The role of grain charge

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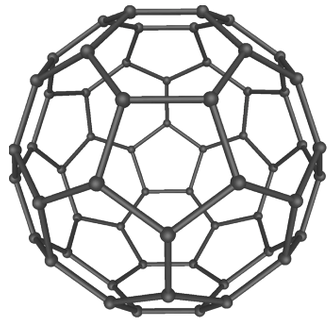
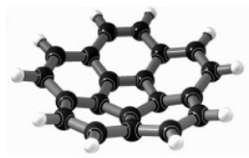
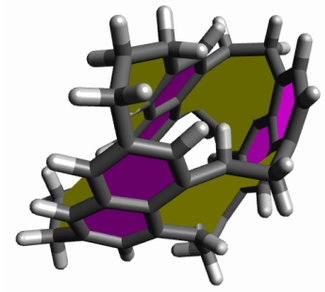
Galactic Lifecycle

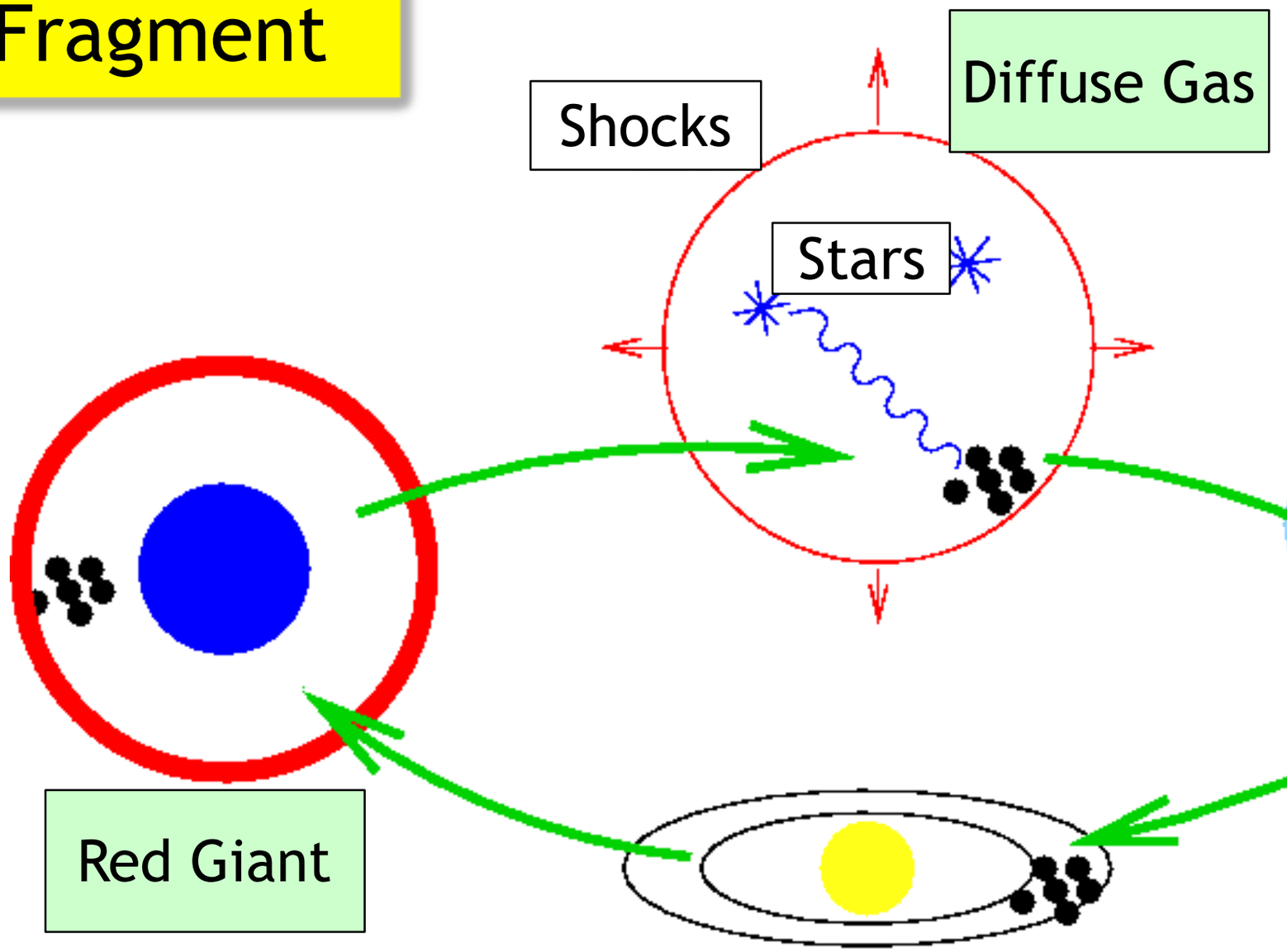


Fragment



dn/da
f(Z)

