of grain species
#
Nbr of size bins

```
# [ a (cm), a4*dn/da, rho(a) ]
#
5
3.000000E-08 2.264156E-01 2.240000E+00
3.703963E-08 2.674749E-01 2.240000E+00
4.573115E-08 3.159897E-01 2.240000E+00
5.646216E-08 3.733180E-01 2.240000E+00
6.971126E-08 4.410674E-01 2.240000E+00
```

The `SIZE_tt.DAT` file can be generated with the `Python` routine `/py/create_vdist.pro`. Note that *(i)* a size-dependent mass density $\rho(a)$ can be given in this file and that *(ii)* these values may be replaced (after size interpolation) by the $\rho(a)$ values if given in the `Q_tt.DAT` file (see end of section 2.5).

2.4   Grain physics

Physical processes affecting the grain properties are taken into account in `DustEM` thanks to population keywords often associated with data files from where parameters are passed. Below is the list of population keywords for the processes included in dustem:

- **mix:** applies a size dependent weighting factor f_{mix} when computing the contribution of the dust population to the extinction and emission. For each population `tt` featuring the `mix` keyword, a file `/data/MIX_tt.DAT` must be given containing a single column with weighting factors for each point of the size grid. The contribution to the emission and extinction of each size bin is then weighted by f_{mix}, allowing the user to generate a size dependent mixing of several dust types. For each size, the weighting factors must be consistent with $\sum_{tt} f_{mix}(tt) = 1$. In the example `GRAIN.DAT` shown above, neutral (`PAH0_MC10`) and ionized PAHs (`PAH1_MC10`) are mixed size by size in the model. The weighing factors (in the `MIX_tt.DAT` files) then corresponds to the fraction of neutral and ionized PAHs. In a coarser way, grain types can also be mixed with their mass fraction.

- **chrg:** if set, the equilibrium charge distribution $f(Z)$ of grains per size and type will be computed using the Kimura (2016) model for the photoemission yield and the Weingartner & Draine (2001b) formalism for the remaining processes. Details of the model can be found in Appendix B. The full Weingartner & Draine (2001b) model can be used by setting the keyword `chrgwd`. The computation of the grain charge requires the following data: the gas state in the file `/data/GAS.DAT` (see 2.6) and the quantities for grain charging in the file `/data/CHRG_tt.DAT`:

  ```
  # DUSTEM : Constants for charge distribution
  #
  # Wf(eV) p_uait(3) p_y(3) : bulk work function, Uait(V) and Y0 for WD01
  # p_6(2) p_se(3) cex : aromatic correction for a-C:H (scale and a/aR), electron sticking, charge exchange
  # p_ke p_le(4) : electron mean KE and le(nm)
  # p_ea(2) s_ea(2) : EA(nm) and cross-section, nr of Ebg values (if 1 Ebg constant)
  # Ebg(eV)
  #
  4.40 3.9 0.12 2.0 9.0e-03 3.7e-02 5.0
  0.0 2.0 0.5 1.0 1.0 1.0
  0.0 143.0 -2.0 5.4e-2 0.5
  0.4 0.7 0.5 3.0 1
  0.0
  ...
  #
  ```

Files with typical values for classical grain types can be found in the /data directory. In the following we detail some important control parameters. The grain charge distribution is sensitive to the electron sticking coefficient which is taken to be $s_e = \alpha(1 - \mathrm{e}^{-\beta a/l_e})$ where a is the grain radius and l_e is the electron mean free path (Kimura 2016) averaged over the distribution of photons above photoemission threshold E_{PE}. The first two values in the array p_se correspond to the Weingartner & Draine (2001b) model for s_e with $\alpha = 0.5$ and $\beta = 1$ [a]. If p_se(3) is positive, eq. (28) of Weingartner & Draine (2001b) (scaled by p_se(3)) is used in s_e. For a-C:H grains a correction to the photoemission thresholds (see appendix B) needs to be applied and is set by the p_6(2) parameter array. The cex parameter if positive allows to take into account charge exchange between C^+ and small grains of the type considered. The rate coefficient of this process is taken from Wolfire et al. (2008) and is scaled with cex. The p_ke parameter ($0 < $ p_ke ≤ 1) sets the fraction of the maximum available energy $h\nu - E_{PE}$ that goes into kinetic energy of the photoelectron released. If p_ke ≤ 0 the Weingartner & Draine (2001b) model is used. The size dependence of the band gap Ebg is controlled by the integer nbg: if nbg = 0 then Ebg = 0, if nbg = 1 the value given is used for Ebg and if nbg = -1 the band gap law for a-C:H grains will be used, namely $E_g(\mathrm{eV}) = \mathrm{MAX}\left[0.1, \, 0.2\left(\frac{5\,\mathrm{nm}}{a} - 1\right)\right]$ (see appendix B). Other size dependance laws of the bandgap can be used with nbg > 0 the number of size bins. The Ebg values are then expected as a single column with nbg lines corresponding to the number of size bins of the grain type (note that, having set the run keyword sdist, you can retrieve the size bin values in the file SDIST.RES). Finally, output on the charge of grains is obtained by adding the run keyword zdist (or zdistf to get the charge distribution $f(Z)$ of all grains).

- **zm:** allows to mix populations of neutral and charged grains with fractions given by the charge distribution $f(Z)$. This must be set for two consecutive grain populations in GRAIN.DAT (see section 2.1). For the first population (neutral grains) chrg-zm must be set and a weighting factor $f_{mix} = f(0)$ is applied for each size to the grain emission and extinction. For the second population (charged grains), chrg-zm is set again and the weighting factor for each size is then $f_{mix} = \sum_{|Z|>0} f(Z) = 1 - f(0)$. This mixing can be applied to any grain population and does not require any MIX_tt.DAT file. It is particularly useful in the computation of the emission and extinction of neutral and charged PAHs. For the gas heating and cooling, it is assumed that the neutral and charged species have same rates which are therefore added up for the first species with chrg-zm. In case this assumption is not verified, the rates for neutral and charged species must be obtained from distinct types each featuring the chrg keyword (i.e. without using zm).

- **spin:** turns on the emission of spinning PAHs following Draine & Lazarian (1998) for the gas-grain interactions and using the emission as derived in DustEM for the radiative IR excitation rates. The permanent electric dipole moment is assumed to be $\mu = m\,N^{1/2}$ where m is given in the file /data/SPIN_tt.dAT with the mean atomic molecular weight of the grain (can be size-dependent) to estimate N the number of atoms in the grain. The gas parameters are given in /data/GAS.DAT (see sec. 2.6). This option triggers the computation of the charge distribution of each grain.

