

# Energetic processing of complex carbonaceous compounds

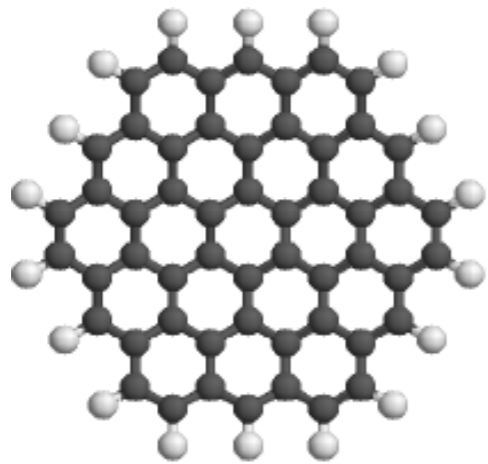
**Elisabetta Micelotta**

University of Helsinki

ISWA 2016 - Campinas, SP, Brazil

July the 4th 2016

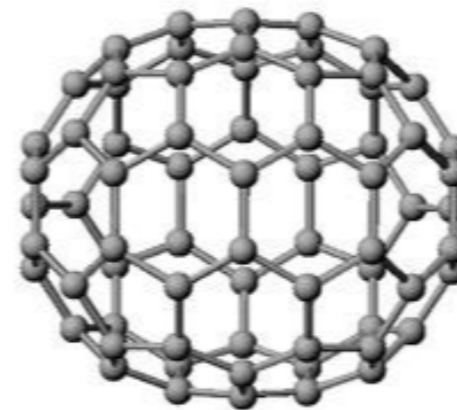
# Complex carbon compounds



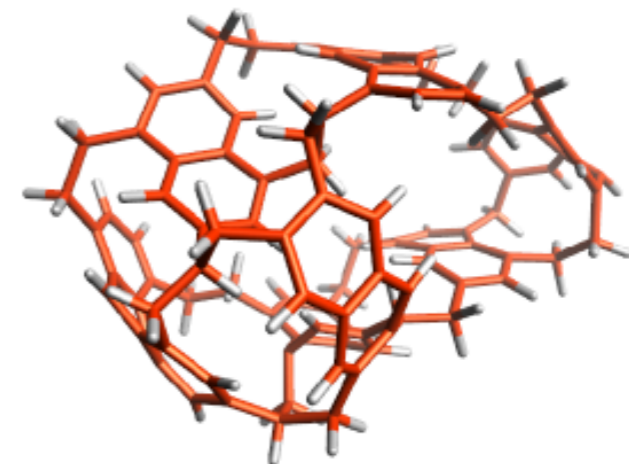
**PAHs**



**C<sub>60</sub>**



**C<sub>70</sub>**



**$\alpha$ -C:H nanoparticles**

# Energetic processing

**How?**



Processing occurs via  
**interactions**  
with these projectiles

**Ions & Electrons**  
(H, He, CNO)



**$E = 10 \text{ eV} - 3 \text{ keV}$**   
 **$E = 5 - 50 \text{ eV}$**   
 **$E = 10 \text{ eV} - 10 \text{ keV}$**   
 **$E = 5 \text{ MeV/nuc} - 10 \text{ GeV}$**