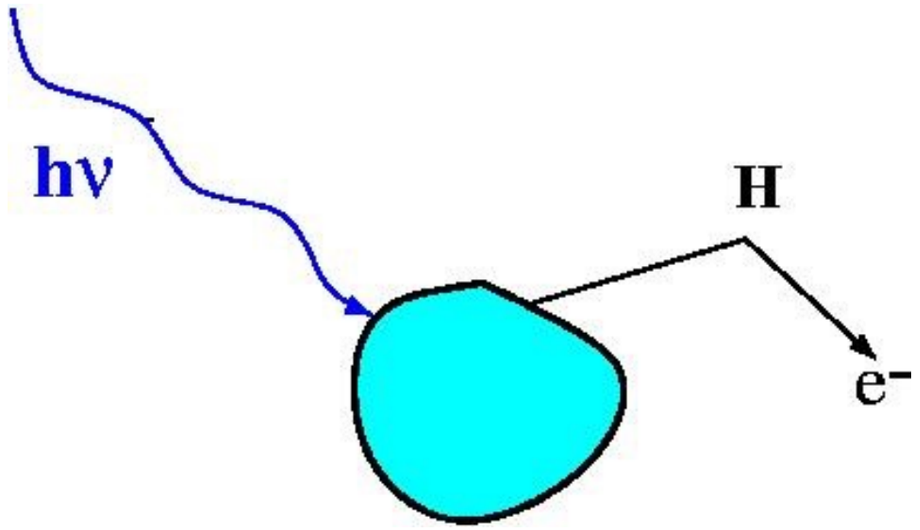




Grow

The dust impact

1% in mass…



✓ Heat the gas

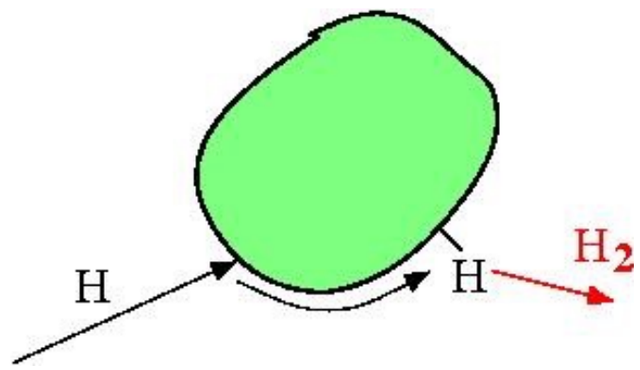
✓ Form H_2

Size a
Charge Z

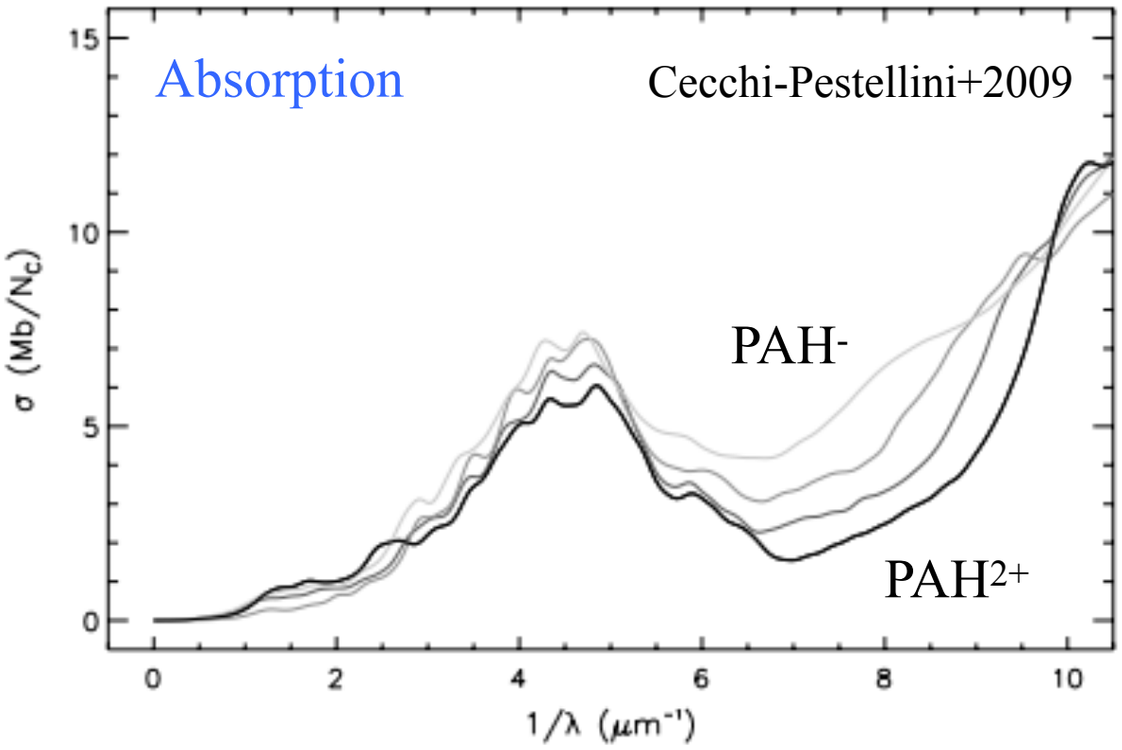
✓ control rad. transfer

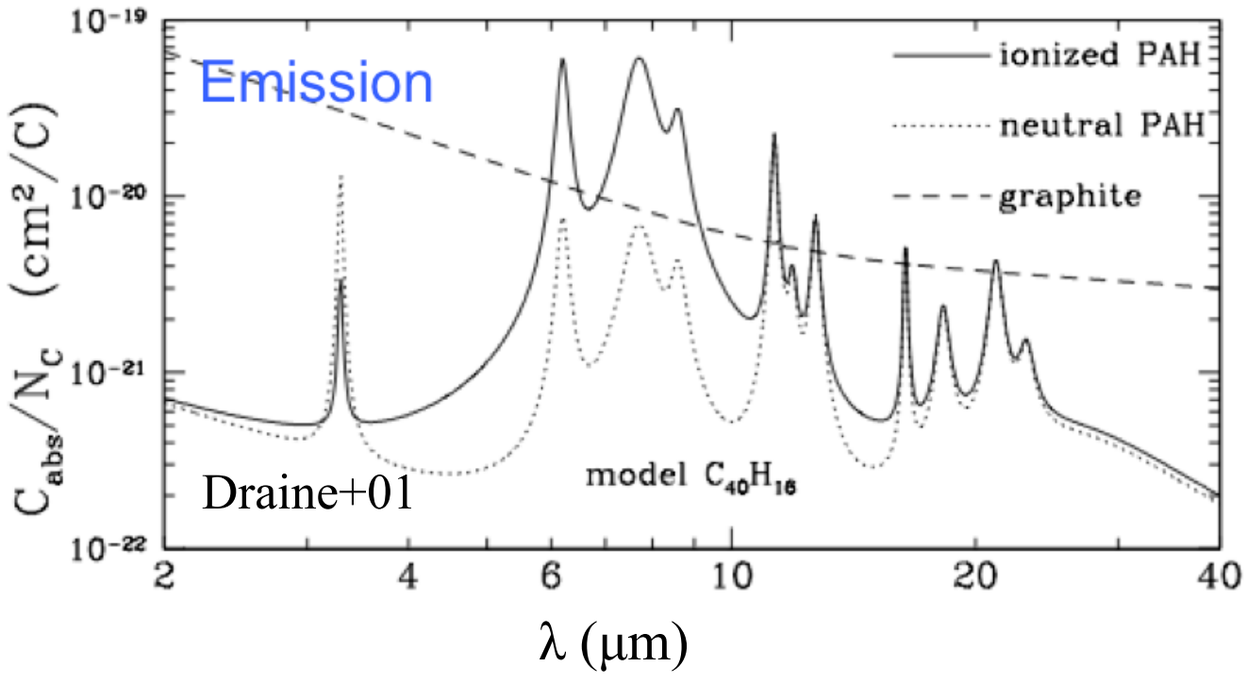
✓ Coupled to $\vec{B}$

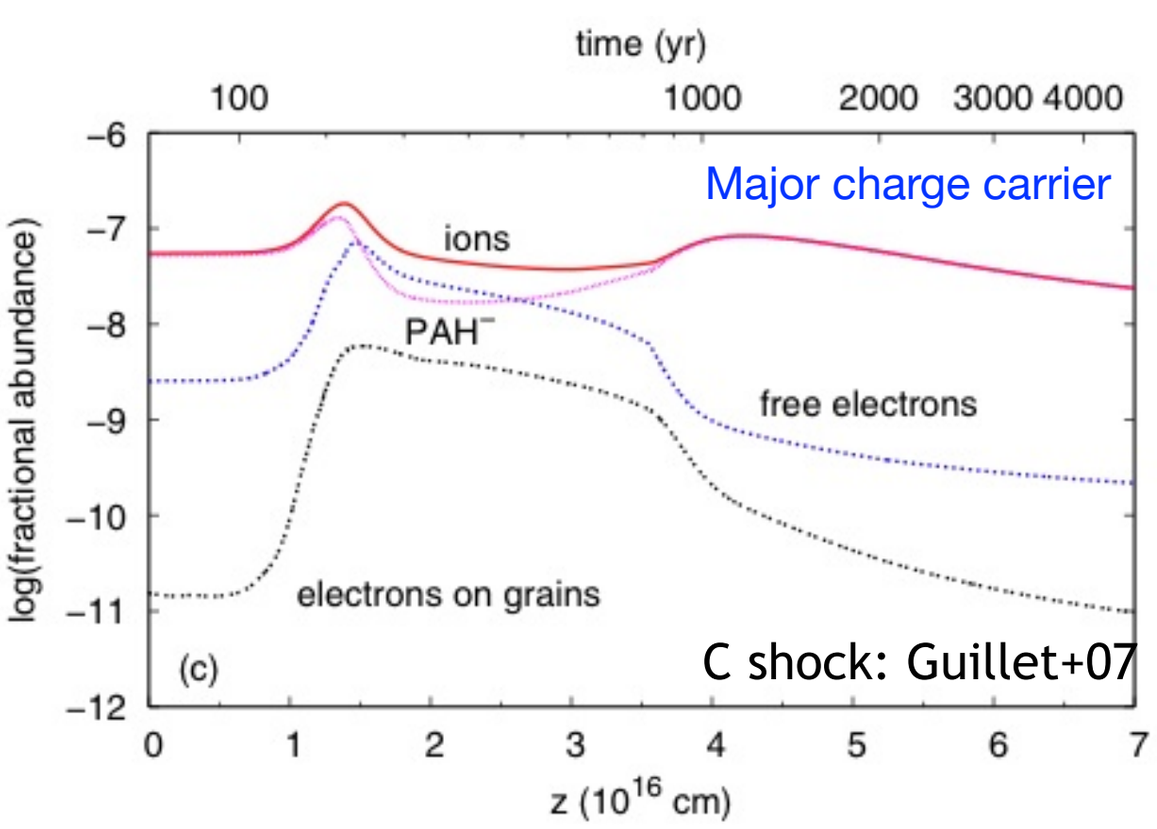
✓ And powerful diagnostic n_H, G_0…

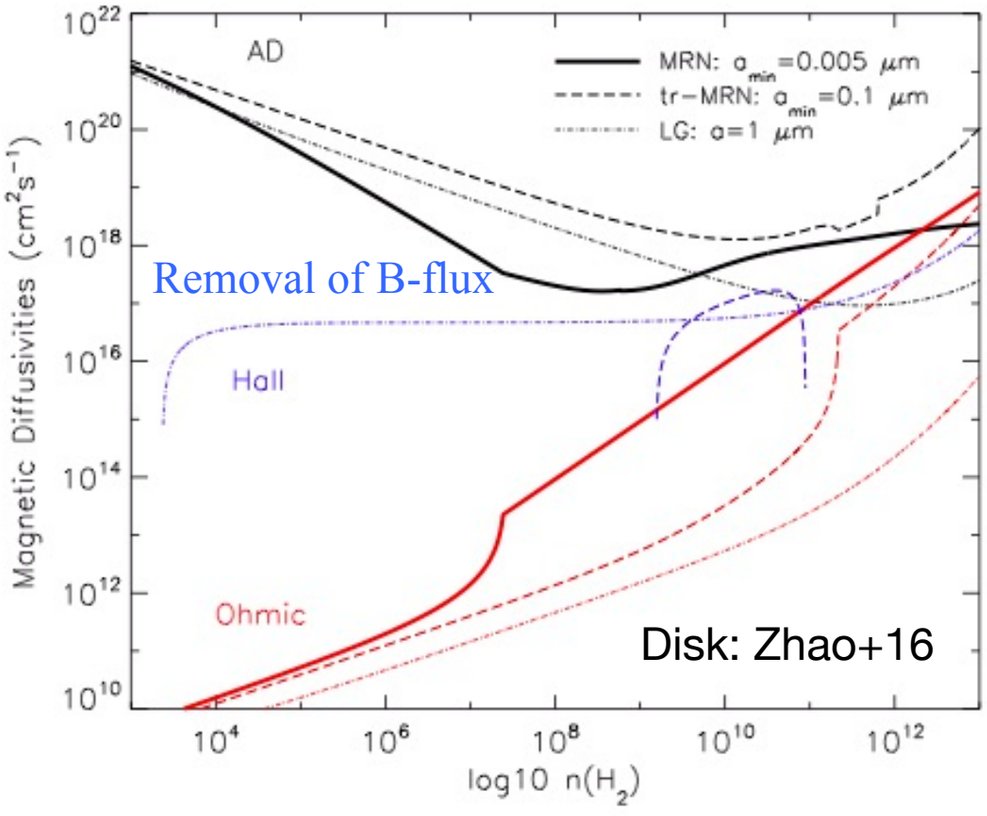


Importance of grain charge









Charge model

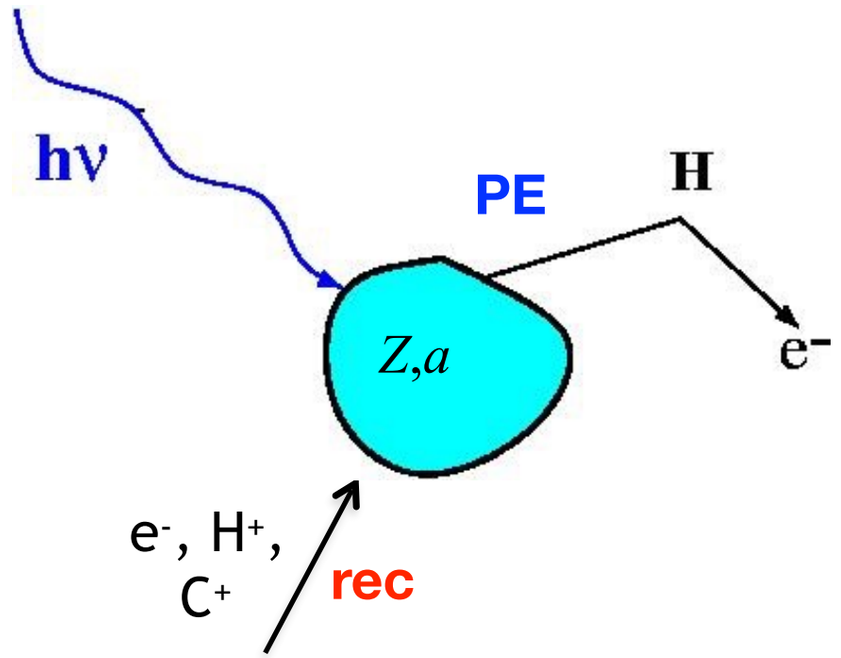
Bakes & Tielens 1994, Weingartner & Draine 2001,2006

Equilibre stationnaire des taux d'échange de charge (s^{-1})

$J_{PE} f(Z) = J_e f(Z+1) + J_i f(Z-1)$ $\quad \tau_Z \sim 10^4$ (100 cm^{-3}/n_H) yrs

Z: charge algébrique du grain, f(Z) distribution
J_{PE} : effet **photoélectrique** (courant cm^{-2} s^{-1}),
J_i et J_e : **recombinaison** des ions (H^+, C^+) les plus abondants et des électrons

dépend de G_0, T, n_e, n_i et de quantités microscopiques probabilités d'effet photoélectrique Y_{PE} et de collage s_i



$$J_{PE}\,(Z,a)\ (s^{-1}) = \int_{IP}^{h\nu_0} 4\pi\, I_\nu\, Y_{PE}\, \sigma_{abs}\, d\nu$$

Effet photoélectrique

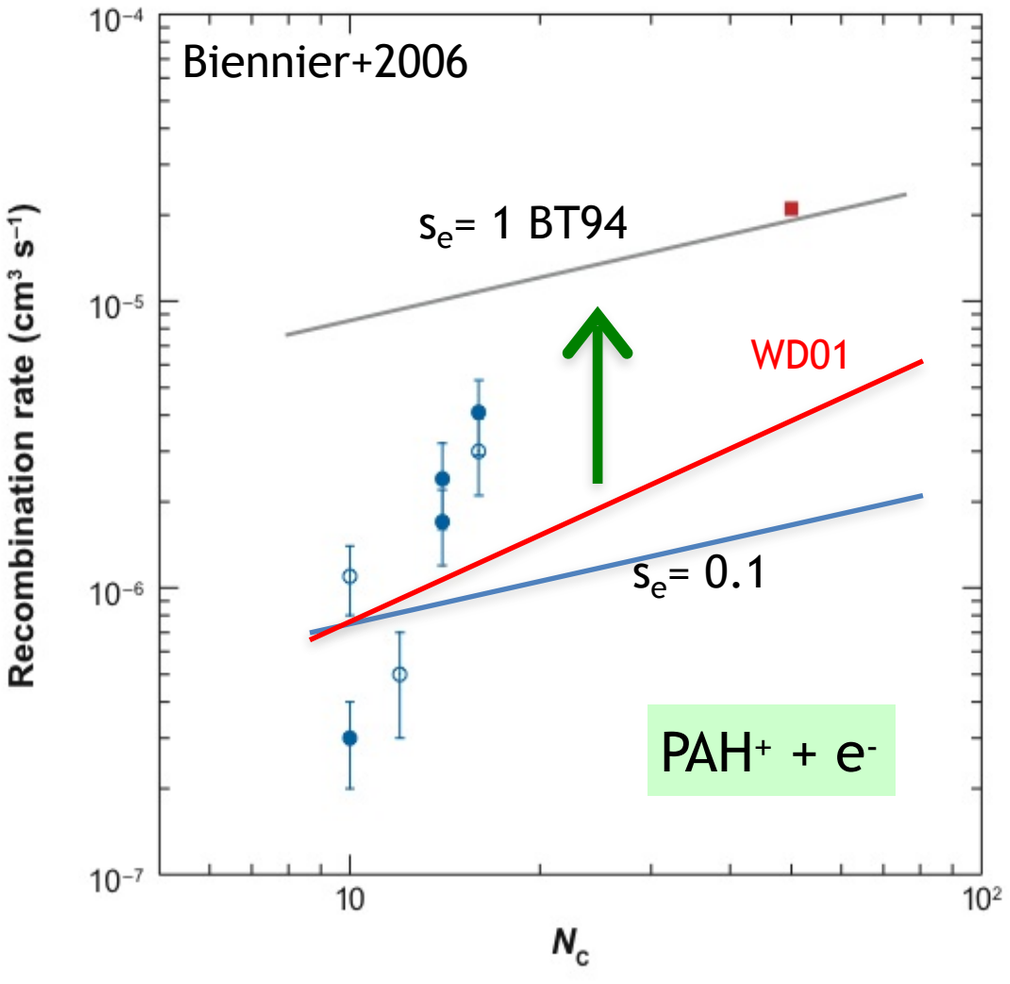
$$J_i(Z) = n_i\, s_i \left(\frac{8kT}{\pi m_i}\right)^{1/2} \pi a^2 \tilde{J}\left(\tau = \frac{akT}{{q_i}^2},\ \nu = \frac{Ze}{q_i}\right)$$

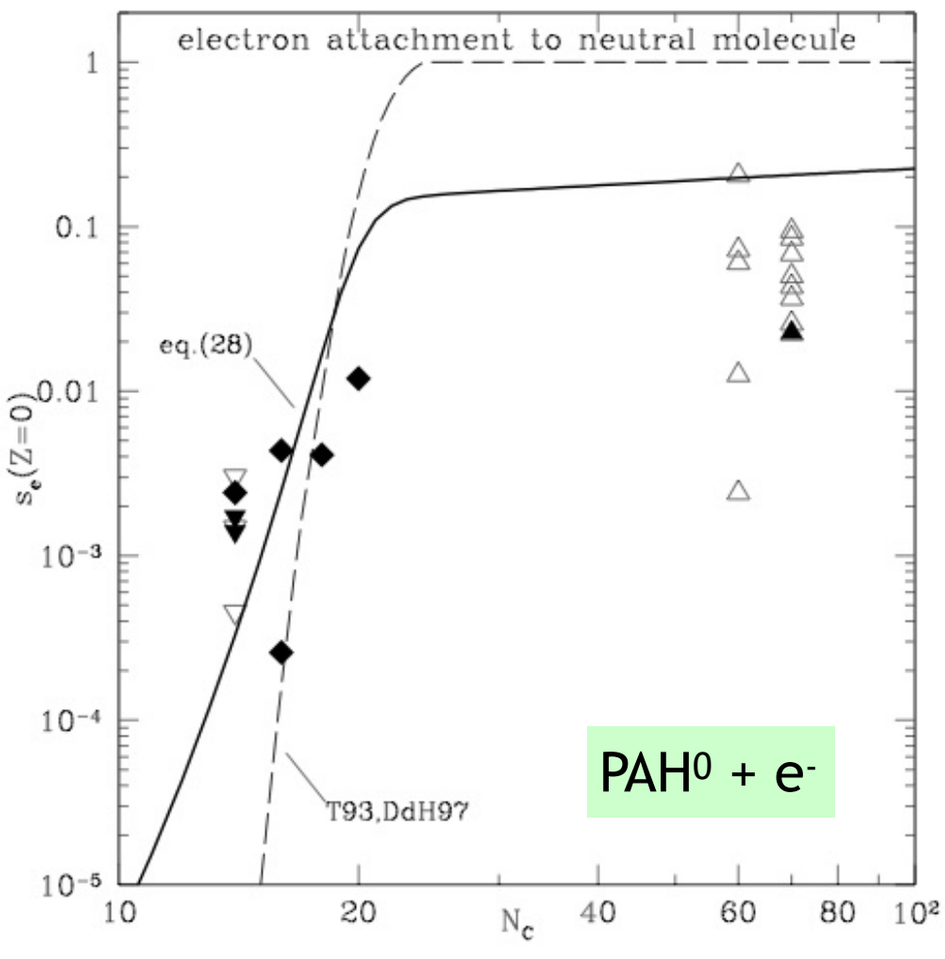
recombinaison de e$^-$, H$^+$, C$^+$

Recombination and attachment

Rates coefficients (cm^3/s) are estimated classically with a sticking coefficient s_i

dust(Z) + i(q_i) $$J_i(Z) = n_i s_i \left(\frac{8kT}{\pi m_i}\right)^{1/2} \pi a^2 \tilde{J}\left(\tau = \frac{akT}{{q_i}^2}, \nu = \frac{Ze}{q_i}\right)$$ i = e^-, H^+ and C^+ (Draine & Sutin 1987)