- **pol:** turns on the computation of the polarized emission and extinction. This requires the files Q1_tt.DAT, Q2_tt.DAT to be in /oprop. These tabulated cross-sections for polarization must be averaged over the grain dynamics around magnetic field lines. The fraction of aligned grains or *alignment function* $f(a)$ is size dependent. We use a parametric step function

$$f(a) = \frac{1}{2}\,f_{\max}\left(1 + \tanh\left(\frac{\ln\left(a/a_{\mathrm{alig}}\right)}{p_{\mathrm{stiff}}}\right)\right).\tag{3}$$

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[a]The widely used Bakes & Tielens (1994) model corresponds to $s_e = 1$, an hypothesis which has noticeable consequences for the gas emission (Verstraete 2011).

where f_{max} gives the maximum fraction of aligned grains, a_{alig} is the size corresponding to $f = 0.5$ and p_{stiff} controls the size range for the transition between $f = 0$ and $f = 1$. Parameters for the polarization model must be given in the file `/data/ALIGN.DAT`, please refer to Guillet et al. (2018) for a detailed description of parameters and files.

```
# DUSTEM: definition of grain alignment
# for each grain TYPE make sure you have the following files in ../oprop
# Q1_TYPE.DAT and Q2_TYPE.DAT
#
# run keywords
# lin (for linear), univ (for universal alignment law)
# degree of anisotropy of the radiation : keep it to 0.
# par (parametric alignment law) followed by parameters a_alig, p_stiff and f_max
#
lin univ
0.00E+00
par 8.0E-02 2.7E-01 6.7E-01
```

If the `univ` keyword is set, the same alignment function $f(a)$ is used for all grain types and only the first parameters line (`par ...  `) in ALIGN.DAT will be used to define $f(a)$. If the `univ` keyword is not set, then parameters lines must come in same number and order as that of the grain types for which the `pol` keyword was added in the file `GRAIN.DAT`.

- **beta:** applies a correction to Q_{abs} to introduce a temperature dependence, namely:

$$Q_{abs}(a, \nu) = Q_0(a, \nu) \, (\nu/\nu_t)^{\delta(T) \, H(\nu_t/\nu)} \tag{4}$$

where Q_0 is the grain emissivity without the temperature dependence, $\nu_t = c/\lambda_t$ is the frequency threshold and $\delta(T) = \beta(T) - \beta_0$ is the index correction with respect to β_0 some reference value. The threshold function in frequency is $H(x) = 0.5 \, (1 + \tanh(4x/s))$ where $x = \log(\lambda/\lambda_t)$ and s controls the stiffness of the transition from 0 to 1 (the width Δx is proportional to s): for instance for $s = 1$ $H(x)$ rises from 0 to 1 for x between 0.5 to 1.5 and $\Delta x = 1$. Parameters for this correction are in `/data/BETA_tt.DAT`:

```
# DUSTEM: parameters for BETA(T) behaviour of Qabs
# first DBETA correction to standard index beta0
# then lambda threshold to apply BETA(T)
#
# beta0 a g bmax
# lthresh(microns) lstiff (dlambda=lthresh/lstiff)
# nbetav (nr of beta values if 0 uses formula)
# tbeta betav (if nbetav >= 0)
#
2.11E+00 1.15E+01 -6.60E-01 5.00E+00
3.00E+01 1.00E+00
13
1.00E+00 1.55E+00
...
```

where $lthresh$ and $lstiff$ stand for the above λ_t and s. If $nbetav = 0$ then $\beta(T) = a \, T^g$ (Désert et al. 2008) and we take $\beta = \min(\beta, bmax)$. If $nbetav > 0$ the $\beta(T)$-values must be given below $nbetav$ in two columns T and β.

- **dtls:** adds the low temperature opacities of amorphous grains as described in Meny et al. (2007). Uses the file `/data/DTLS_tt.DAT`:

```
# DUSTEM: constants for the DCD and TLS effects
# a_dtls lc(nm) c_delta
#
```

vt(cm/s) P*mub²gamma_e(eV)
omega_m(s-1) tauO(s-1) Vo(K) Vmin(K) Vm(K)
ldtresh(microns)
#
5.81 1.34e+01 4.75e+02
3.00e+05 1.40e-03 5.00e-01
2.69e+12 1.00e-13 410.0 50.0 550.0
1.00e+02

where all parameters are from Meny et al. (2007), with a_{dtls} the relative weight of the DCD to TLS effects and *ldtresh* is the wavelength threshold above which these effects are taken into account. The absorption efficiency per grain type and size is thus:

$$Q_{abs}(\lambda) \quad = \quad Q_{DCD} + a_{dtls}Q_{TLS}, \quad \lambda \geq ldthresh$$
$$Q_0, \qquad\qquad\qquad \lambda < ldthresh$$

where Q_0 is the absorption efficiency without the DCD-TLS effects as read in the Q_tt.DAT file (see sec. 2.5). The DCD-TLS absorption efficiencies are defined such that for $\lambda = ldthresh$ one has $Q_0 = Q_{DCD} + a_{dtls}Q_{TLS}$.

2.5 Grain data

For a given type of grain `tt`, the grain properties are provided as a function of the size a in the data files, namely: `Q_tt.DAT` files for the absorption and scattering efficiencies, $Q(a, \lambda)$, and `C_tt.DAT` files for the heat capacity per unit volume, $C(a, T)$. The Q and C values are provided over the broadest possible size range (usually 0.3 to 10^4 nm). A grain type can be used once these `Q` and C-files exist in the `DustEM` data file set, in the optical properties `/oprop` and heat capacity `/hcap` directories respectively. The sizes requested in `GRAIN.DAT` or `SIZE_tt.DAT` have to fit into those of the above files (i.e. extrapolation is not allowed). When `DustEM` is coupled to radiative transfer codes (e.g. `PDR, CRT, SKIRT`), the g-factors[b] are required at all wavelengths and for all sizes: they are given in `/oprop/G_tt.DAT`. In the case of spherical grains, the `Q` and G-files are generated with the Mie theory (`bhmie` Bohren & Huffman 1983) while for spheroidal grains the T-matrix method is used (Mischenko & Travis 1998). We briefly outline below the format of these files.

The `Q`-files are as follows:
QABS and QSCA to be used by DUSTEM
#
nsize (number of sampled sizes in this file)
sizes (microns)
50
3.0000E-04 3.7104E-04 4.5891E-04 5.6759E-04 7.0200E-04 8.6824E-04 1.0738E-03 1.3281E-03 ...
#
QABS
1.3461E-03 1.6642E-03 2.0571E-03 2.5419E-03 3.1398E-03 3.8762E-03 4.7819E-03 5.8952E-03 ...
...
QSCA
5.0179E-07 1.1650E-06 2.6935E-06 6.1884E-06 1.4083E-05 3.1594E-05 6.9380E-05 1.4766E-04 ...

The first uncommented line gives the number of sizes present in the file. The line next gives the sizes (in microns). Then for each grain size (one column per size), the absorption Q_{abs} and scattering Q_{sca} efficiencies are given. The G-files have a similar format as the Q-files with the

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[b]The anisotropy factor for scattering defined as $< \cos\theta >$ where θ is the scattering angle.