**Photons**



**UV:  $E = 6 - 15 \text{ eV}$**   
**X-rays:  $E = 0.3 - 10 \text{ keV}$**

# Where?

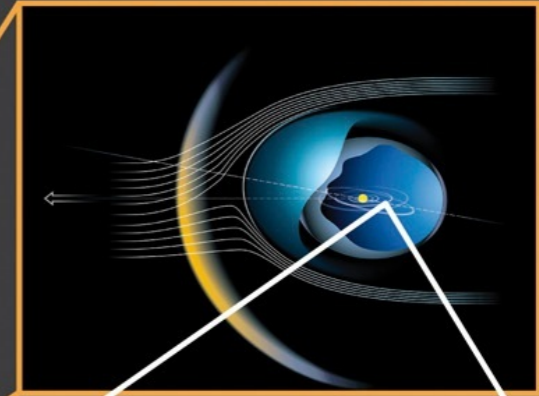
Young star LL Ori



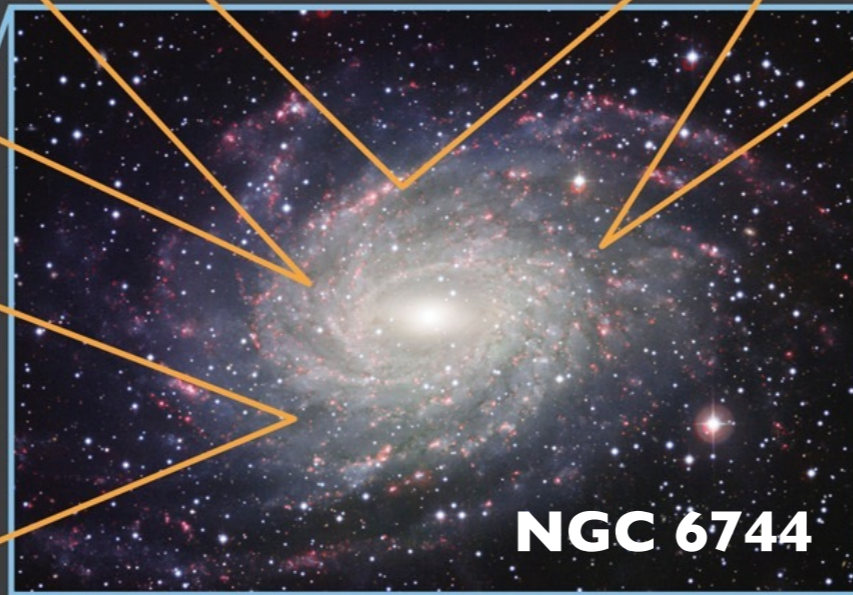
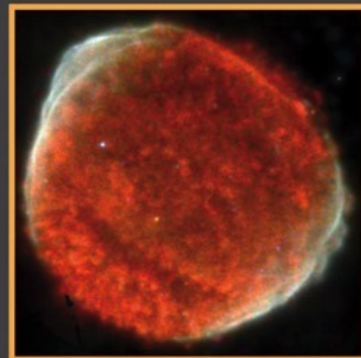
Red Spider Nebula - PN