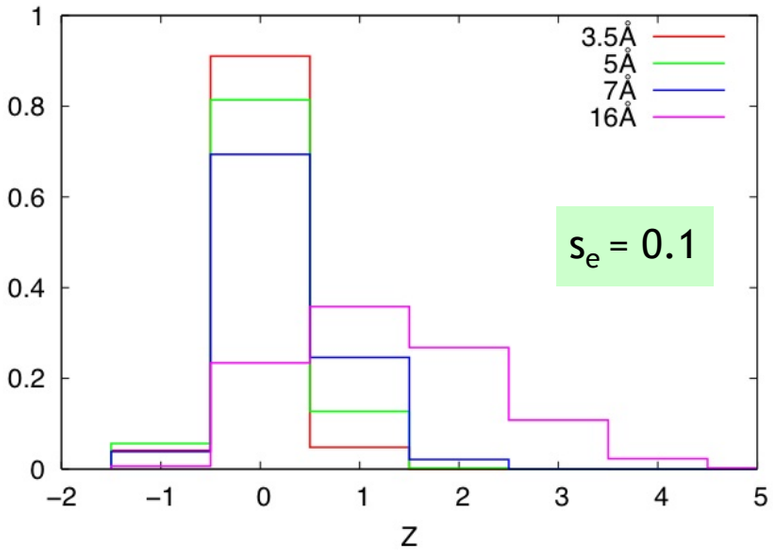


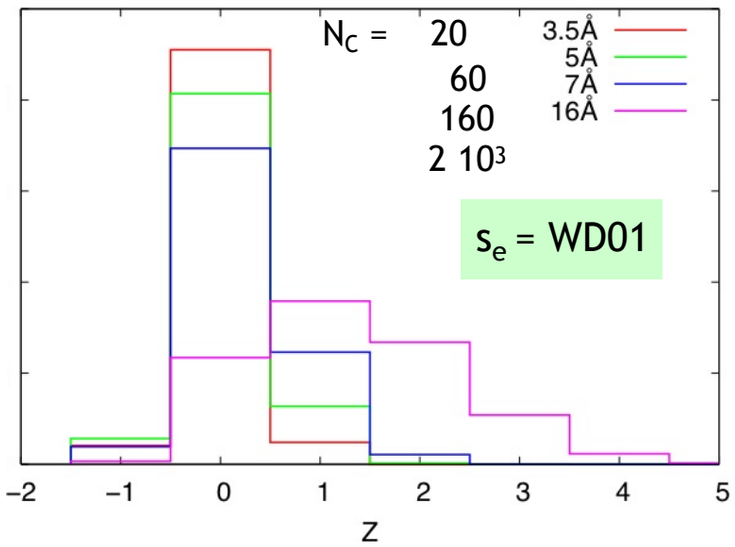
Experiments also show a steeper T-behaviour $J_e \sim T^{-3/2}$ ($T \geq 80$ K)

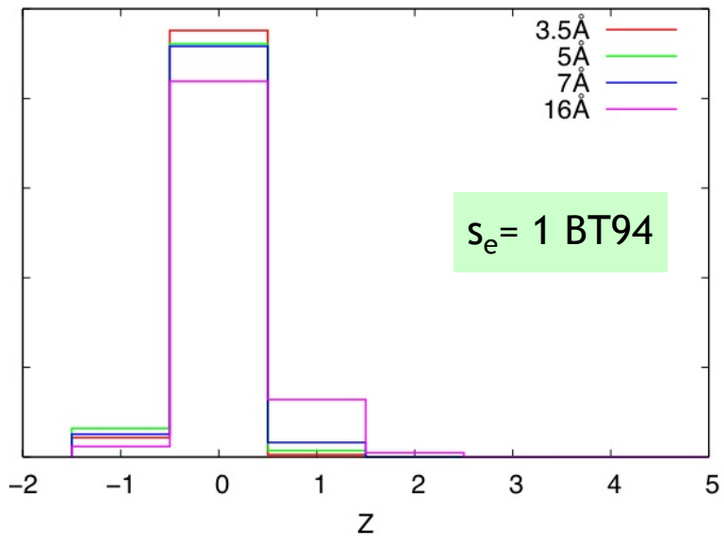
Sticking coefficients for higher charge states are assumed to be the same.

Charge distribution of Cold Diffuse medium: n_H = 100 cm^{-3} and Mathis ISRF

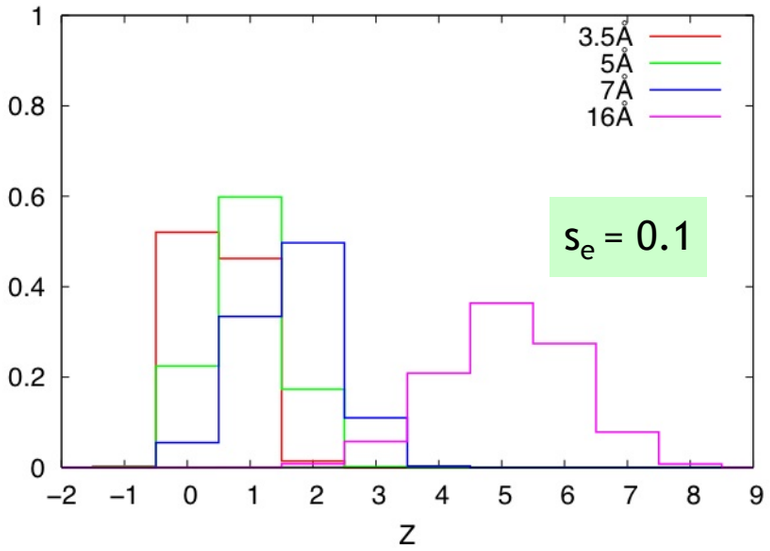
G_0 = 1 T = 55 K, x = 2.4 10^{-4} **$G_0\ T^{1/2} / n_e$ ~ 300**

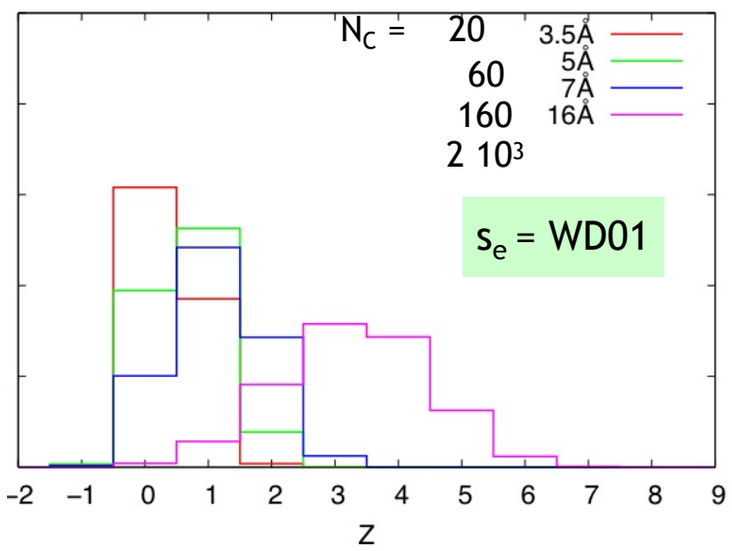


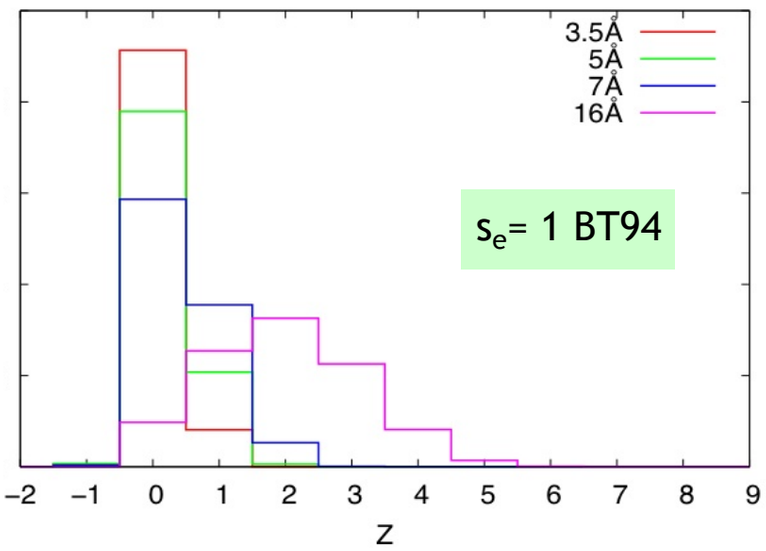




G_0 = 10 T = 192 K, x = 2.6 10^{-4} **$G_0\ T^{1/2} / n_e$ ~ 5,300**

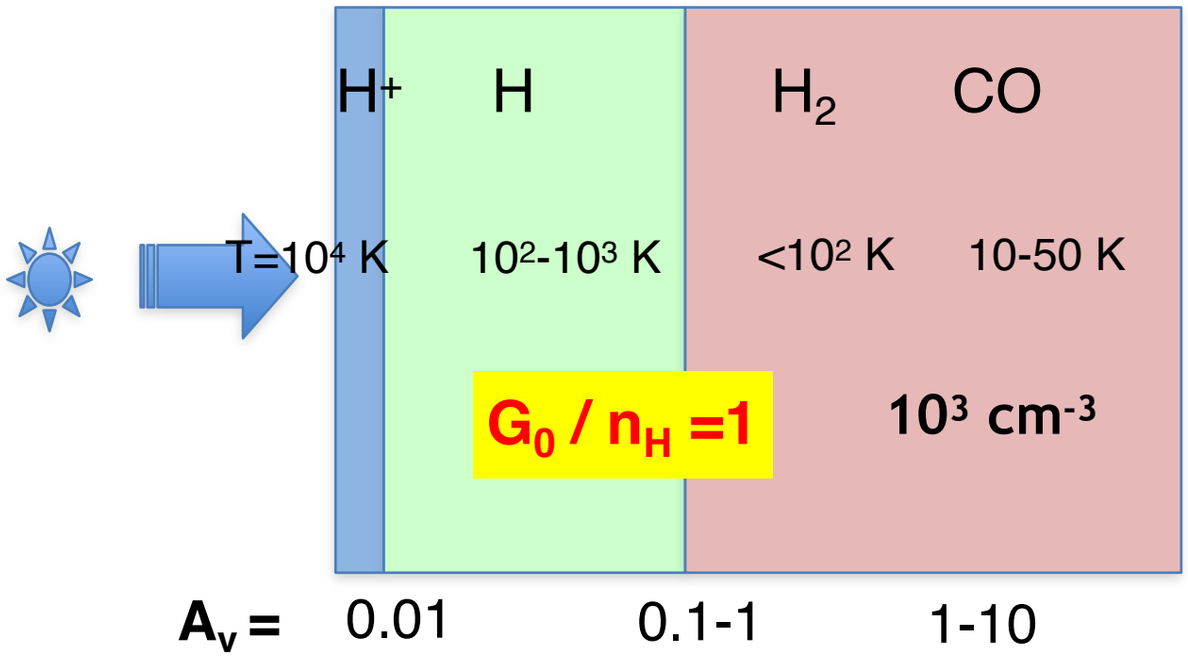


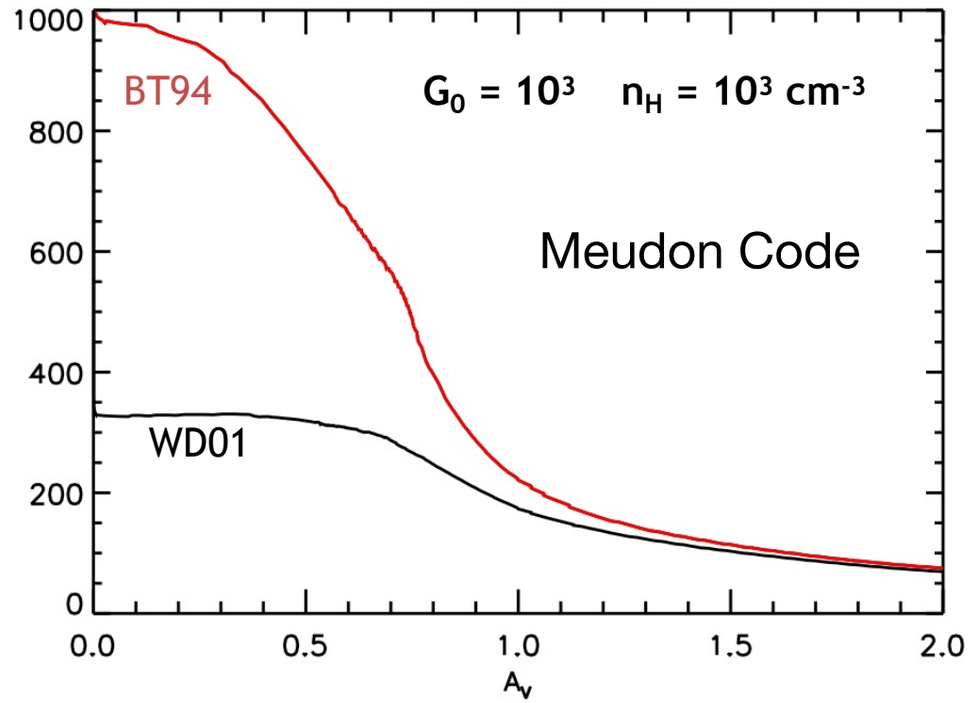




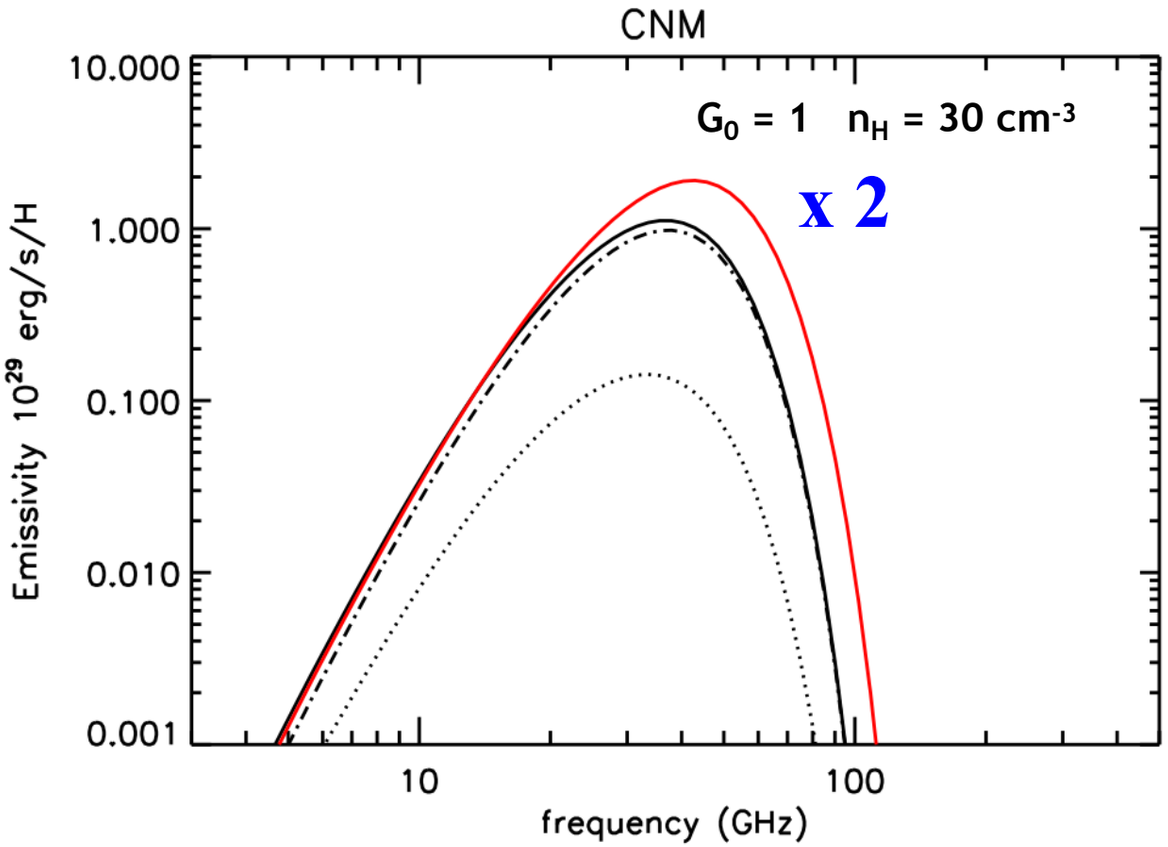
Astrophysical impact

Photon-dominated regions

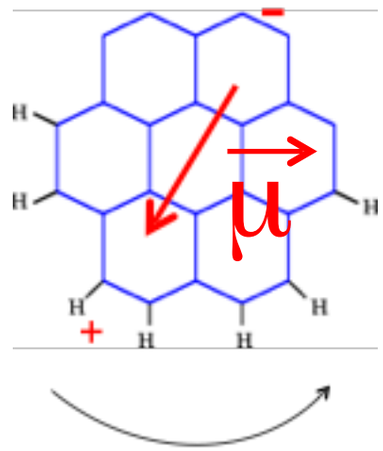




Alter **face-on** Line fluxes up to 30% (C^+, O^0 or H_2-rot), **edge-on:** up to factor 2