QABS field replaced by $g(a,\lambda)$ and no QSCA field. The `Q` and `G`-files are all generated with th common wavelength grid given in `/oprop/LAMBDA.DAT`.

The `Q1` and `Q2`-files for polarization have a content similar to that of `Q`-files.

The `C`-files look like this:
DUSTEM heat capacity
#
nr of sizes ns
sizes (microns)
nr of T-values
log T(K) log C_1...log C_ns (erg/K/cm3)
50
3.0000E-04 3.7104E-04 4.5891E-04 5.6759E-04 7.0200E-04 8.6824E-04 1.0738E-03 1.3281E-03 ...
30
-1.0000E+00 4.8983E-01 4.8983E-01 4.8983E-01 4.8983E-01 4.8983E-01 4.8983E-01 4.8983E-01 4.8983E-01 ...

The first uncommented line gives the number of sizes present in the file and the second line gives the sizes in microns. The third line gives the number of points in the temperature grid. The following gives the $\log_{10}$ of temperatures (in Kelvin, column 1) and the $\log_{10}$ of heat capacities (one column for each size) in units of erg/K/cm3 . The same temperature grid (30 points from 0.1 to 5,000 K with a constant log step) is used for all `C`-files. This temperature grid is given in `/hcap/TEMP.DAT`.

The grain data is generated with the `DustProp` IDL package (based on publically available codes and not included in the `DustEM` distribution). We list below the grain types for which `Q` and `C`-files are available in the current `DustEM` distribution:

- **PAH0_DL01, PAH1_DL01:** PAHs as defined in Draine & Li (2001) for neutral and singly charged PAHs, respectively.

- **PAH0_DL07, PAH1_DL07:** PAHs as defined in Draine & Li (2007) for neutral and singly charged PAHs, respectively. It takes into account the transition to graphite optical properties for $a > 50$ (Draine 2003),

- **PAH1_MC08:** PAHs described in Compiègne et al. (2008),

- **PAH0_MC10, PAH1_MC10:** PAHs as defined in Compiègne et al. (2011) for neutral and singly charged PAHs, respectively,

- **Gra:** graphite grains. The Q-values have been generated with the Mie method for spherical particles. The refractive index and heat capacity are as described in Draine & Li (2001); Li & Draine (2001),

- **amCBEx:** amorphous carbon grains. The Q-values have been generated with the Mie method. The refractive index is from Zubko et al. (1996) and the Q_{abs} have been extrapolated above 0.9 mm (see Compiègne et al. 2011). The heat capacity is the same as that of graphite,

- **aSil:** astronomical silicates. The Q-values have been generated with the Mie method. The refractive index and heat capacity are as in Draine & Li (2007),

- **BG_MC08:** big grain as originally defined in Désert et al. (1990) and modified by Compiègne et al. (2008),

- **CM20:** carbonaceous grains as defined in Jones et al. (2013). Grains up to 20 nm consist purely of aromatic-rich H-poor amorphous carbon, a-C, whereas bigger grains have a core/mantle structure, where the core is made of aliphatic-rich H-rich carbon, a-C:H, and the mantle of a-C with a thickness of 20 nm,

- **aOlM5 + aPyM5:** silicates as defined in Köhler et al. (2014). These core/mantle grains consist of amorphous silicate cores (olivine and pyroxene-normative composition, Mg-rich) and 5 nm mantles of a-C,

- **amCBE_0.3333x:** spheroidal amorphous carbon grains (see above) including the data for polarized emission and extinction (Guillet et al. (2018),

- **aSil_0.3333_p20B, aSil2001_0.3333_p20B** and **aSil2001BE6pctG_0.4x**: spheroidal astronomical silicates (see above) including the data for polarized emission and extinction (Guillet et al. (2018).

Finally, data files for the Désert et al. (1990) model are also available corresponding to the grain types **PAH0_DBP90, PAH1_DBP90, VSG_DBP90** and **BG_DBP90**.

Grains with size-dependent mass density $\rho(a)$ can also be handled. The mass density values need to be calculated on the size grid of the `Q_tt.DAT` file and must be given in that file right after the size array. To use these $\rho(a)$ values for a given grain type `tt` you then need to turn negative the corresponding mass density in the `GRAIN.DAT` file. If the keyword `size` is used for the grain type `tt`, the $\rho(a)$ values from the Q-file will supersede those given in the `SIZE_tt.DAT`.

2.6 Astrophysical data

The radiation field used by `DustEM` is in `/data/ISRF.DAT`. This file contains 2 columns, the wavelength (microns) and the flux $4\pi I_\nu$ in erg/s/cm^2/Hz. The wavelength range must fit in that of the `LAMBDA.DAT` file. It can be generated with the `create_rfield.pro` routine in `/pro`. Note that in order to estimate the energy absorbed by a grain, this radiation field will be interpolated on the wavelength grid for the optical properties (`LAMBDA.DAT`). The current distribution includes `ISRF_MATHIS.DAT`, the standard radiation field of Mathis et al. (1983) and `ISRF_CMB.DAT` where the CMB contribution has been added to the Mathis field.

Parameters for the gas are given in `/data/GAS.DAT` as

DUSTEM : Gas quantities

#

Gas temperature (K), hydrogen density, H2 density, CR rate, G0 (if>0 supersedes GRAIN.DAT), nr of charge type (e-, H+, C+, ...)

ion density (cm-3), mass (amu), charge, polarizability (Ang3)

>>>>> 1st line is electron <<<<<<

>>>>> 2nd line is proton <<<<<<

>>>>> 3d line is ionized carbon <<<<<<

>>>>> ... etc other massive cations <<<<<<

#

1.00E+02 3.00E+01 0.00E+00 5.00E-17 1.00E+00 3

3.00E-02 5.4858E-04 -1.00 0.00

2.40E-02 1.00794 1.00 0.67

6.00E-03 12.0107 1.00 1.54

If the gas temperature value *tval* given in `GAS.DAT` is negative, it will be used to estimate the gas temperature from a thermal pressure-G_0 relationship (Joblin et al. 2018), namely $T_{\mathrm{gas}} =$

$tval \times G_0/n_H$. Similarly, if the given H_2 density value is negative, the density computed from the formation-dissociation equilibrium of H_2 is used (with an assumed dissociation rate of 5^{-11} s^{-1}). If negative the G_0 value in GAS.DAT will not be used. Otherwise, if positive, this G_0 value will supersede the value given in GRAIN.DAT.

The abundances of the main charged species (e^-, p and C^+) are important for the grain charge and the gas photoelectric heating. Values for the electron and C^+ density must be given in the GAS.DAT file. The proton density value will be superseded by $n_p = n_e - n_m$ with n_e the electron density and n_m the density of heavy cations (usually only C^+ so that $n_m = n_{C^+}$ [c]). Positive values for n_e and n_{C^+} as given in /data/GAS.DAT will be used directly.