Solar System



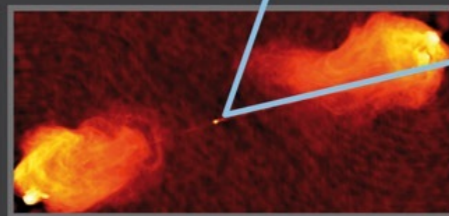
SN 1006



NGC 6744



Earth



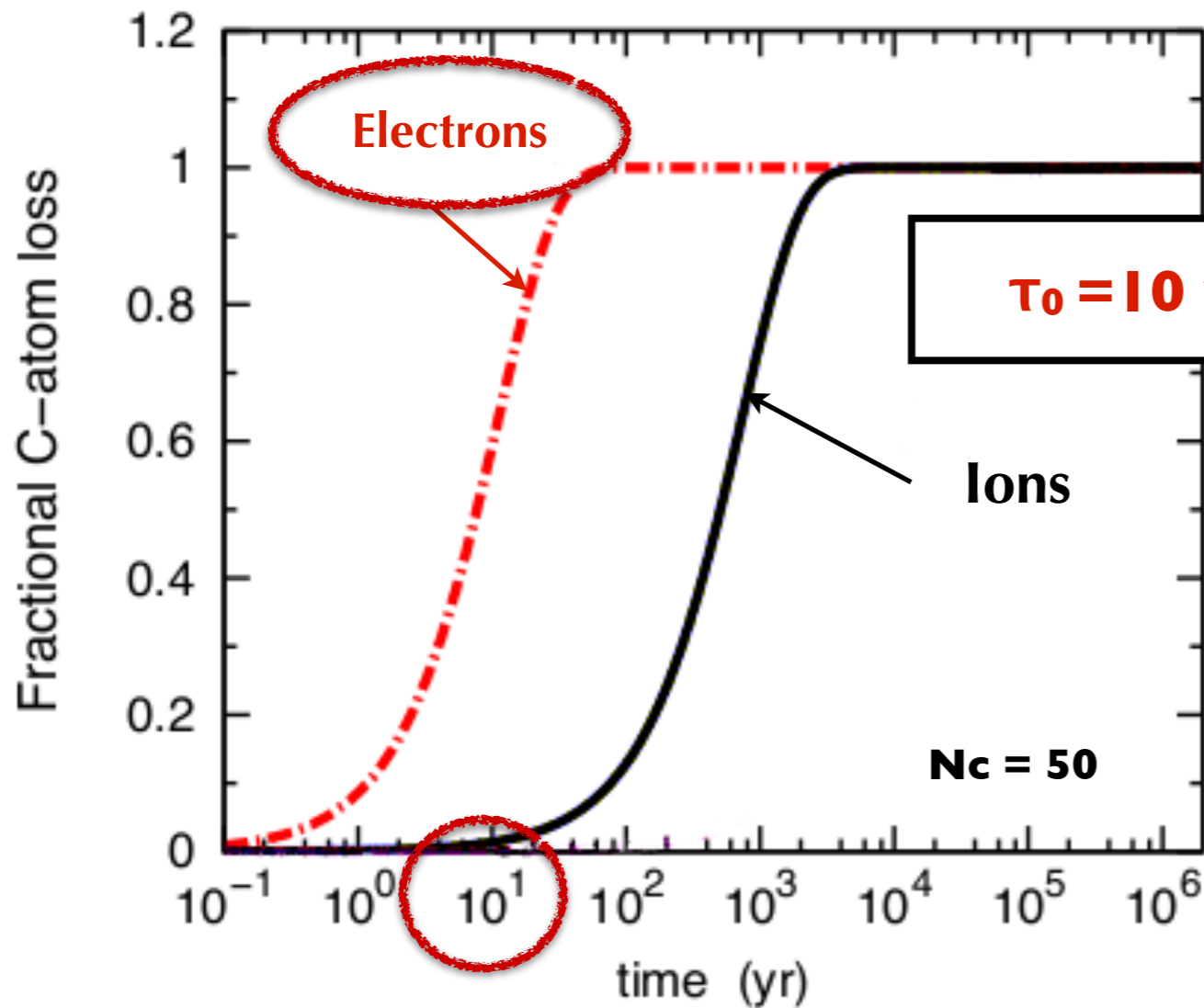
Cygnus A - radio lobes



Bullet Cluster - merging

[PhysOrg.com](http://PhysOrg.com)  
NASA/ESA, Hubble Heritage

# PAHs in hot shocked gas: M82



$v_{\text{SHOCK}} \sim 600$  km/s

Temperature of gas:

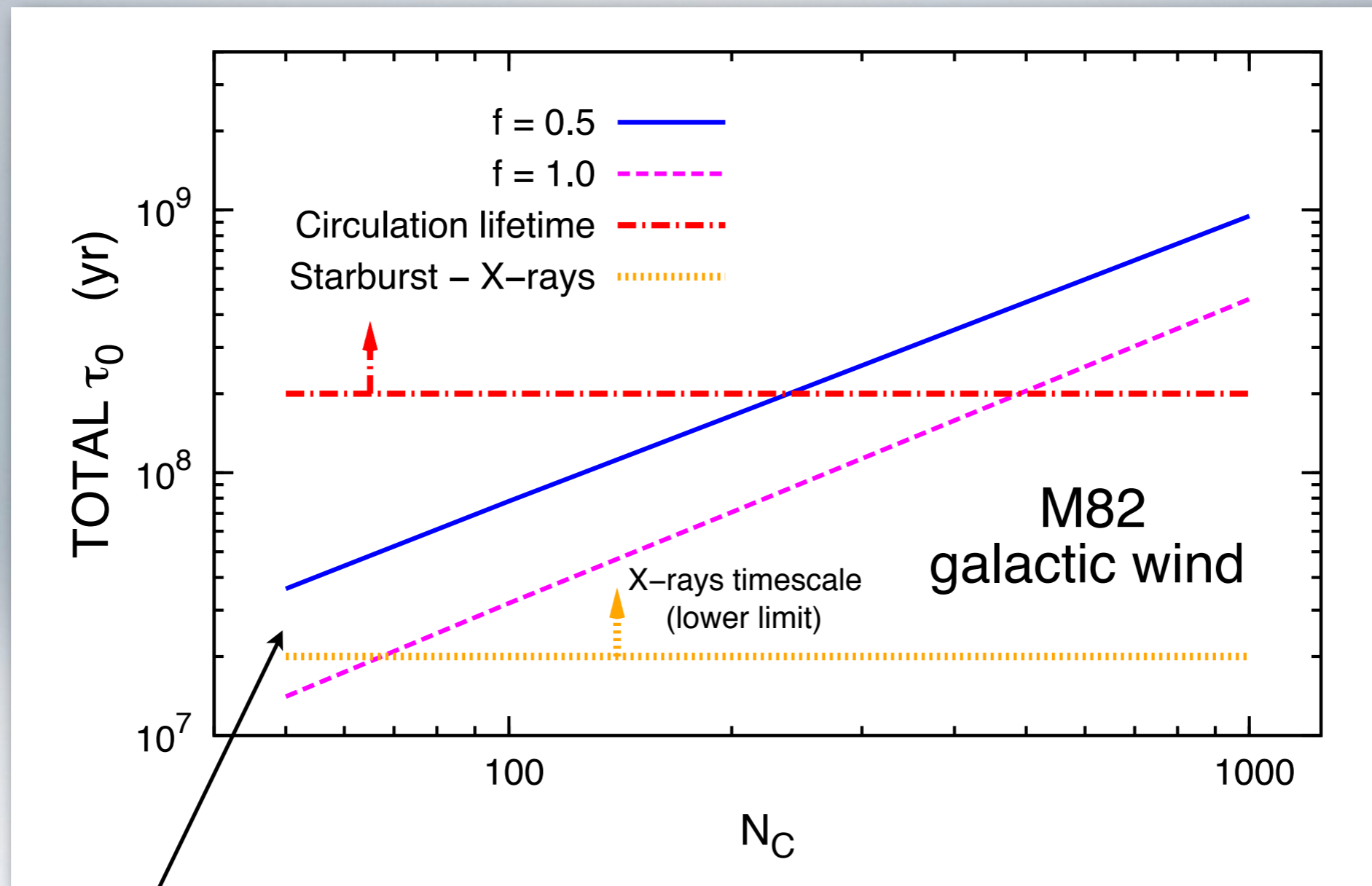
$T \sim 5.8 \times 10^6$  K

Thermal motion:  $E = 500$  eV

Adapted from **Micelotta** et al. 2010b, A&A, 510, A37