Spinning dust emission



Traces the abundance of small dust grains

A new model of Photoemission

Photoelectric effect (PE) important for grain charging and gas heating.
More efficient on small grains (Watson 1973, Draine 1978)
First studies need to be furthered to take into account finite-size effects:

- light attenuation by a finite grain (not the bulk)
- grain curvature and PE threshold in the yield Y_{PE}
- PE needs to be revisited for composite, evolved grains, such as those of THEMIS.

Photoelectric effect described as a 3 step process:

i) absorption of a UV photon and excitation of an electron into a propagating state threshold IP and attenuation length l_a $\exp(-a/l_a)$

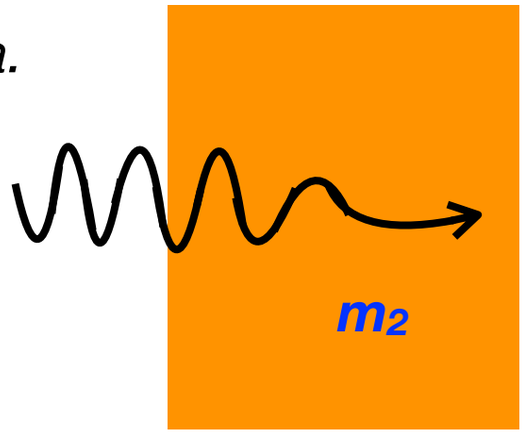
ii) random walk of the electron to the surface mean free path l_e $\exp(-a/l_e)$

iii) electron escapes from the grain escape probability p_{esc}

Light attenuation by a grain

$\beta = a / l_a$: describes the light attenuation efficiency within a grain of size *a.*

Since extinction efficiency $Q_e = \sigma_e / \pi a^2$ must have $\beta \sim Q_e$

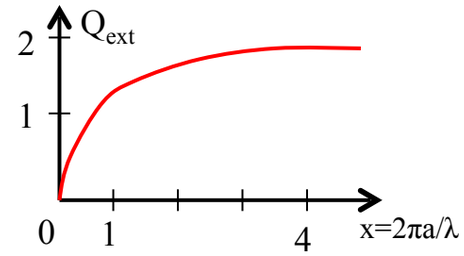


So far **bulk description**:

$\beta = 2kam_2 = 2xm_2$ ($m = m_1 + im_2$ ref. index of grain material)

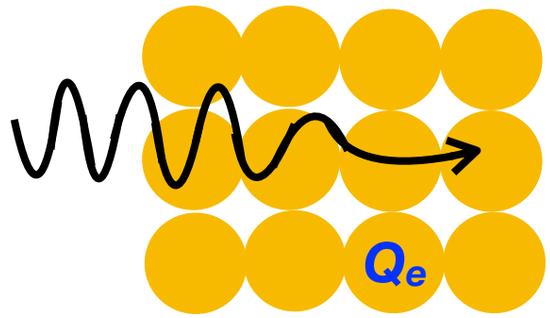
and $\beta \sim a$ in contradiction with Mie theory, $Q_e \rightarrow 2$ as *a* increases

Also require the knowledge of *m:* difficult to define in the case of composite, evolving grains e.g. calculated with DDA



But grain is finite:

Q_e which contains all the information of the light interaction with 1 grain (**DustEM**)



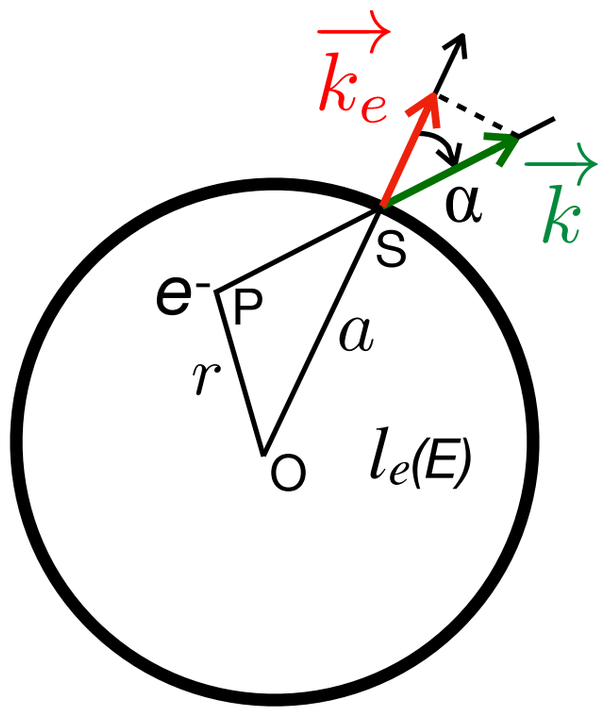
$\beta = a\, n\sigma_e = 3Q_e / 4$ with $n = 3 / 4\pi a^3$ density of absorber

→ Attenuation efficiency saturates with size, large grains are more prone to PE effect

e.g. for *a* = 100 nm, <Z> is ~ 2 times larger than bulk model (carbon grain)

While no change for *a*<30nm

Finite-size effects for the photoelectric yield



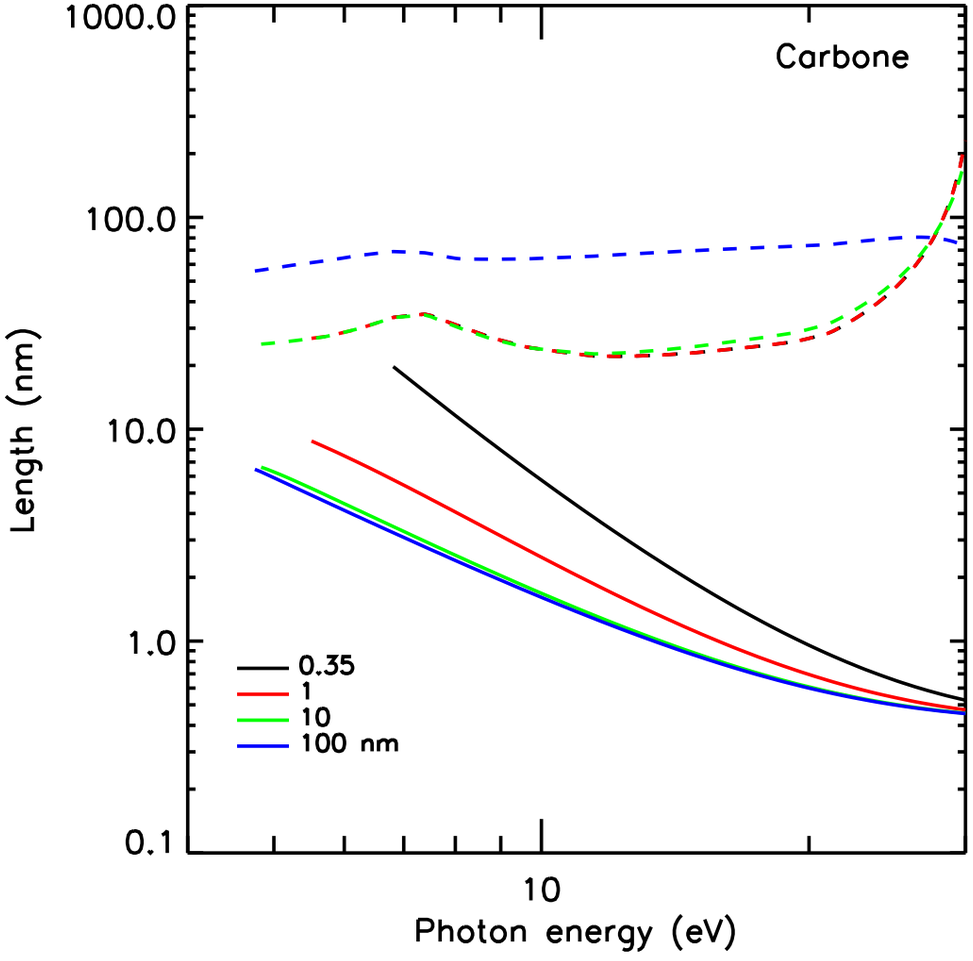
Recently considered by Kimura (2016, K16):

to leave the grain the produced photoelectron must have a radial component of its wave number such that its total energy exceeds the threshold: $E \cos^2\alpha > \mathrm{IP}$

PE yield enhancement then **depends on IP** and rapidly decreases with size (≠ Watson). To use eq. (A12) of K16, use $l_e(E)$ with

$$E = \langle K \rangle + \mathrm{IP}$$

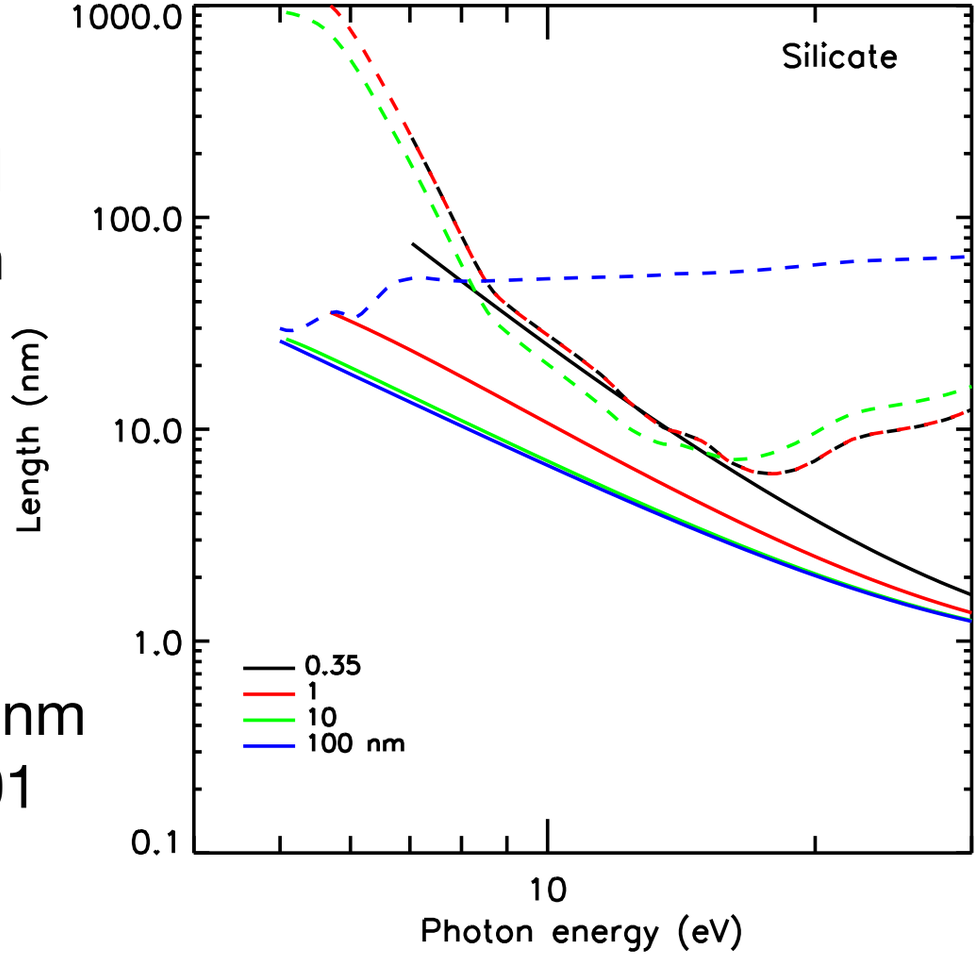
where $\langle K \rangle$ is the mean kinetic energy of the ejected electron estimated with a parabolic K-distribution



l_e: solid

l_a: dash

NB: l_e=*1* nm in WD01



Finite-size effects for the photoelectric yield...