If n_e is negative, the value at ionization equilibrium (cosmic ray ionization balanced by proton recombination) is used complemented by the approximation of Williams et al. (1998) in dense, cold gas and

$$n_e = n_H \, \text{MAX}(x, x_{dc}) \tag{5}$$

with $x_{dc} = 10^3 \left(\frac{\zeta}{n(H_2)}\right)^{1/2}$ and $x = n_e/n_H = 0.5 \left(x_m - x_{cr} + \sqrt{(x_m + x_{cr})^2 + 4x_{cr}}\right)$ where x_m is the abundance of ionized metals (C^+, Si^+, Fe^+,...etc), $x_{cr} = \zeta/(n_H\alpha)$ with ζ the cosmic-ray (CR) ionization rate per proton and α the proton recombination rate (in cm^3/s, taken from Röllig et al. 2006).

If the given n_{C^+} is negative, the electron density n_e is first computed from the coupled equilibria of protons (eq. 5) and C^+ possibly involving charge exchange reactions with grains[d]. The C^+ density is then calculated assuming $n_m = n_{C^+}$. Finally the proton density is derived as described above. These results also depend on the total carbon gas abundance which is taken to be the absolute value of the (negative) number given for n_{C^+} in the GAS.DAT file.

Several template GAS.DAT files can be found in the /data directory:

- **GAS_MC.DAT** for molecular gas from Draine & Lazarian (1998),

- **GAS_CNM.DAT** and **GAS_CNM_WD01.DAT** for the Cold Neutral Medium from the work of Wolfire et al. (1995) and Draine & Lazarian (1998); Weingartner & Draine (2001b) respectively,

- **GAS_WNM.DAT** and **GAS_WNM_WD01.DAT** for the Warm Neutral Medium from the work of Wolfire et al. (1995) and Draine & Lazarian (1998); Weingartner & Draine (2001b) respectively,

- **GAS_PDR.DAT** for photon-dominated regions from Draine & Lazarian (1998).

3 Output files

The utput files produced by DustEM are stored in /out. They give the dust emission and extinction. Each file begins with documentation lines (first character is #). Any DustEM run will produce the 2 following files:

---

[c]Other more massive cations (S^+, Si^+, Mg^+, Fe^+) could be included but this would require the knowledge of their polarizability.

[d]This derivation couples two equilibrium equations: the cosmic ray/proton recombination and the photoionization/neutralization of C^+, the latter process involving reactions with H_2 and charge exchange with PAHs (see Ysard et al. 2011). The charge exchange with grains of type tt is controlled from the CHRG_tt.DAT file by setting the charge exchange parameter to 1.0 (see sec. 2.4).

- **SED.RES:** contains the emission per proton for each grain population $4\pi\nu I_\nu/N_H$ in erg/s/H as a function of wavelength (N_H is the proton column density). The last column is the total of all previous columns.

- **EXT.RES:** contains the extinction opacity for a column density $N_\mathrm{H} = 10^{21}$ H cm^{-2} for each grain population. The last column is the sum of all previous columns, *i.e.* the dust optical depth:

$$\tau(\lambda) \;\; = \;\; N_\mathrm{H} \sum_{tt} \left(\sigma_{abs}^{tt}(\lambda) + \sigma_{sca}^{tt}(\lambda) \right) \tag{6}$$

$$A_\lambda \;\; = \;\; 1.086 \times \tau(\lambda) \tag{7}$$

If the run keywords `temp`, `zdist` or `sdist` are used, the files `TEMP.RES`, `ZDIST.RES` or `SDIST.RES` will be written and will contain, respectively, the temperature, charge or the size distribution of the dust populations. Full temperature and charge distribution per grain type and size are obtained if `tempf` or `zdistf` are set. All these files have a documented header.

Use of the population keywords `pol` or `spin` will generate the following files:

- **SED_POL.RES:** contains the polarized emission of aligned grains, with the same format as `SED.RES`.

- **EXT_POL.RES:** contains the polarized extinction by aligned grains, with the same format as `EXT.RES`.

- **SPIN.RES:** contains the emission of spinning grains with the same format as `SED.RES`.

Using the run keyword `res_a` will generate the files `SED_A.RES`, `SED_POL_A.RES` and `SPIN_A.RES` which contain the same information, namely, the emission per grain in size bin $[a, a + da]$ or $4\pi\nu I_\nu/N_d(a)$ in erg/s/grain ($N_d(a)$ is the column density of grains of size a).

4 DustEM Python

Below is a list of the Python routines in the `/py` directory with the use for each. To use a routine `rname`, documentation is obtained by typing

```
> from rname import *
> rname().
```

- **get_band_flux** (in `band_flux`) : returns structure (dictionary) with band or spectral flux (MJy/sr) in instrument filter,

- **create_rfield**: generates the radiation field in erg/cm2/s/Hz for DustEM,

- **create_vdist** : generates a normalized dust size distribution for DustEM,

- **dm4cldy** : generates a grain opacity file for Cloudy from DustEM data,

- **rebin_oprop** : rebin DustEM optical properties of a given grain type,

- **show_dustem** : shows the results of DUSTEM overlaid on diffuse ISM data,

- **show_tdist** : shows temperature distribution of grains computed by DustEM,

- **show_zdist** : shows charge distribution of grains computed by DustEM.

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A Comparison to other models