**Destroyed unless protected**

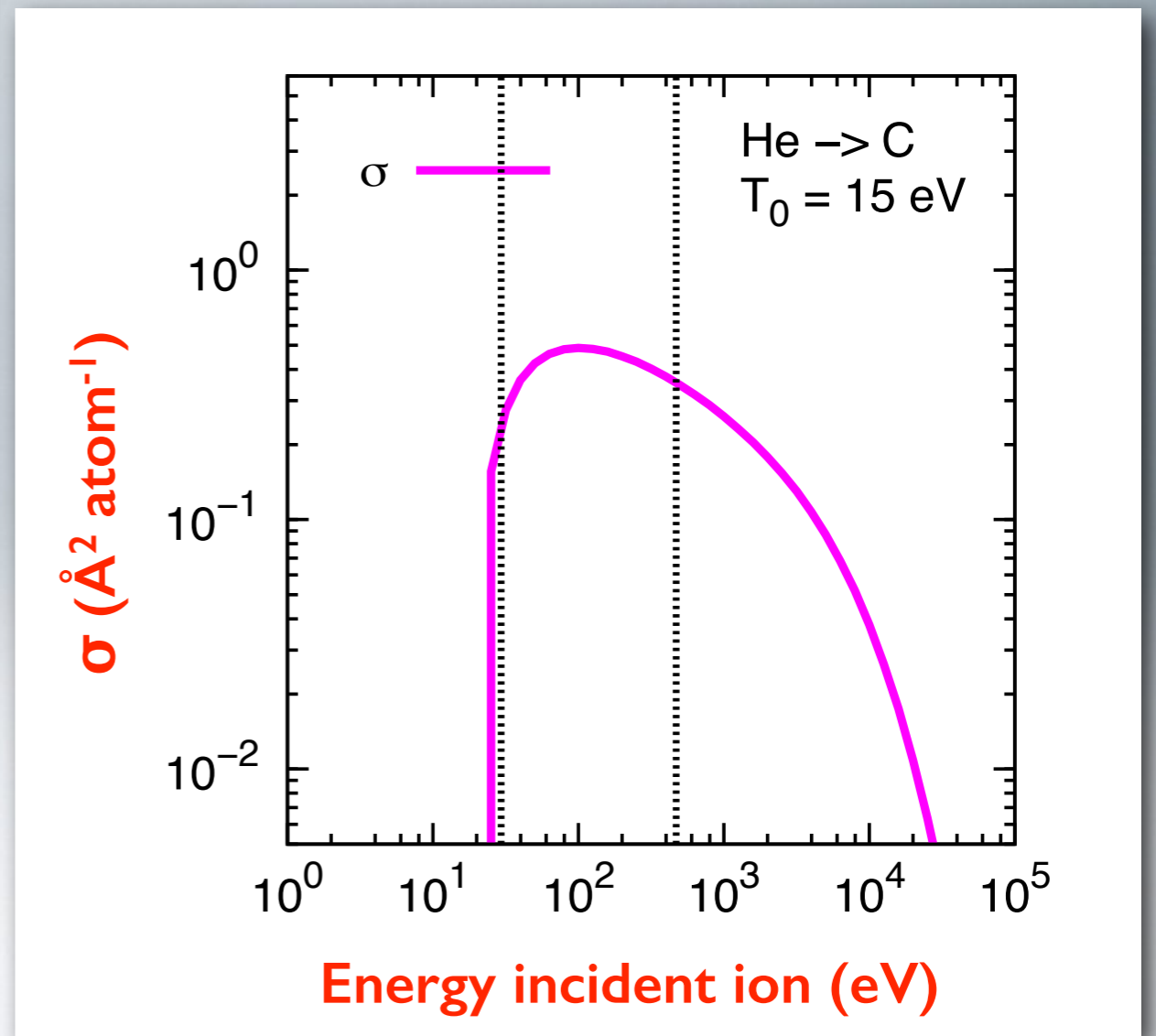
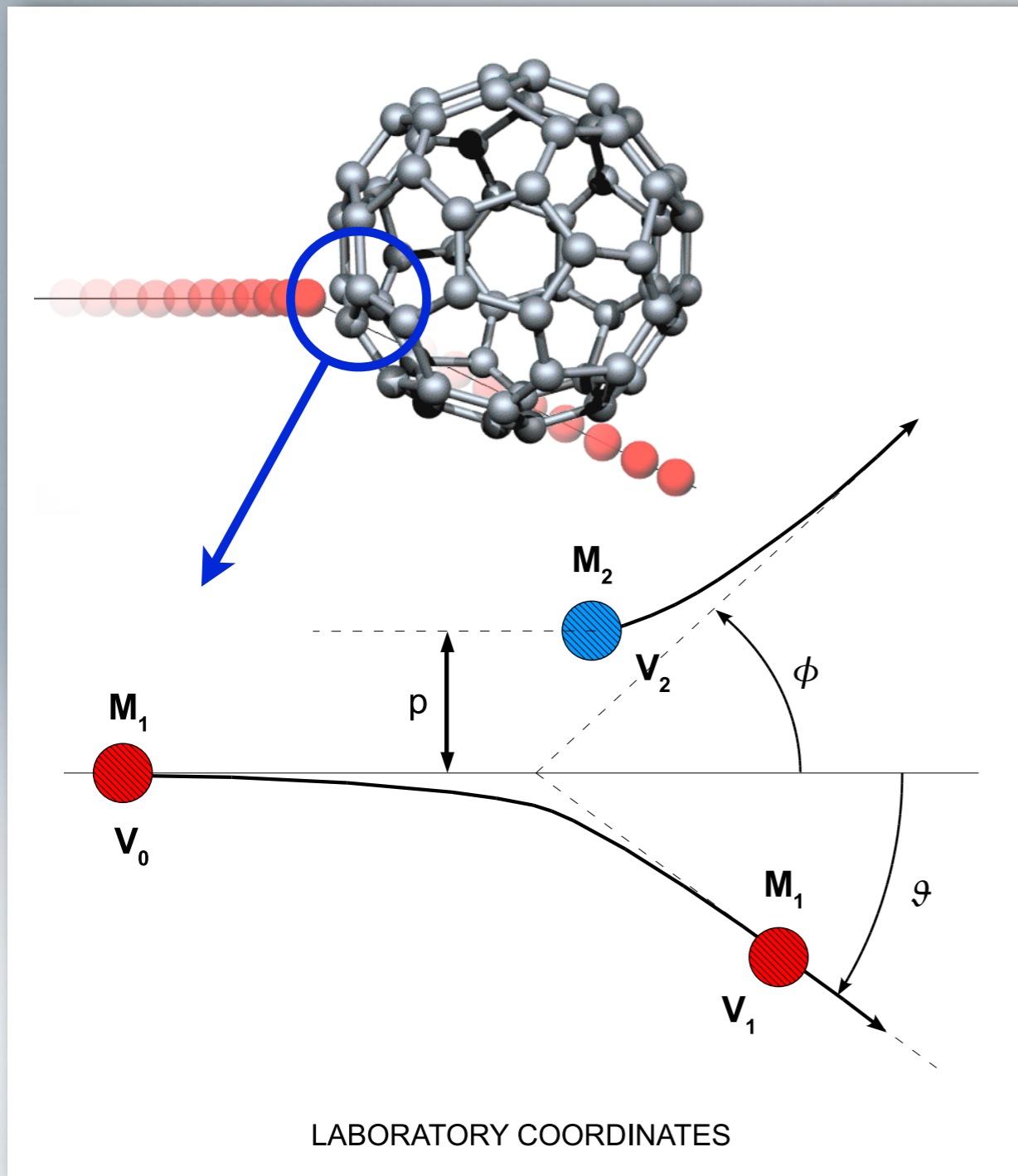
# PAHs in M82: add X-rays + CRs