Total yield $Y_t = Y_a\, Y_2$ with Y_2 the fraction of attempting electrons leaving the grain

and Y_a the photoelectric quantum yield (K16) corresponding to $Y_0\, Y_1$ in WD01

A good approximation to Y_a is (K16)

$$Y_a(h\nu) = \frac{1}{2}\left(1-\sqrt{\frac{W}{h\nu}}\right)\left(\frac{\beta}{\alpha}\right)^3 \frac{\left(1+\sqrt{W/h\nu}\right)\alpha^2\left(1-e^{-\alpha}\right)+\left(\alpha^2-2\alpha+2-2e^{-\alpha}\right)(\alpha-\beta)}{(\alpha-\beta+1)\left(\beta^2-2\beta+2-2e^{-\beta}\right)}.$$

where $\alpha = a/l_{\rm a} + a/l_{\rm e}$ and $\beta = a/l_{\rm a}$

W is the grain ionization potentiel *IP* and in general $h\nu$ must be replaced by *E* the total energy of the electron

Image potential term in threshold: adopt BT94 $\quad W = W_\infty + \left(Z+\frac{1}{2}\right)\frac{e^2}{a}$

instead of K16 $\quad W = W_\infty + \left(Z+\frac{3}{8}\frac{\epsilon-1}{\epsilon}\right)\frac{e^2}{a}$

(see discussion in BT94 note that ε>>1)

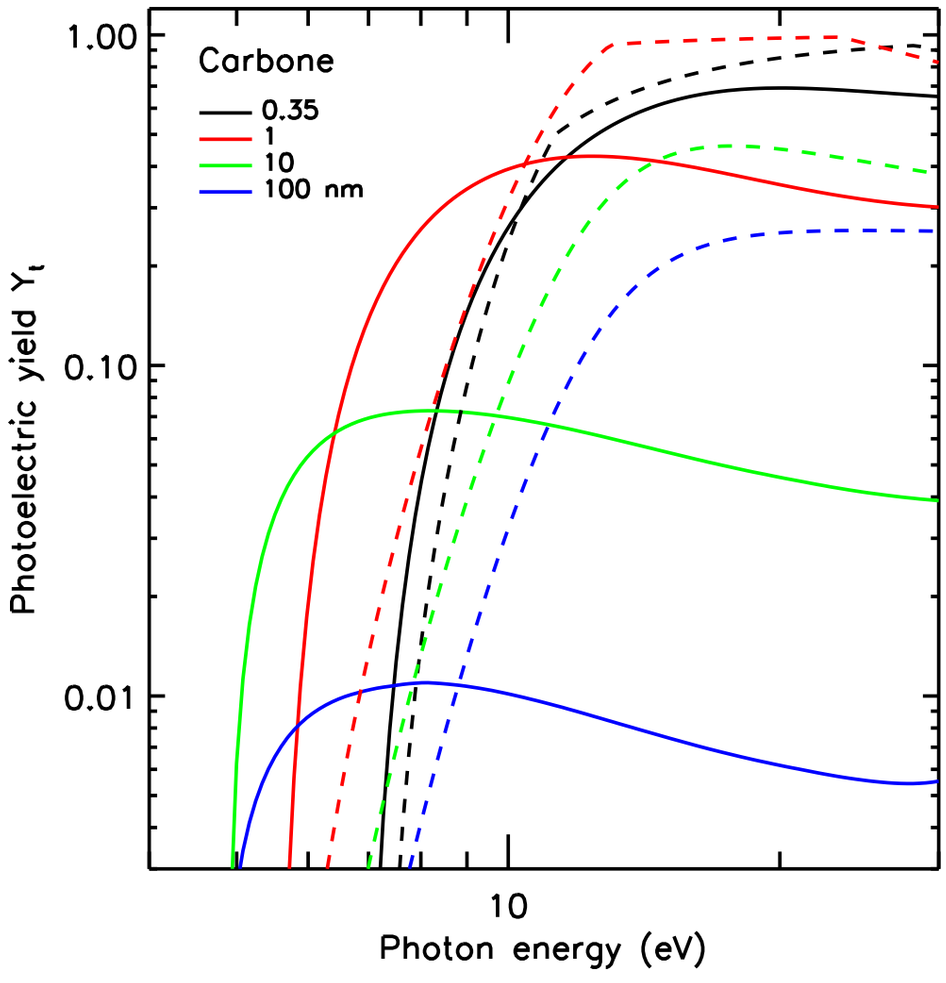
Finite-size effects for the photoelectric yield…

The resulting total PE yield Y_t

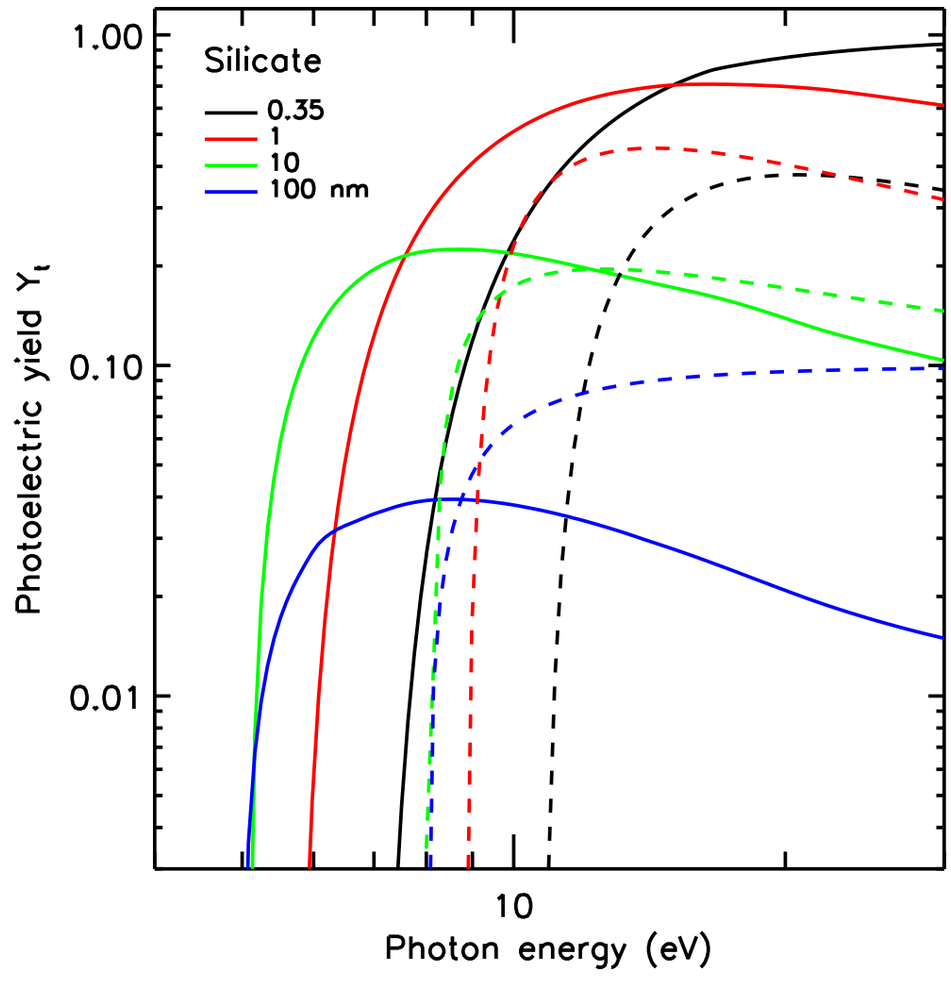
Note: (i) similar yields for small grains a<1 nm. (**NB** WD01 model normalized to lab data, not K16)

(ii) as sizes increases WD01 yields are higher, disagrees with lab data (see WD01 note 4 p.268)

(iii) from lab data (Feuerbacher+1972), K16 chooses a lower work function for silicates, W_f = 4.97 eV. Adopt W_f = 4.4 eV threshold for sp2 carbone (K16 takes 4.75 eV).



solid: K16
dash: WD01

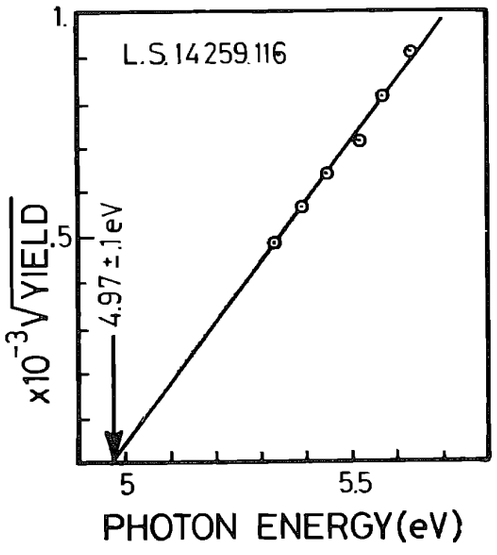


Why changing the work function of silicates ?

From lab data the PE yield of lunar dust and graphite are similar. Lunar dust is a proxy for IS silicates.

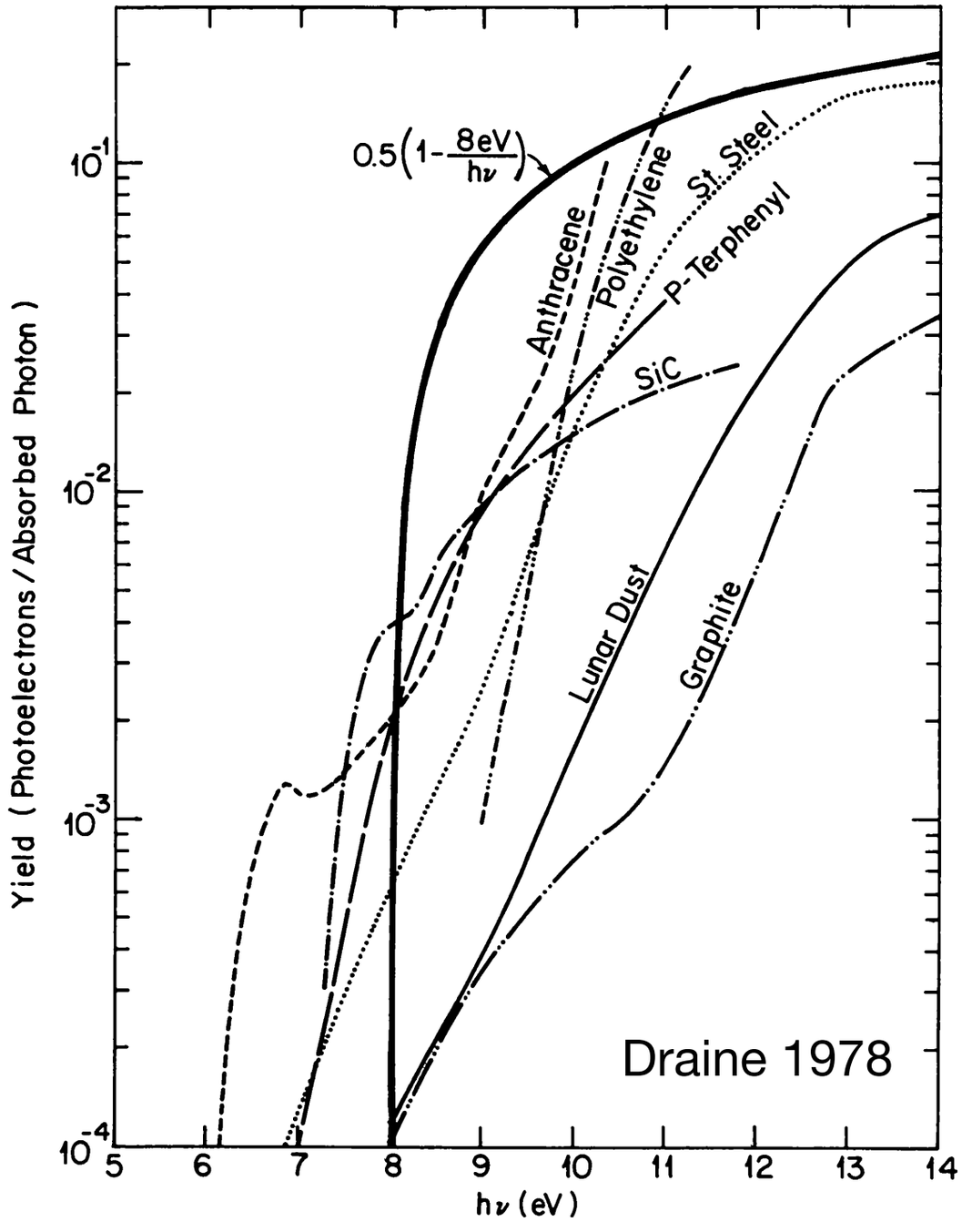
The bulk threshold or work function W of graphite is W = 4.4 eV why should that of silicates be 8 eV ?