Figure 1 shows the comparison between the Draine & Li (2007) model as tabulated and re-trieved on the B.T. Draine webpage[e] and the `DustEM` output obtained using the input file `GRAIN_DL07.DAT`.
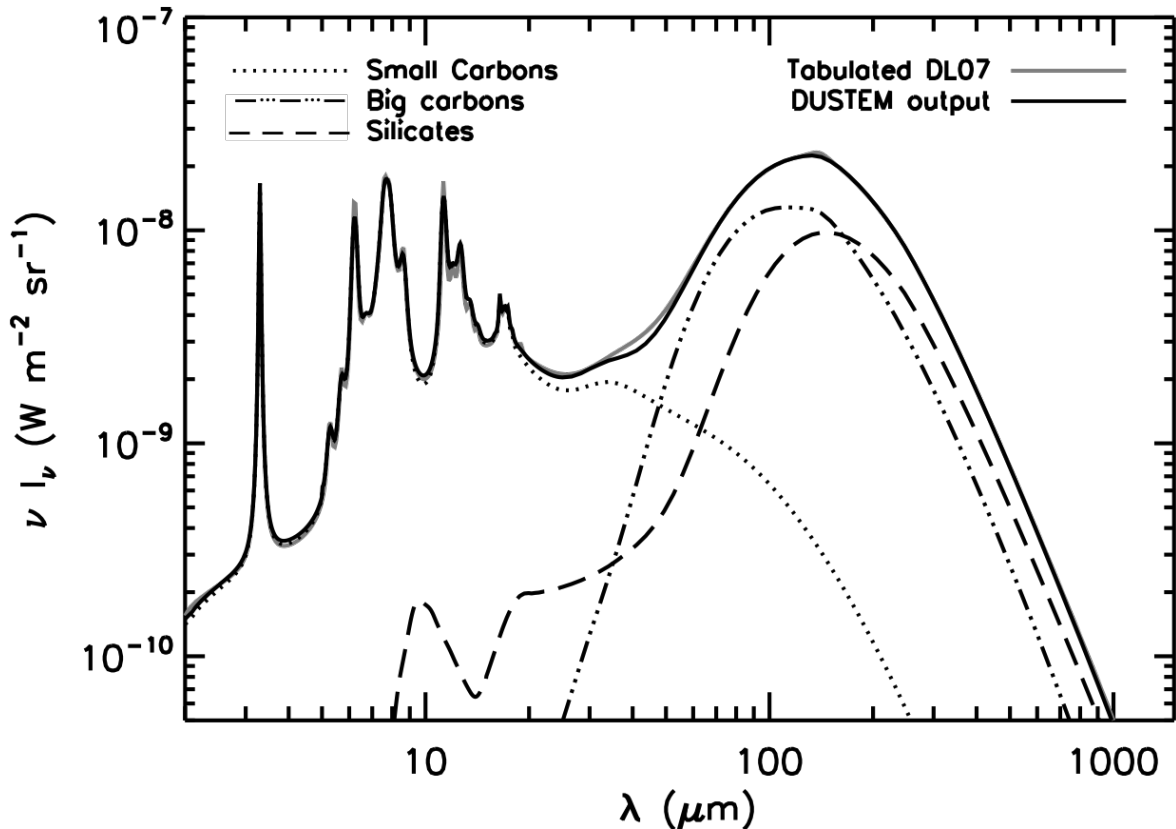

Figure 1: Comparison between the tabulated version and the output of `DustEM` for the Draine & Li (2007) model.

B Grain charge model

The `DustEM` grain charge model follows the work of Weingartner & Draine (2001a); van Hoof et al. (2004); Weingartner et al. (2006) with significant amendments: the photoemission model of Kimura (2016) has been implemented and we have adapted the photoemission thresholds for a-C:H and silicate grains.

The plain Weingartner & Draine (2001a) model can still be used in `DustEM` by setting the `chrgwd` grain type keyword (see sec. 2.4).

B.1 Photoemission model

In the classical photoemission models of Draine (1978), Bakes & Tielens (1994) and Weingartner & Draine (2001a) the photoemission process is described from bulk properties of the grain material. Since the gas photoelectric heating is dominated by the contribution of small nanometric grains (e.g. Bakes & Tielens (1994)), finite-size effects must be taken into account in the pho-toemission model. Still assuming spherical grains, the Kimura (2016) model revisits the work of Watson (1973) by considering that the photoelectrons produced can escape the grain only if a
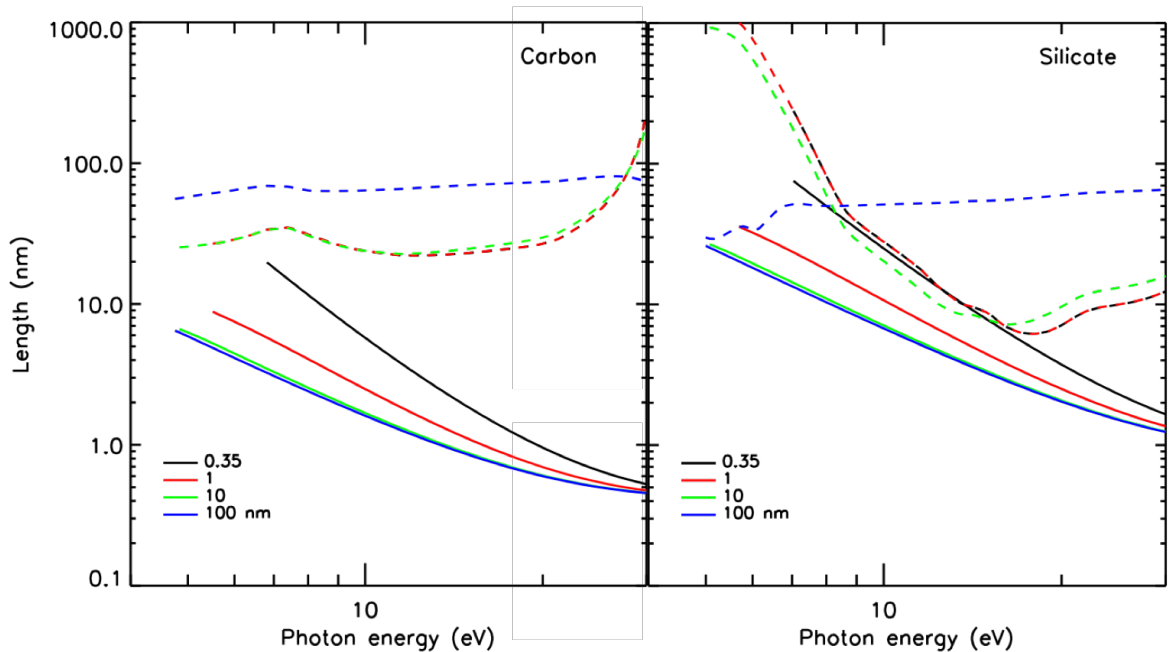
---

[e]http://www.astro.princeton.edu/~draine/

Figure 2: Photon attenuation length (dashed line) and electron mean free path (solid line) for grains of radius $a = 0.35, 1, 10$ and 100 nm. Left shows the case of carbonaceous grains (`amCBE`) and right that of silicates (`aSil`).

component of their kinetic energy perpendicular to the grain surface exceeds the work function W. As a consequence the photoemission yield depends on the work function and on the grain curvature, thus featuring a dependence on the grain radius different from that of Watson (1973).