**Cosmic Rays:  $E = 5 \text{ MeV} - 10 \text{ GeV}$**

*Micelotta et al. 2011, A&A, 526, A52*

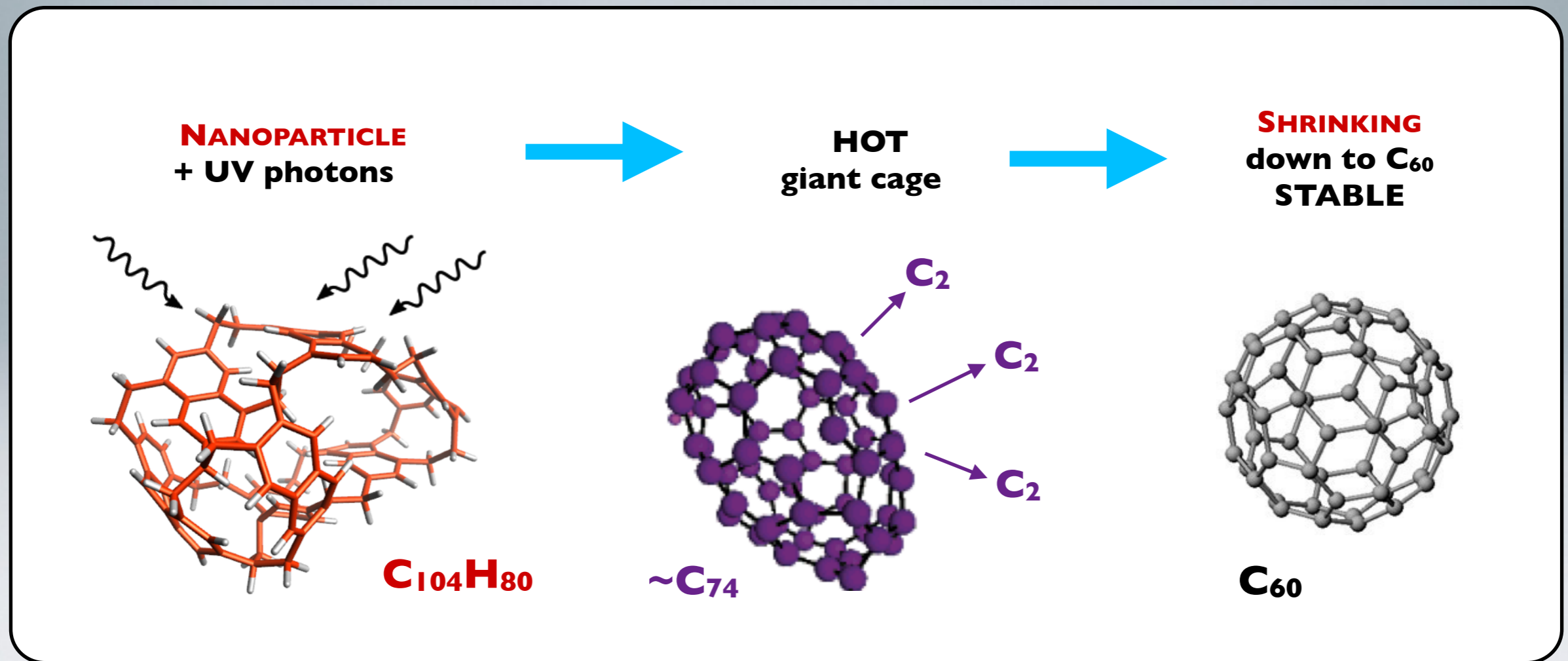
# Ions - C<sub>60</sub> collisions



**Micelotta** et al. 2013, Proc. IAU Symp. 297, 339