Feuerbacher+1972 found $W = 4.97$ eV



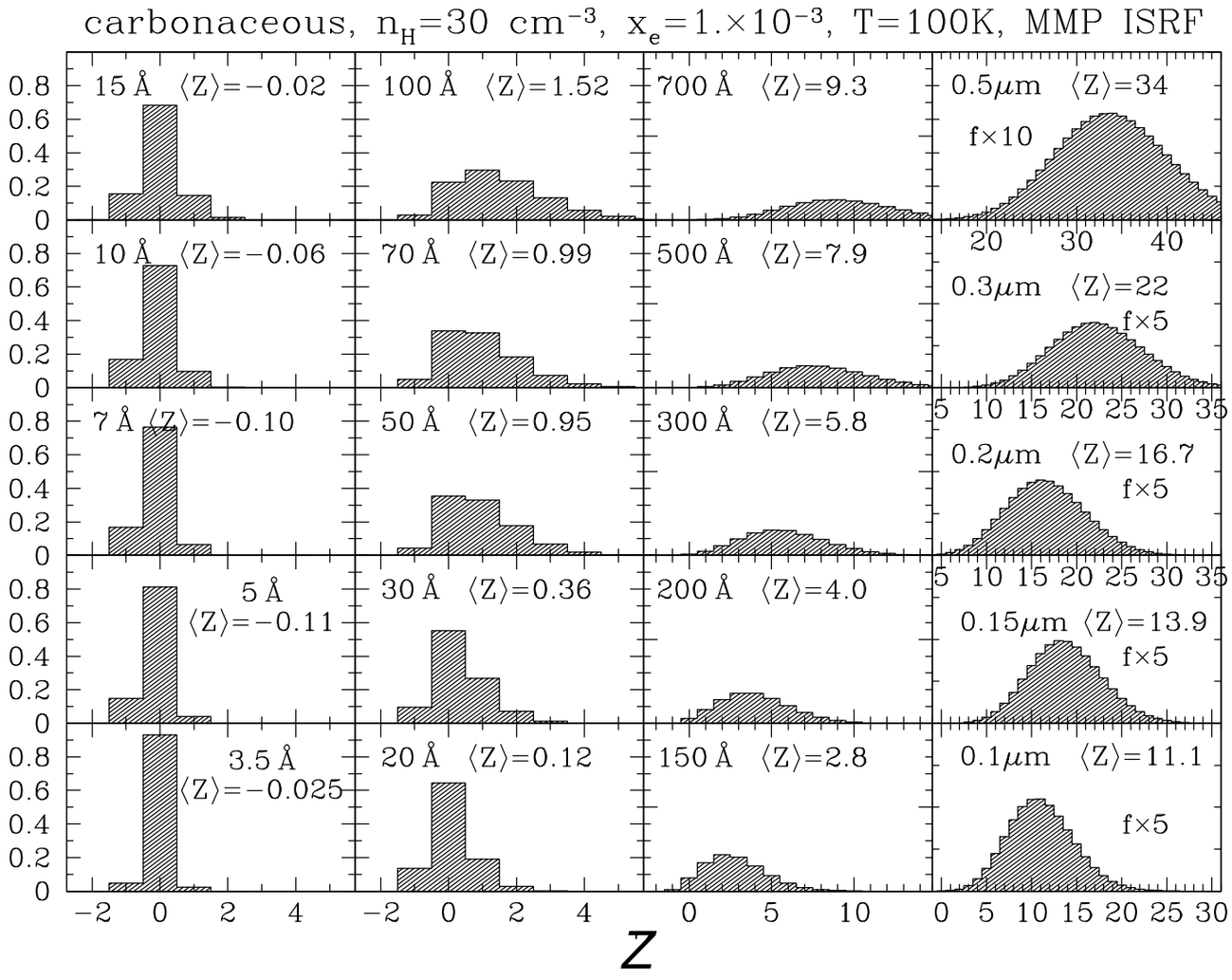
$$Y \sim (h\nu - W)^2$$

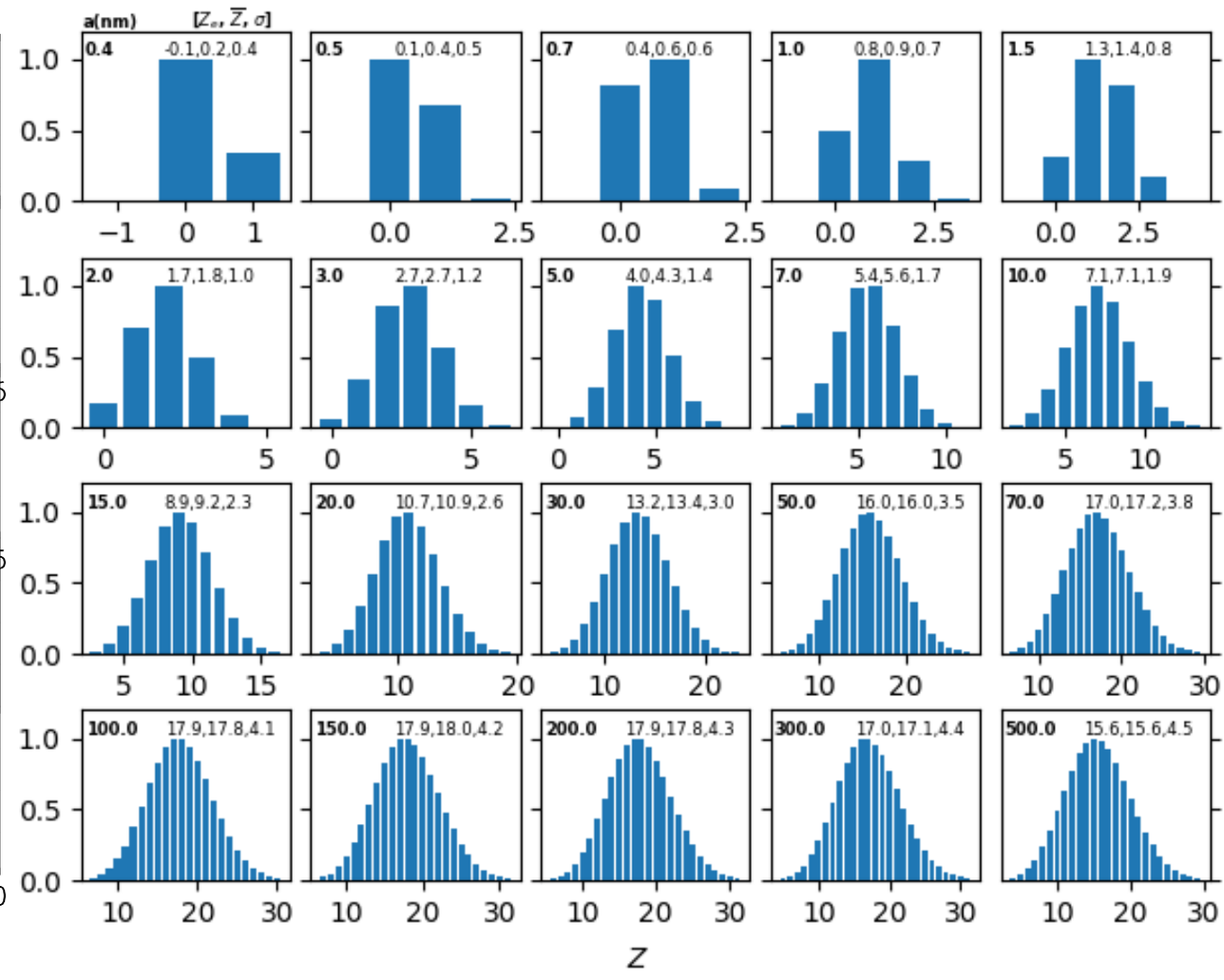
$W = 8$ eV was the value in the « standard model » of Draine 78, meant to represent both carbone and silicate materials