Nanometric dust grains also have specific optical properties that are best described from their absorption and scattering efficiencies (in the `Q`-files, sec. 2.5). In a medium composed of dust grains of radius the photon attenuation length can be expressed from the optical theorem (Krügel 2003) as $l_a = \left(n_g\, \pi a^2\, Q_e\right)^{-1}$ where n_g is the density of grains. In the case of a single grain, $ng = \frac{3}{4\pi a^2}$ and we therefore estimate l_a as

$$l_a = \frac{4a}{3Q_e} \tag{8}$$

where $Q_e = Q_{\mathrm{abs}} + Q_{\mathrm{sca}}$ the extinction efficiency and a the grain radius. This expression replaces the bulk estimate derived from the refractive index (eq. (14) of Weingartner & Draine (2001a)). In particular, eq. (8) allows to take into account the case of heterogeneous or composite grains. Kimura (2016) also introduced a more realistic description of the photoelectron mean free path l_e by taking into account its dependence on the electron energy E. Figure 2 shows the derived l_a as well as the mean free path of the photoelectron l_e as a function of the photon energy $h\nu$[f] As discussed in Draine (1978), typical values for carbon material are $l_e = 1$ nm and $l_a = 10$ nm but fig.2 shows that more realistic values deviate significantly, in particular for l_e. This affects significantly the photoemission yield which depends on length related quantities, namely $\alpha = \beta + a/l_e$ and $\beta = a/l_a = 3Q_e/4$ (see eq. (A12) of Kimura (2016)).
In figure 3, we show the photoemission yield of several grain sizes and types as computed from the Kimura (2016) model and from the Weingartner & Draine (2001a) model. Note that Y_a corresponds to the product $Y_0 Y_1$ defined in Weingartner & Draine (2001a). In this comparison we note striking differences. In the case of carbon grains, we first see that the Kimura (2016)

---

[f]For each photon energy value, we took $E = <K> + W$ where $<K>$ is the kinetic energy of the photoelectron averaged over a parabolic distribution (Weingartner & Draine 2001a).
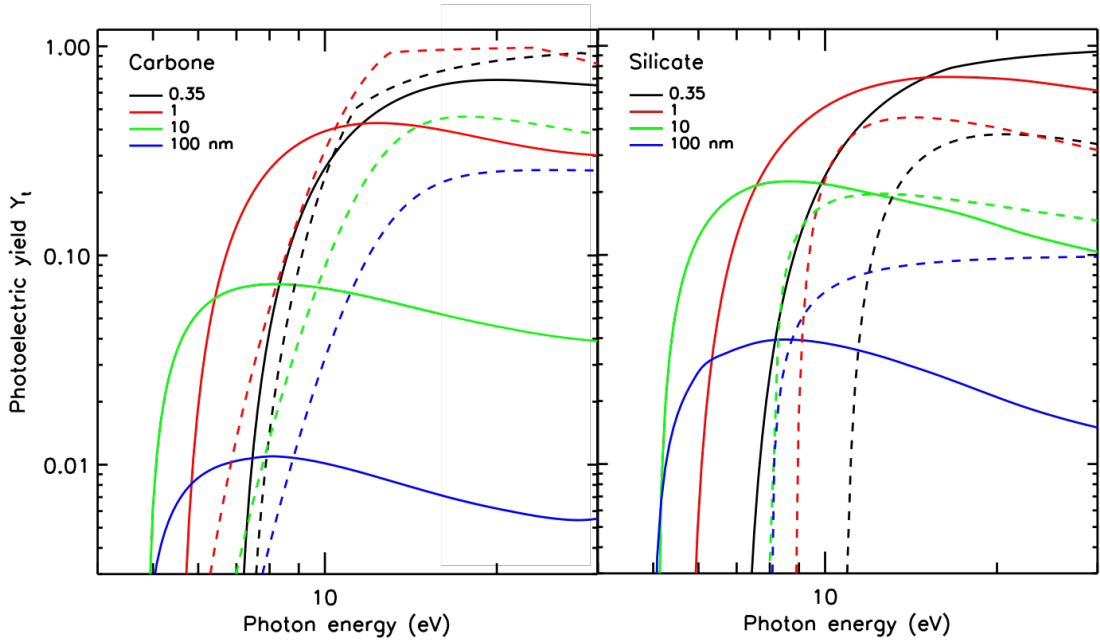
Figure 3: Total photoemission yield $Y_t = Y_a Y_2$ for various grain sizes. Y_a is the photoemission yield and Y_2 is the fraction of these electrons that actually escape the grain (Weingartner & Draine 2001a). The dashed line shows the yield of Weingartner & Draine (2001a) and the solid line that of Kimura (2016). In both models the Y_2 function of Weingartner & Draine (2001a) has been used. For carbon grains we used the optical properties of graphite in Li & Draine (2001) and adopted $W = 4.75$ eV. In the case of silicates we used the optical properties from Draine & Li (2007) and took $W = 4.97$ eV as in Kimura (2016).

yield decreases faster with the grain size than the Weingartner & Draine (2001a) does, in better agreement with experiments as already noted by Weingartner & Draine (2001a) (the note 4 of their paper) and further discussed by Kimura (2016). This decrease of the yield with size is mitigated by the broader plateau in the Kimura (2016) model (see for instance the red curves). Also noteworthy is the case of the smallest carbon grains $a = 0.35$ nm where the two yields are
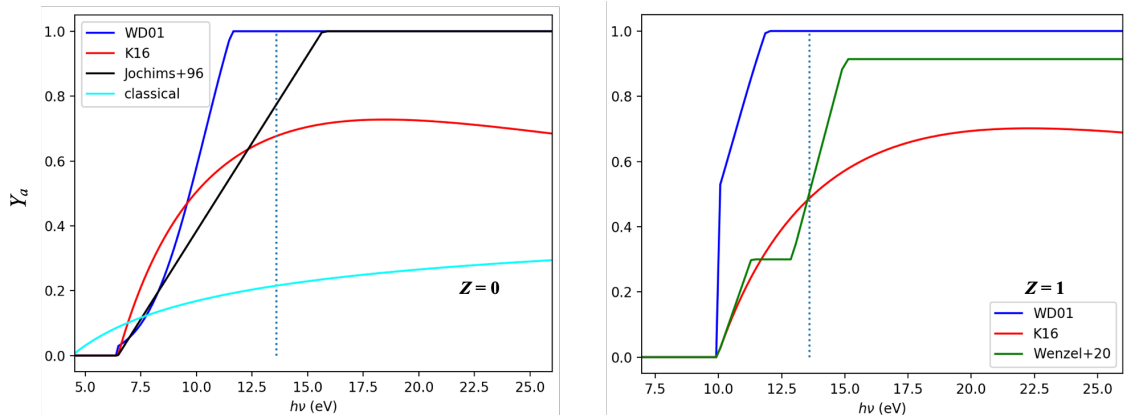

Figure 4: Photoemision yield Y_a as a function of the absorbed photon energy for a carbon grain of radius $a = 0.44$ nm with 40 C-atoms. The red solid line shows the yield from Kimura (2016) and the blue solid line shows the yield from Weingartner & Draine (2001a). The dotted line shows the Lyman limit at $h\nu = 13.6$ eV. *Left:* comparison of the yield of a neutral grain to the measurements of Jochims et al (1996) on small PAHs and to the semi-classical model $Y = \frac{1}{2}\left(1 - \sqrt{\frac{W}{h\nu}}\right)$ (cyan curve, Kimura (2016)). *Right:* comparison of the yield of a singly positively charged grain with the measurements of Wenzel et al. (2016) on PAHs.

quite comparable (black solid and dashed lines) and also in good agreement with yield measurements on small PAHs (Weingartner & Draine 2001a). However, while the Weingartner & Draine (2001a) model assumes the bulk yield y_0 to have the right form and absolute level (eq. (16) of their paper) to match the measurements, the Kimura (2016) model provides a direct match to measurements without any fudge factors. For the case of silicates we follow Kimura (2016) and adopt $W = 4.97$ eV (instead of 8 eV in the Weingartner & Draine (2001a) model, see next section). This smaller W-value for silicates explains why the Kimura (2016) yields are higher, however showing the same trends as those of carbon grains (fast decrease with size and broader plateau). On figure 4 in the case of small carbon grains, we compare the model yield of Weingartner & Draine (2001a) and Kimura (2016) to laboratory measurements. For photon energies below 13.6 eV (which corresponds to the common case of neutral interstellar regions), the best fit to the measured yield is obtained with the Kimura (2016) model while the Weingartner & Draine (2001a) model clearly overestimates the measurements. Conversely, the Weingartner & Draine (2001a) yield is a better representation for photon energies above 13.6 eV relevant for fully ionized interstellar regions, if small carbon grains can survive in these harsh conditions.

In figures 5 and 6, in the case of the cold neutral medium (CNM as defined in Table 1 of Draine and Lazarian 1998), we compare the charge distributions obtained with `DustEM` and the Kimura (2016) photoemission model to the Weingartner & Draine (2001a) results. As can be expected from the behaviour of the photoemission yield, the mean charge of grains increases less rapidly as a function of size in the Kimura (2016) model. We also note that the charge distribution for grains of radii less than 1 nm are comparable, leading to comparable gas photoelectric heating rates of the order of a few 10^{-26} erg/s/H.

In figure 7 we show the mean ($\overline{Z}$) and equilibrium (Z_{eq}) charge in the case of CM20 grains (Jones et al. 2013) and for the diffuse cold neutral medium. We note that both quantities reach a maximum at size $a \simeq 90$ nm (a similar result is obtained for graphite and silicates grains). Not observed with the Weingartner & Draine (2001a) model, this maximum is a consequence of the rapid decrease of the photoemission yield with size (see above and fig. 3). This maximum charge only disappears in molecular cloud conditions. Figure 7 also shows the gas photoelectric heating power per unit grain mass. We see that this heating power increases strongly as the grain size decreases, a consequence of the drop of the photoemission yield with grain size (see fig. 3). We also note that the increase of the photoelectric heating at sizes below 7 nm is a result of the threshold increase (aromatic correction) discussed below.
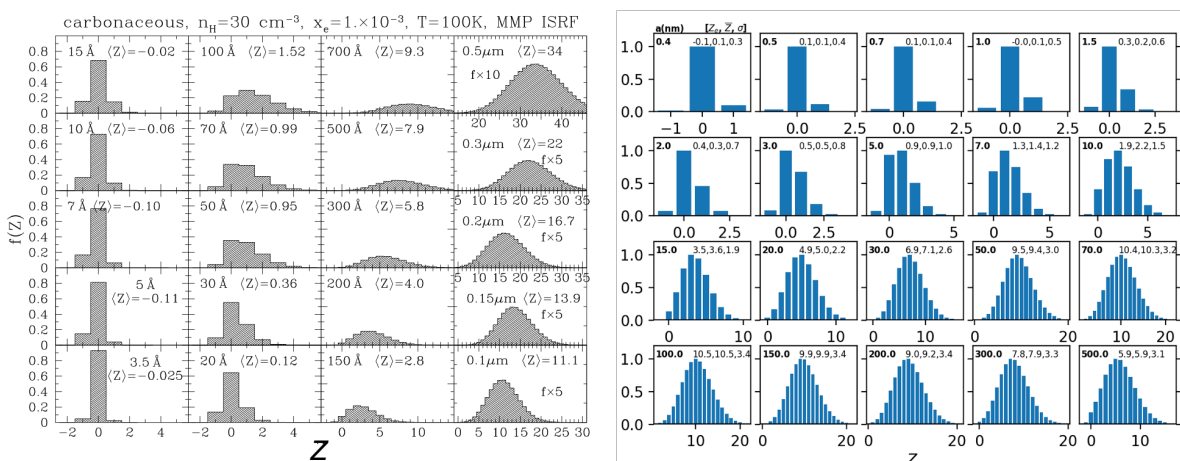

Figure 5: Charge distribution $f(Z)$ for graphite grains in the conditions of the CNM (see text). *Left:* $f(Z)$ from the Weingartner & Draine (2001a) model and *right:* $f(Z)$ from DustEM where the bold number gives the grain size in nm and the 3 other numbers give respectively the mean and equilibrium charges as well as the standard deviation of $f(Z)$.
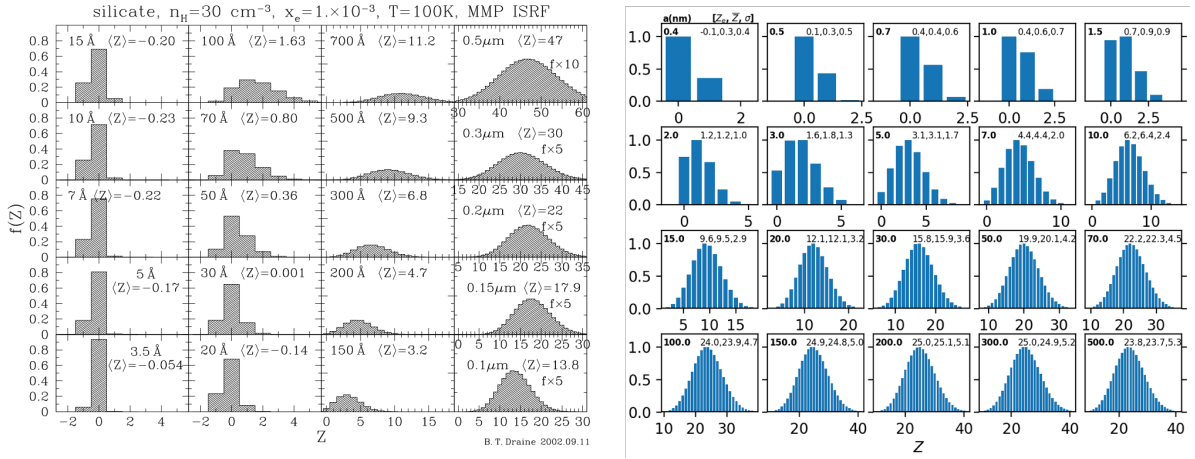
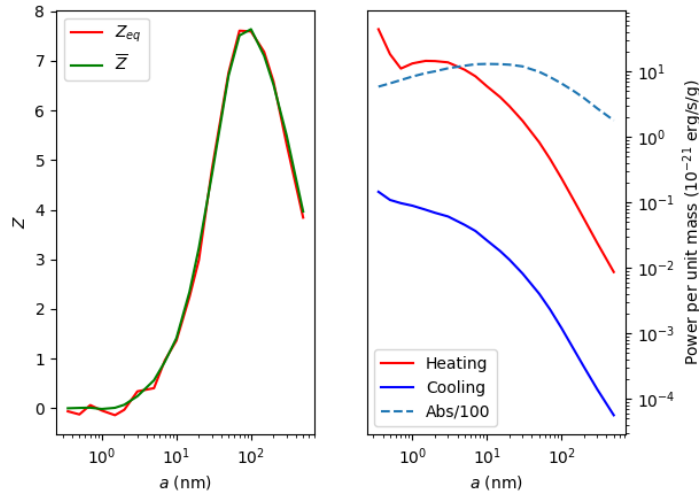Figure 6: Same as figure 5 but for silicate grains and with $W = 4.97$ eV (see text).