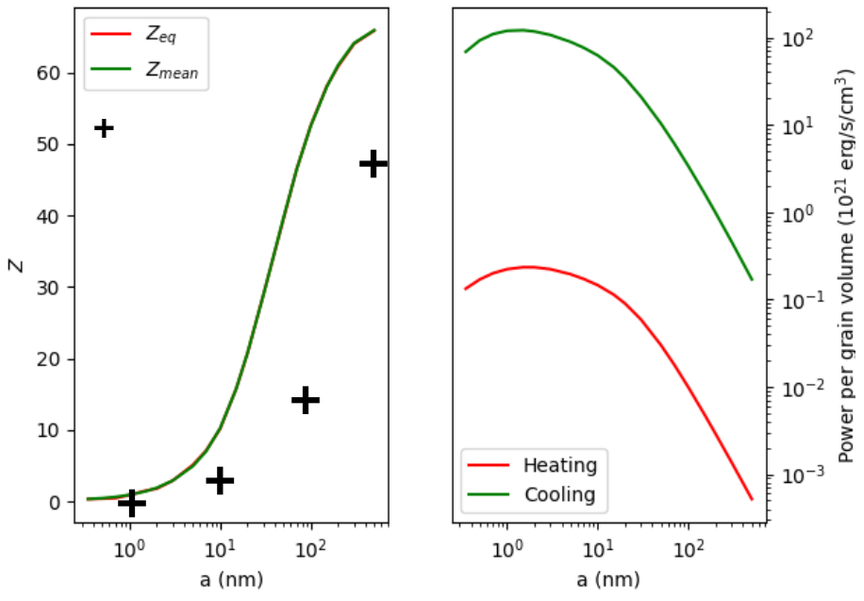
Charge distribution

Diffuse gas: *f(Z)* WD01 vs K16

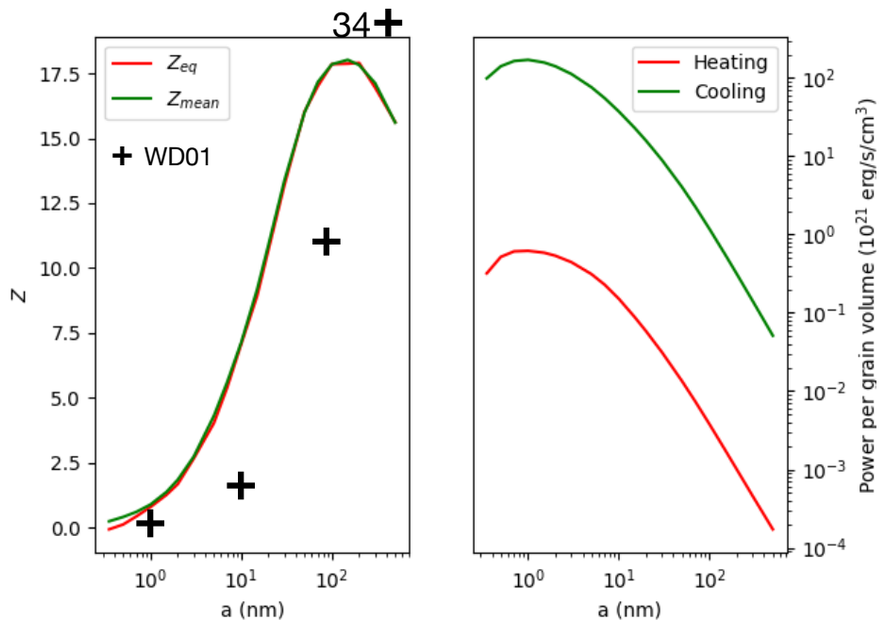




aSil

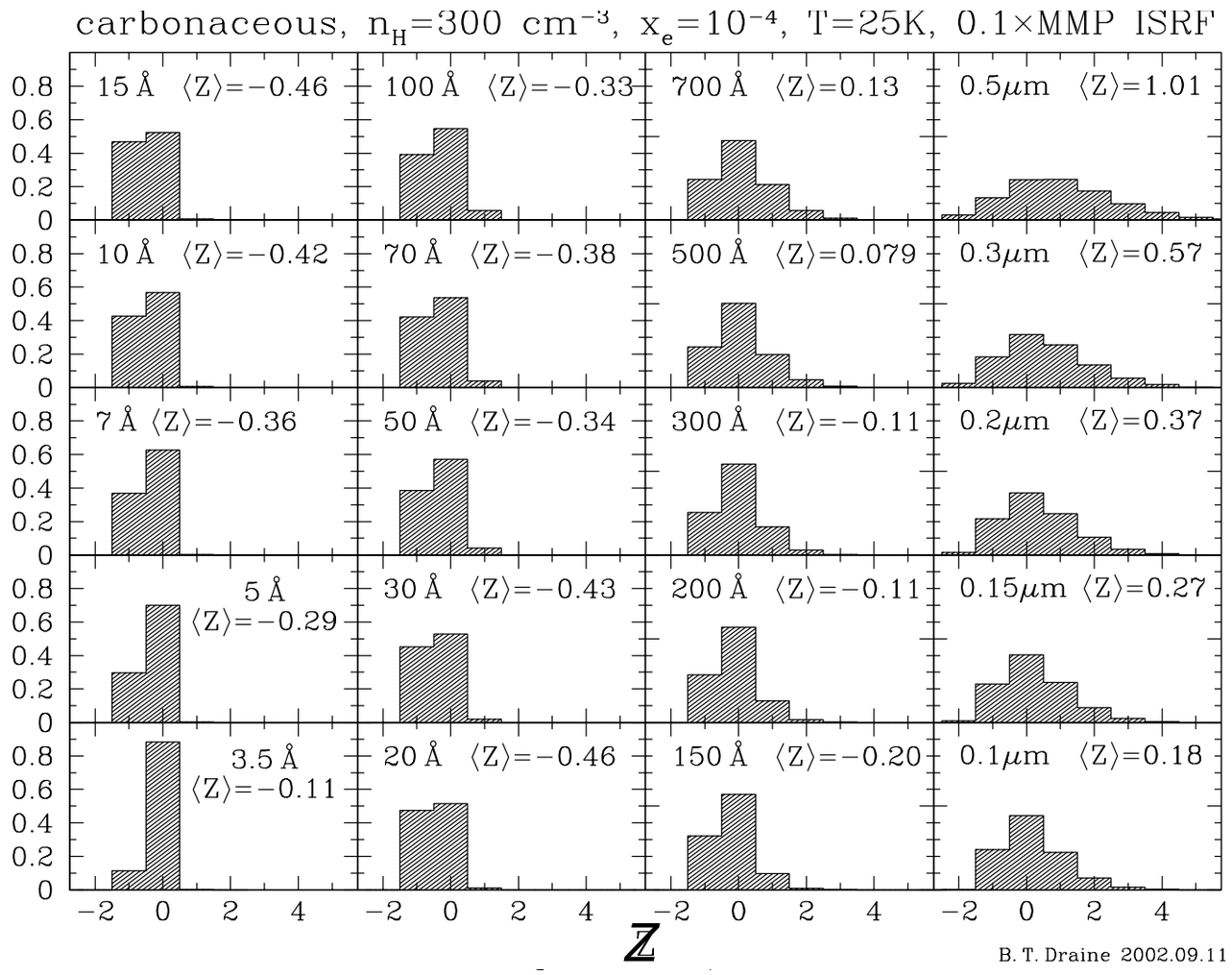


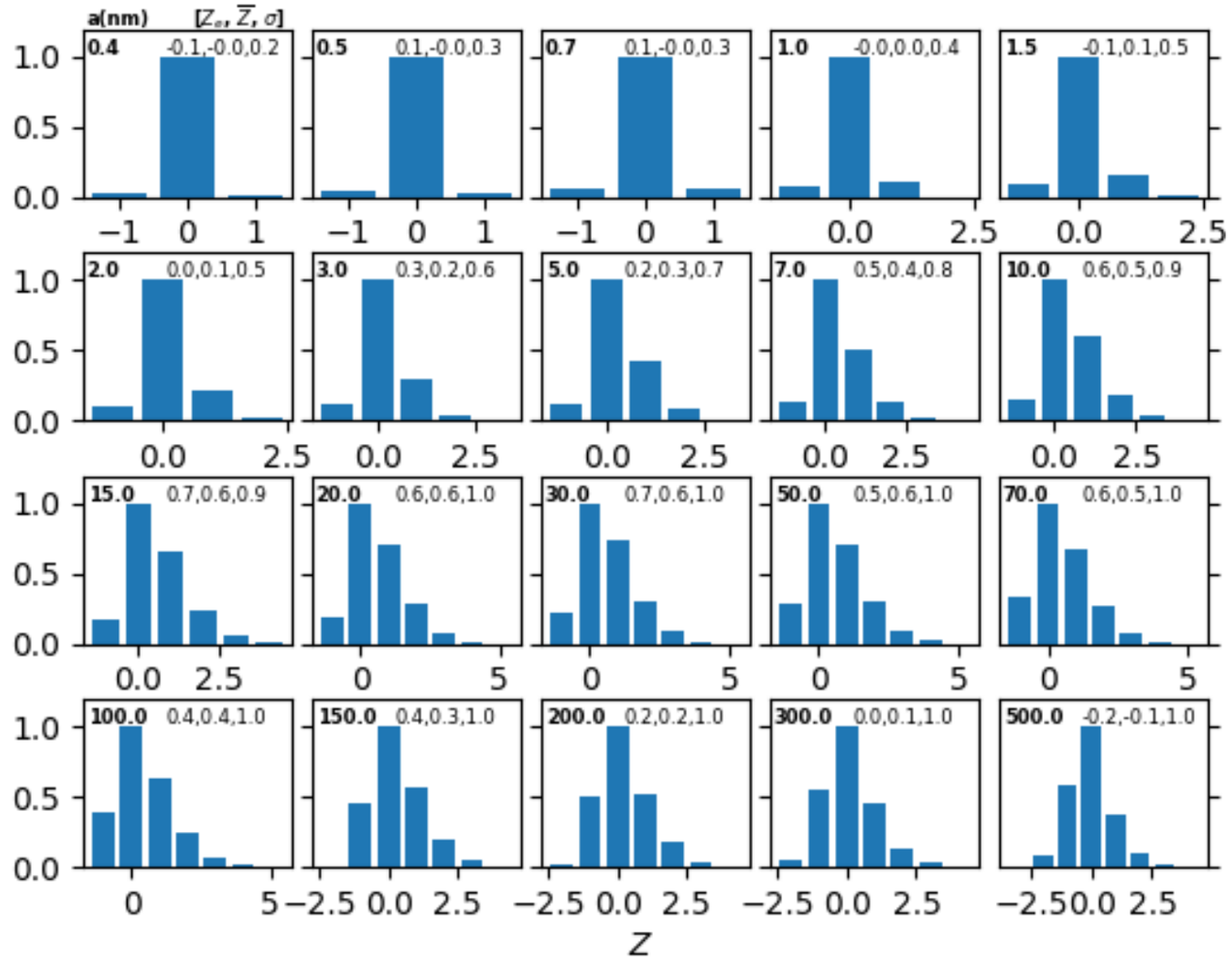
Gra

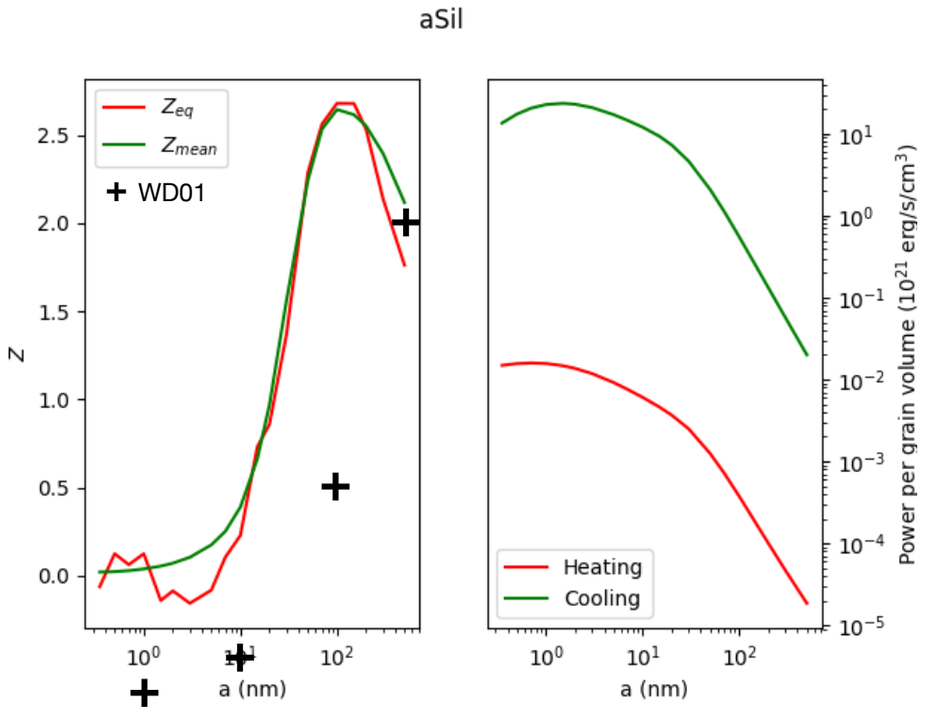


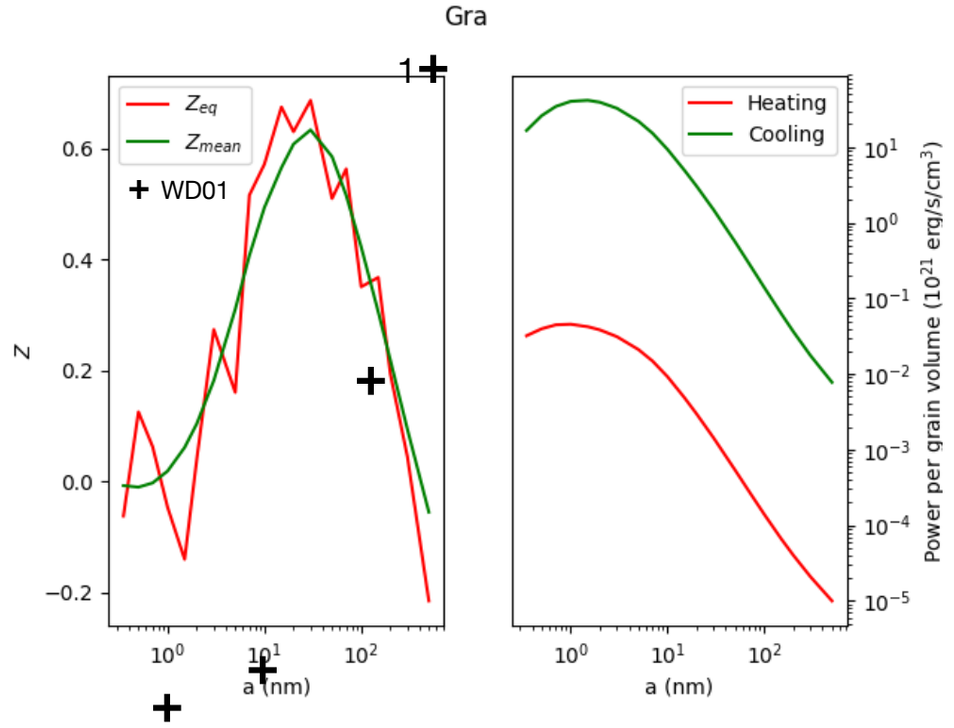
Charge distribution…

Molecular gas: *f(Z)* WD01 vs K16



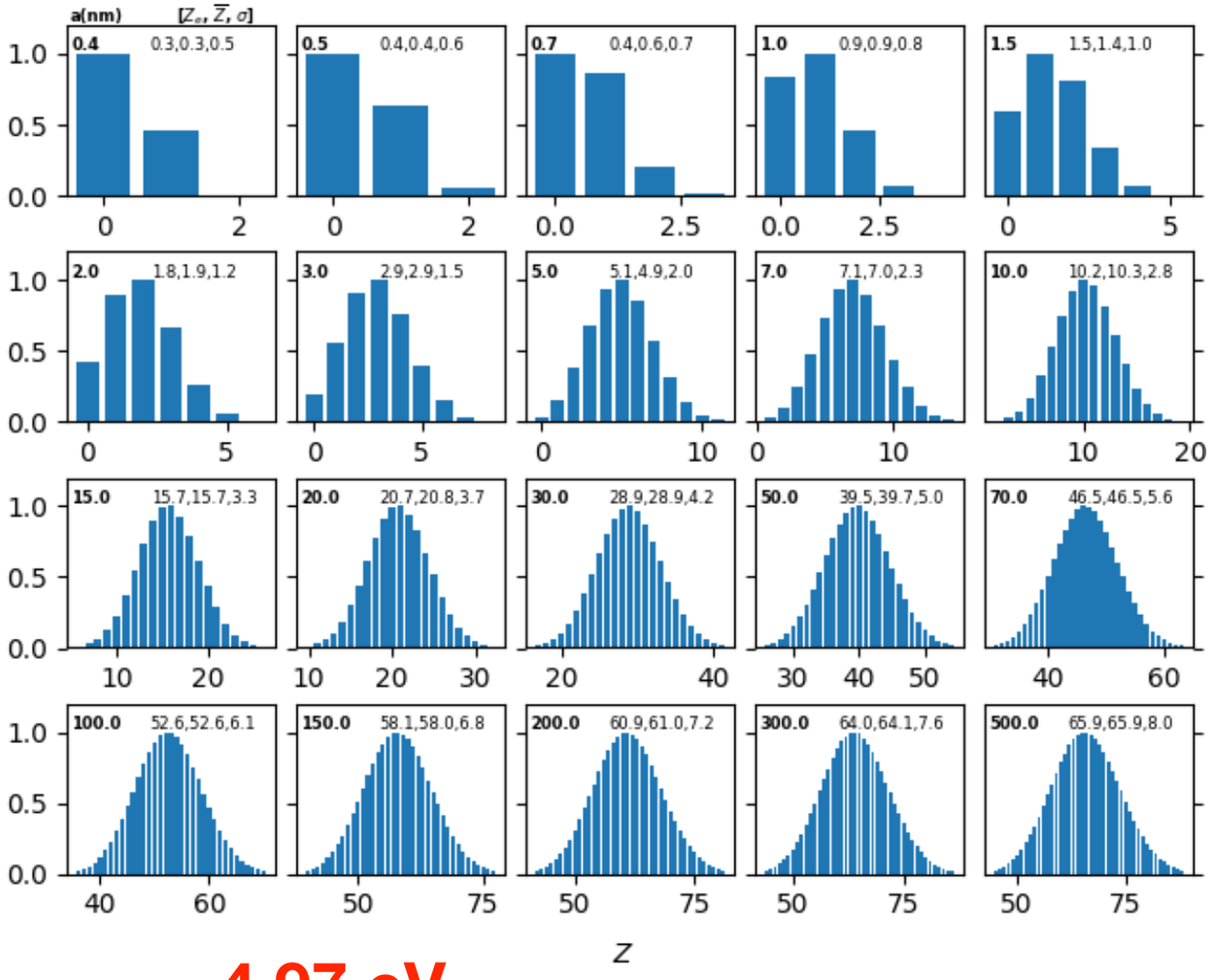






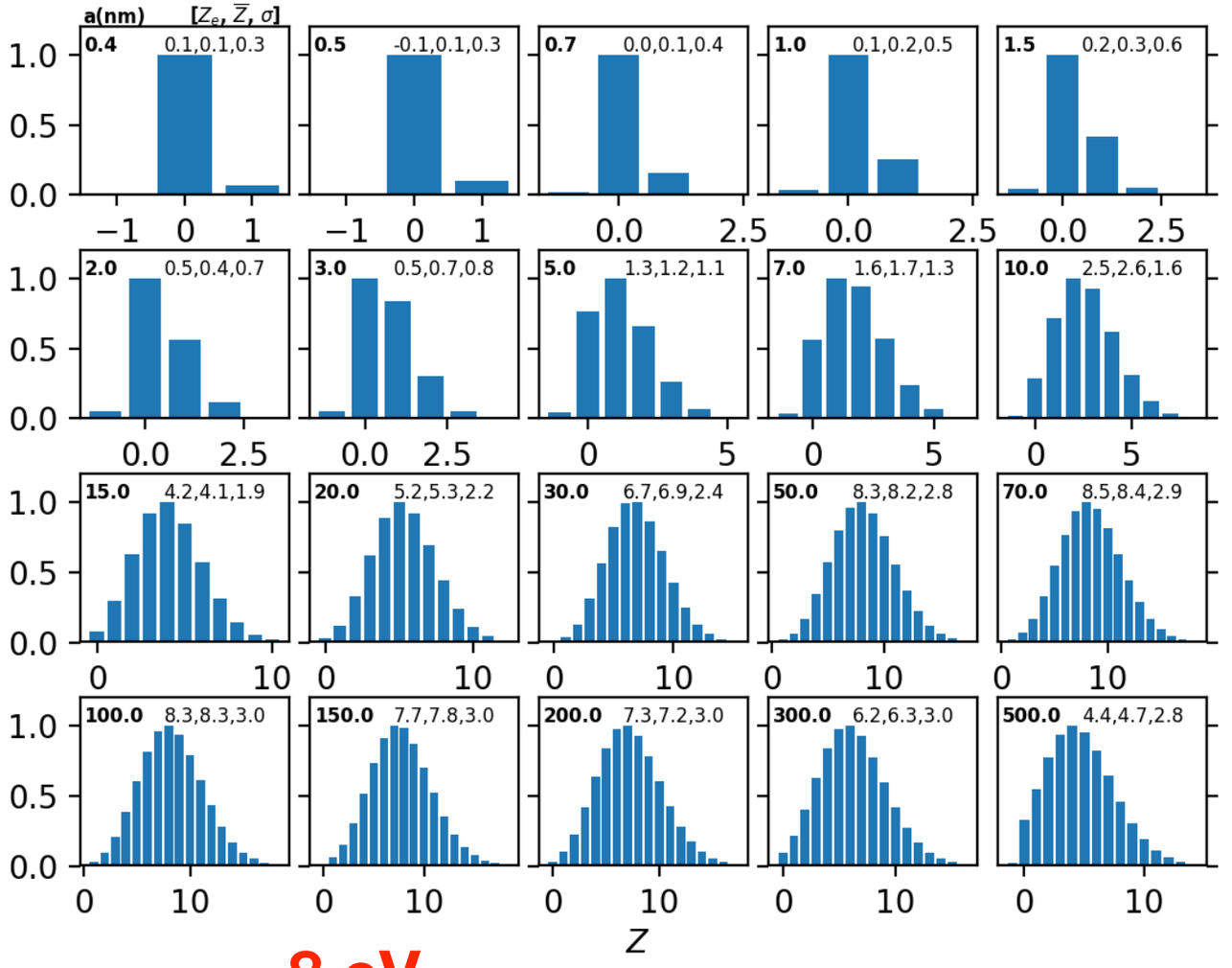
Effect of silicates IP

Diffuse gas, silicates



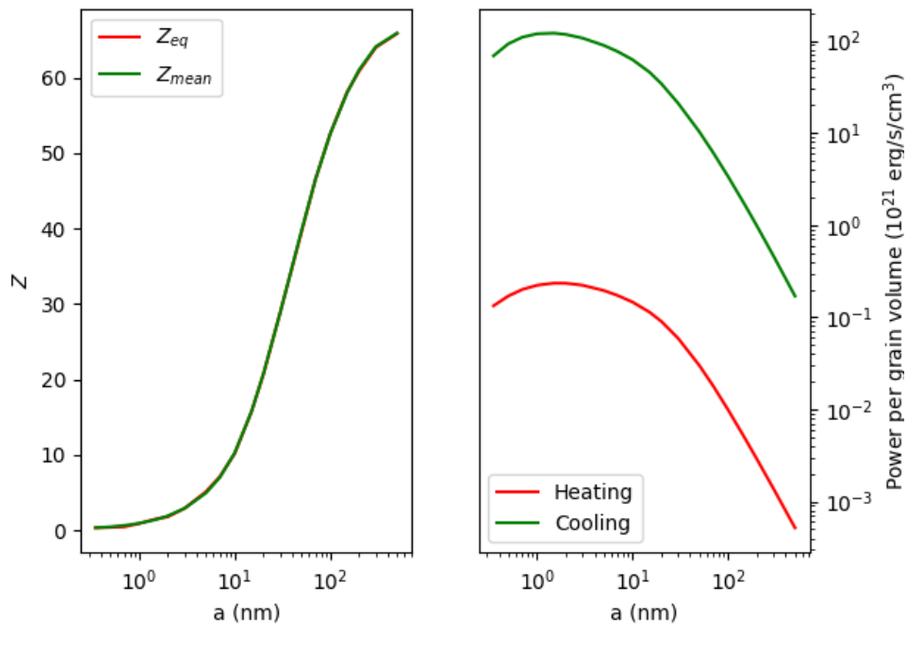
4.97 eV

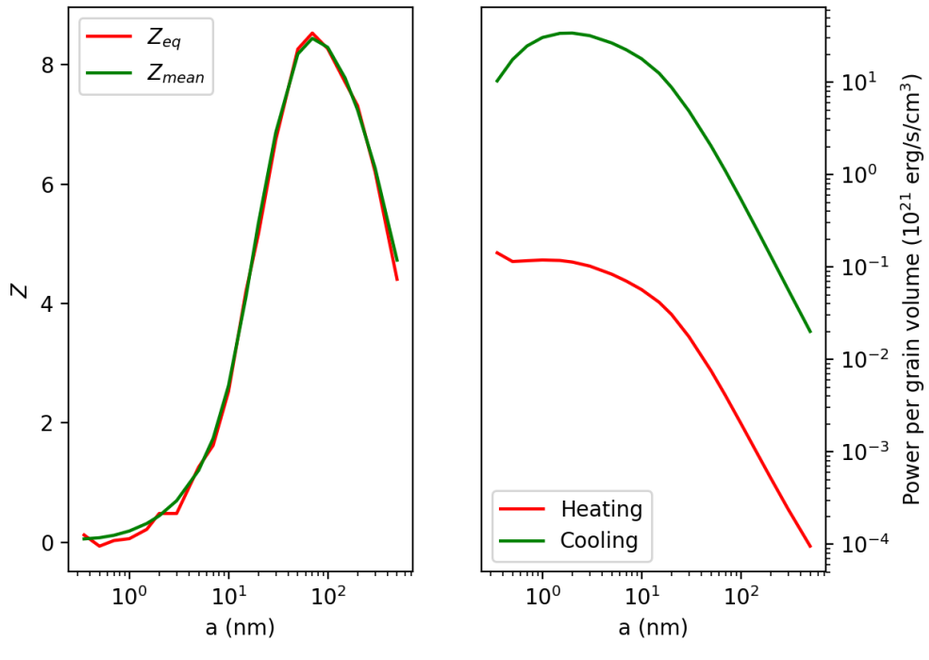
aSil



8 eV

aSil





New photoemission model: a summary

Treating light attenuation and photoelectric yield in the case of finite-size grains leads to effects mitigating each other:

- the light attenuation saturates: more PE effect with increasing size while
- Photoelectric yield Y_{PE} decreases with size

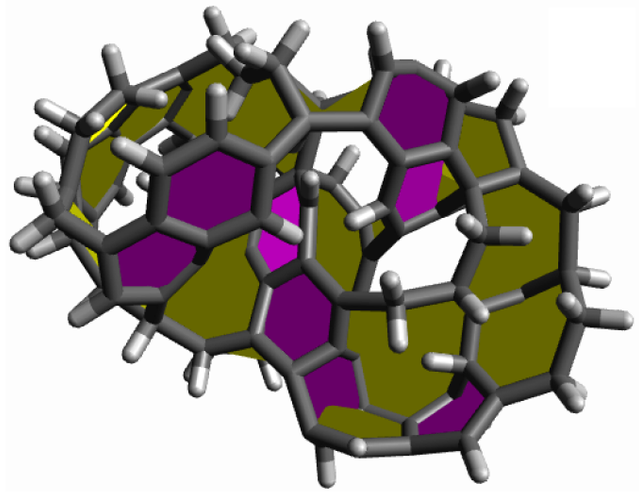
In general, grains more charged, positively.

The charge distribution of small grains (a<3 nm, carbone or silicates) is less affected:
The **gas heating** is similar (although somewhat below, Z>0) to WD01, with a notable **contribution from small silicates** (up to 10%), a consequence of the lower work function.

Heterogeneous grains: the case of a-C:H

In a-C:H grains the threshold for PE effect IP is set by the least binding states, i.e., the sp^2-electrons of the largest aromatic domain of radius a_R.
This leads to a correction A_C of the capacitive energy to be overcome by the electron.

In addition the band gap E_g is size dependent.



$$\mathrm{IP} = W + \frac{e^2}{2C_R} + \frac{Ze^2}{a} = W + \left(Z + \frac{1}{2}\right)\frac{e^2}{a} + A_C$$