Figure 7: In the case of CM20 grains in CNM conditions, *Left:* mean and equilibrium charge as a function of grain size and *right:* powers per unit mass as a function of size for photon absorption, photoelectric gas heating and gas cooling by recombination of electrons, protons and C^+ atoms.

B.2 Photoemission thresholds for a-C:H and silicate grains

As discussed in Jones et al. (2013), amorphous hydrogenated carbon grains (or a-C:H grains) are predominantly composed of carbon [g] and hydrogen atoms engaged in sp, sp^2 and sp^3 bonds. Among these, the π-bonds from aromatic domains have low thresholds for the ejection of an electron. Thus photoelectrons will come from the largest aromatic domain (of radius a_R) which has the lowest threshold. If the grain is neutral or positively charged, the electron is taken from the valence band and the threshhold is called ionization potential (IP). In the case of a negatively charged grain, the electron stems from the lowest accessible state above the valence band: in that case the threshold is the electron affinity (EA). For the case of a-C:H grains we write the thresholds as

$$
\begin{aligned}
\text{IP} &= W + \frac{e^2}{2C_R} + \frac{Ze^2}{a} = W + \left(Z + \frac{1}{2}\right)\frac{e^2}{a} + A_C \\
\text{EA} &= W - E_g - \frac{e^2}{2C_R} + \frac{Ze^2}{a} = W - E_g + \left(Z - \frac{1}{2}\right)\frac{e^2}{a} - A_C
\end{aligned}
\tag{9}
$$

---

[g] Other atoms such as N and O may come in place of C. Due to the lower abundance of these atoms with respect to C we will not discuss this case.

18

where $W \simeq 4.75$ eV is the amorphous carbon work function, E_g the band gap and Z the relative number of charges born by the grain. The threshold includes the energy required to bring the electron away from the electrical influence of the grain. The $e^2/2C_R$ term is the energy to separate an electron from the largest aromatic domain, taken to be a conductive disk of radius a_R with capacitance $C_R = \frac{2}{\pi} a_R$. The term Ze^2/a is the energy required to take the electron out of the grain Coulomb potential. We see that the classical thresholds of Bakes & Tielens (1994) need to be corrected with A_C, the aromatic correction, $A_C = \frac{e^2}{2a} \left[\frac{\pi}{2} \frac{a}{a_R} - 1 \right]$. The radius of the largest aromatic domain a_R is tightly correlated to the grain band gap as well as with its radius. In particular, the largest aromatic domain has the lowest band gap (Robertson 1986) relevant for EA. The size distribution of aromatic domains in a-C:H grains is poorly known and we simply assume that the largest aromatic domain has a radius half that of the grain, $a_R = a/2$. We now
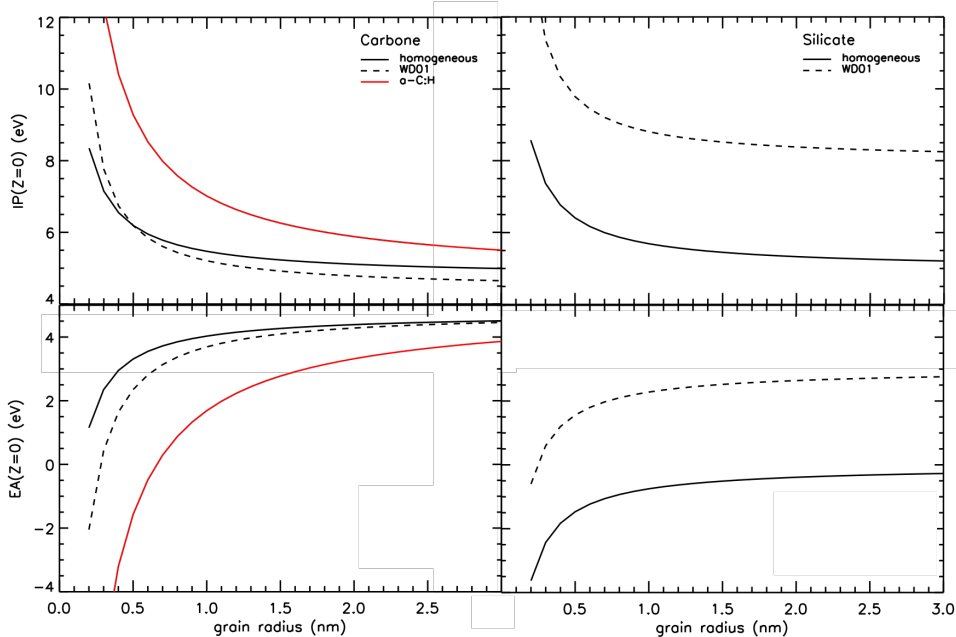

Figure 8: Thresholds for photoemission by carbonaceous and silicate grains. The red curve shows the case of CM20 grains with aromatic correction A_C. The black solid for silicates correspond to $W = 4.97$ eV.

turn to the expression of the lowest band gap. As discussed in Jones (2012), the size of the grain itself limits the size of the largest aromatic domain allowed which then fixes the lowest allowable band gap. This leads to an empirical band gap lower limit

$$E_g \,[\mathrm{eV}] = 0.2 \left(\frac{5\,\mathrm{nm}}{a} - 1 \right). \tag{10}$$

As a further limitation, we consider a minimum band gap at $E_g = 0.1$ eV for the larger ($a > 3$ nm) grains (Jones 2012).

In the case of silicates, we follow Kimura (2016) and adopt a work function $W = 4.97$ eV, a value determined on lunar dust by Feuerbacher et al. (1972). In fact, the value of 8 eV used by Weingartner & Draine (2001a) applied to the standard model of gas photoelectric heating from Draine (1978, see p. 597 of the paper), meant to describe both carbonaceous and silicate material. The resulting thresholds are shown in fig. 8. In the case of carbon grains, the aromatic correction A_C (red curve) tends to increase the threshold, keeping CM20 grains neutral thus more prone to let an electron go for gas heating.

Finally, for all types of grains, `DustEM` takes into account the van Hoof et al. (2004) modification for the photodetachment (see also Weingartner et al. (2006)).