$$\mathrm{EA} = W - E_g - \frac{e^2}{2C_R} + \frac{Ze^2}{a} = W - E_g + \left(Z - \frac{1}{2}\right)\frac{e^2}{a} - A_C$$

with $C_R = \frac{2}{\pi} a_R$ the capacity of the aromatic domain a_R

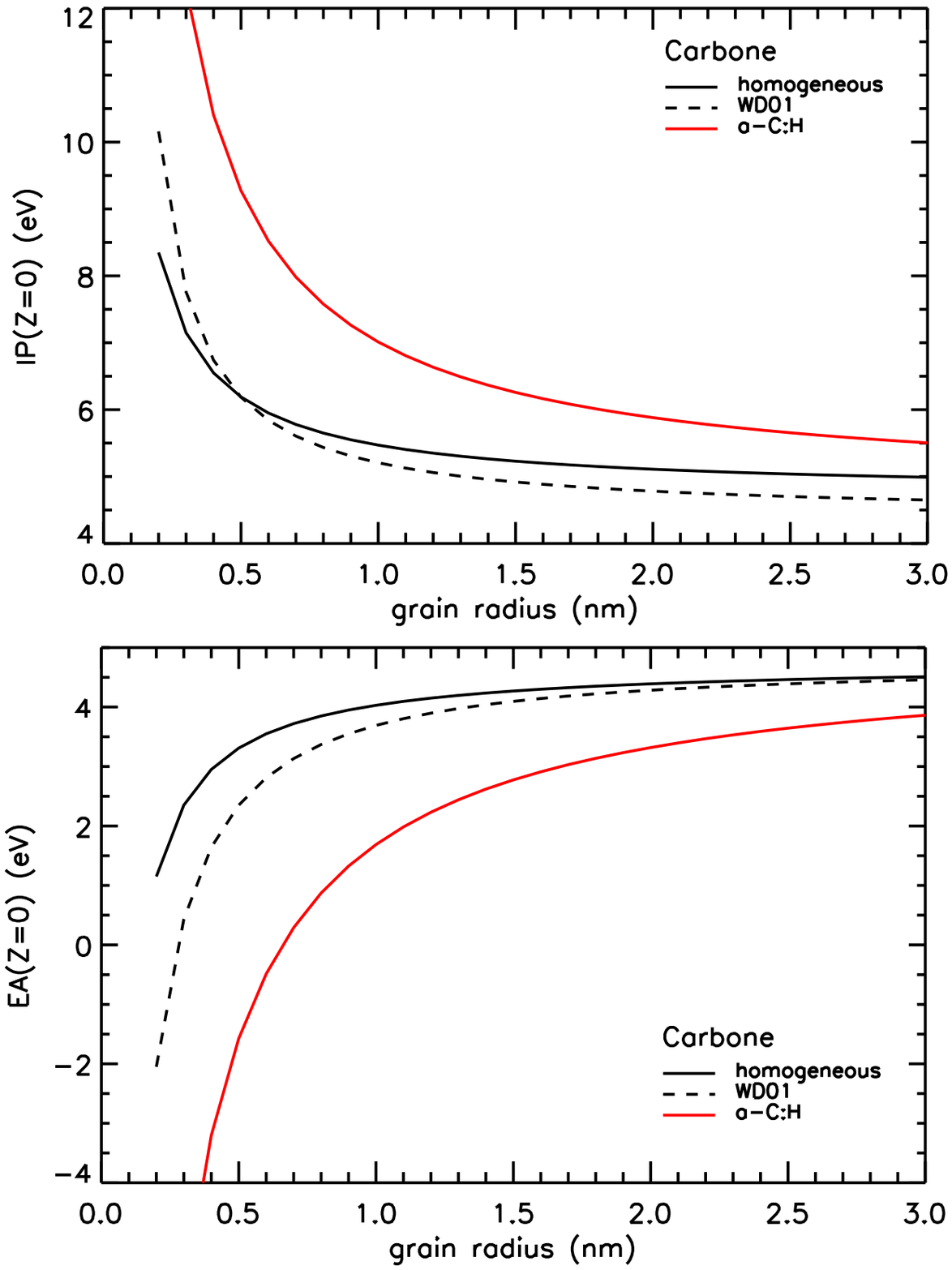
$$A_C = \left(\frac{\pi}{2}\frac{a}{a_R} - 1\right)\frac{e^2}{2a}$$

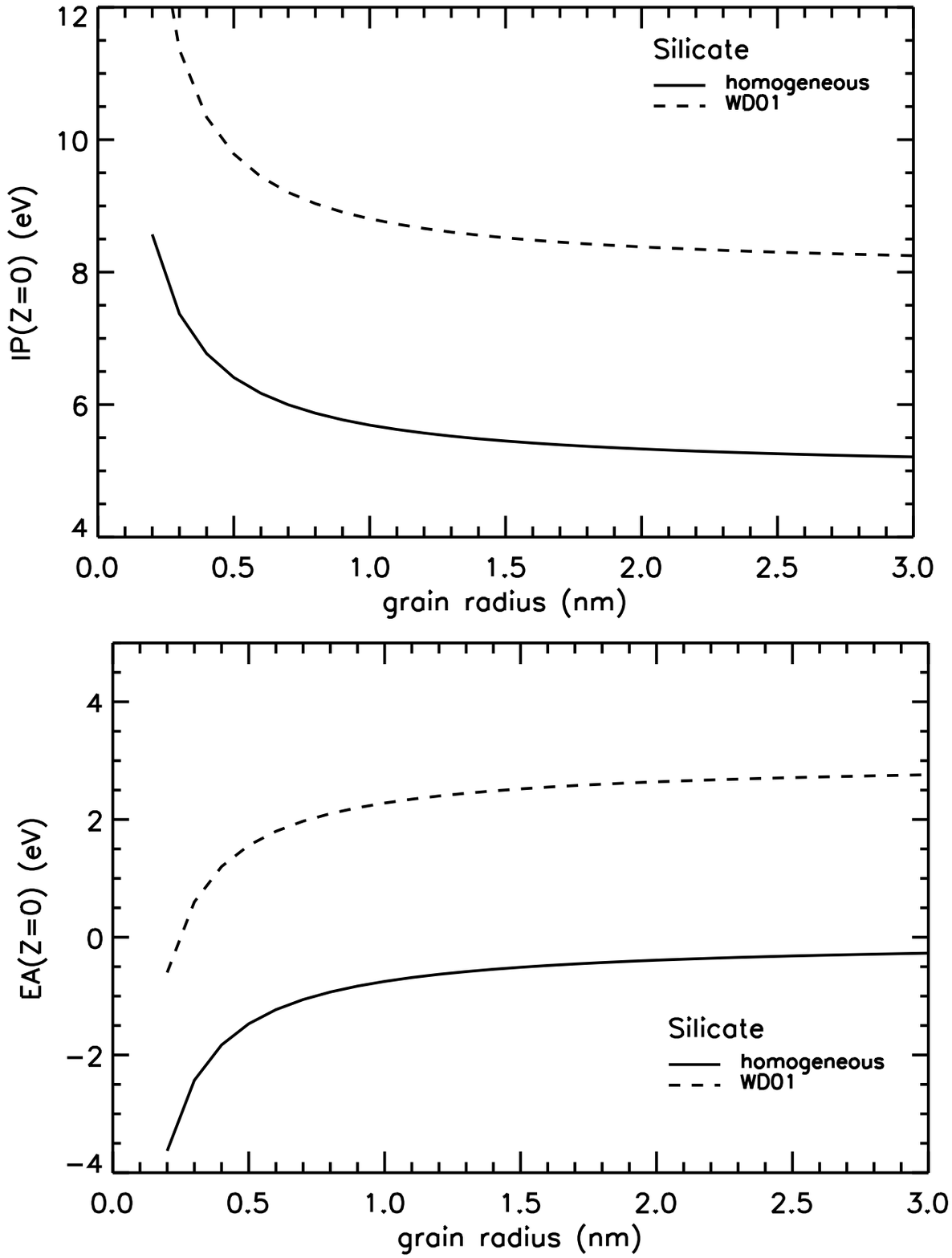
and $E_g(\mathrm{eV}) = \mathrm{MAX}\left[0.1,\ 0.2\left(\frac{5\,\mathrm{nm}}{a} - 1\right)\right]$

Hyp: $a_R = a / 2$

(Jones+2017)

Heterogeneous grains: thresholds





Heterogeneous grains: a summary

➡ For **silicates**, thresholds are shifted down (8 -> 5 eV) while PE yield is smaller (K16) and are more **positive**

for MC, CNM and WNM: <Z>~ (-0.1 ; 2) / (0.4 ; 66) / (1.1 ; 500) for (a=0.35 ; 500nm)

➡ For **a-C:H grains**, thresholds (IP and EA) move apart: this tends to keep the **charge around 0** (except when electrons are rare, cf low density WNM)

for MC, CNM and WNM: <Z>~ (-0.1 ; -0.2) / (-0.1 ; 16) / (0.1 ; 260) for (a=0.35 - 500nm)

Rapid test with IP and EA on amCBE shows that:

- A_C has the strongest effect but moderate in most cases (MC,CNM and WNM),
- **gas heating little affected**

Summary of summaries

- A more realistic model of dust grains photoemission has been developed taking into account finite size effects (Q_e, $l_e(E)$, E_g(a)) and in DustEM

- Increases mean charge of grains (silicates): less heating ? coagulation ? more B-coupling ?

- Case of amC:H grains: charge tend to be around 0

- gas heating little affected (but no transfer)

- Assess in a variety of physical conditions with transfer and gas heating, from PDR to the MC

- Refine amC:H picture: size of largest aromatic domain a_R (a) ? E_g on LUMO states only ?