# C<sub>60</sub> formation in space

Conventional routes **DO NOT WORK**  $\implies$  **NEW MECHANISM!**

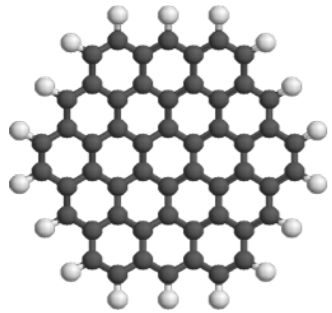


*Micelotta et al. 2012, ApJ, 761, 35*

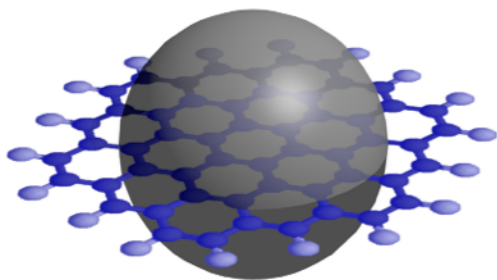


# Photo-processing

## Aromatic Infrared Bands - Proposed carriers

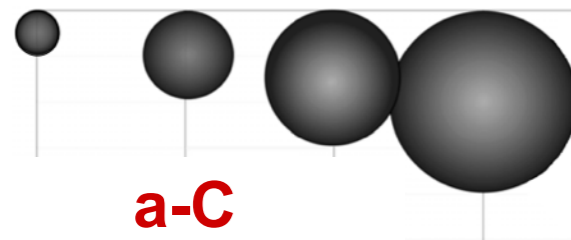


“Classical” PAHs

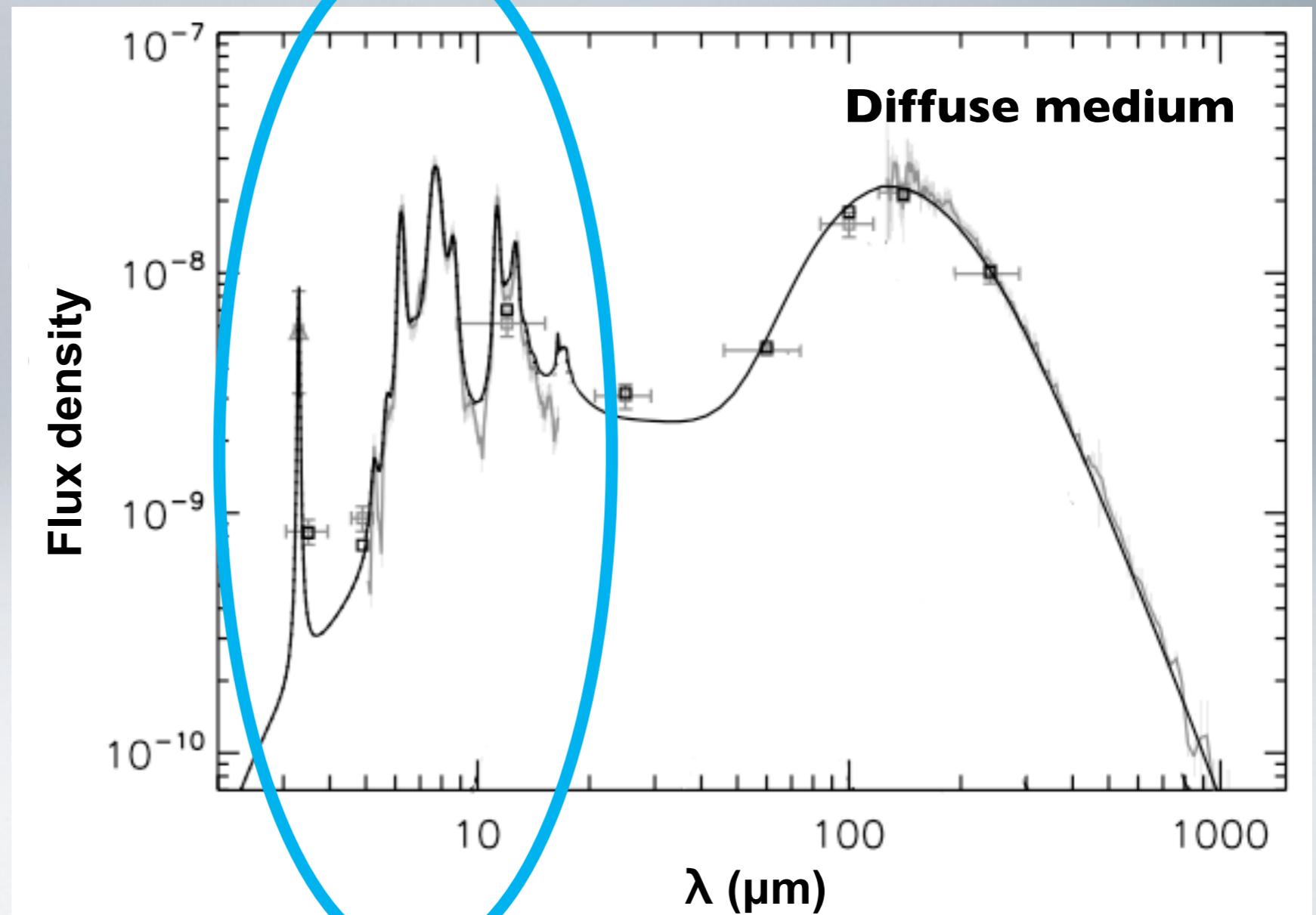


“Astronomical” PAHs

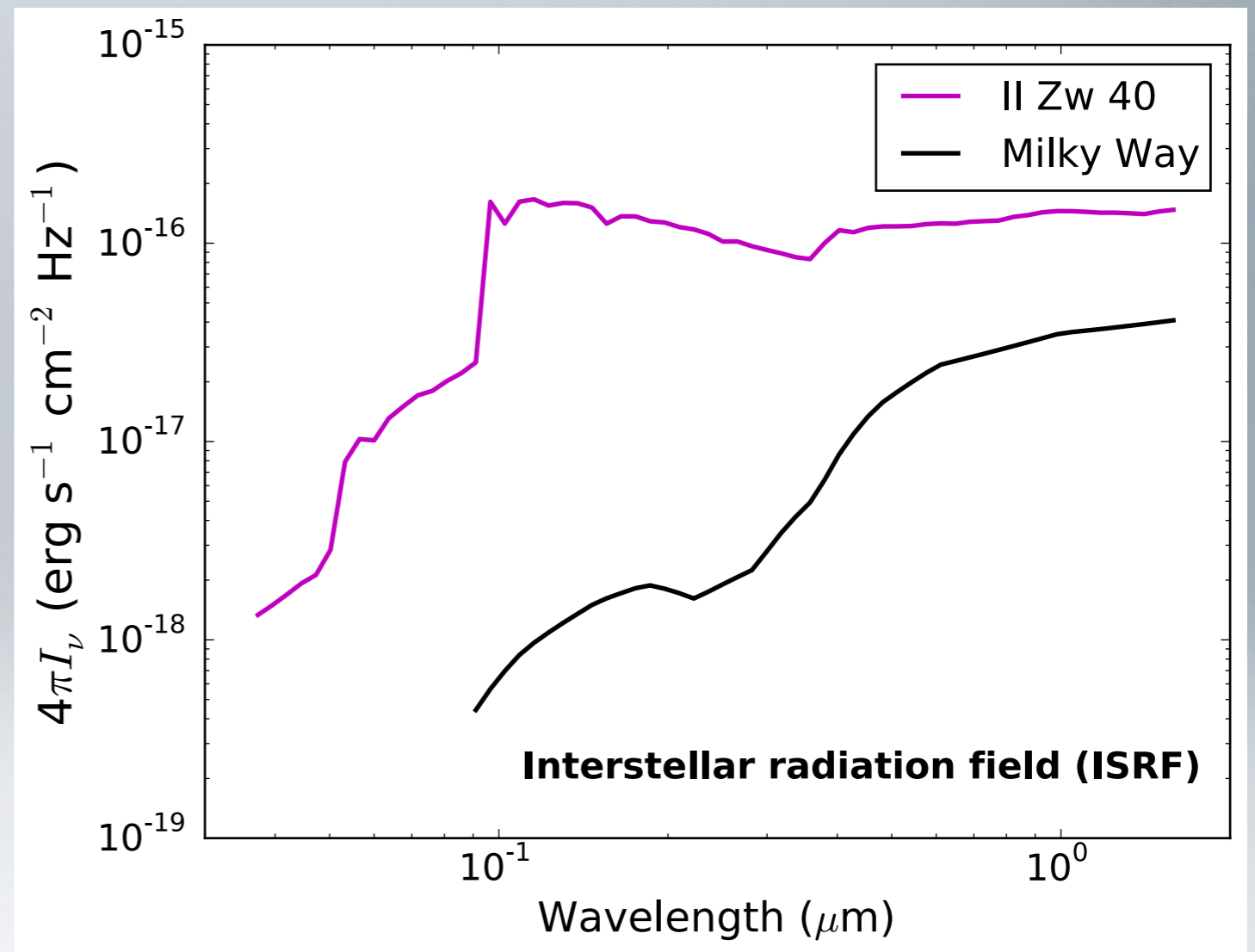
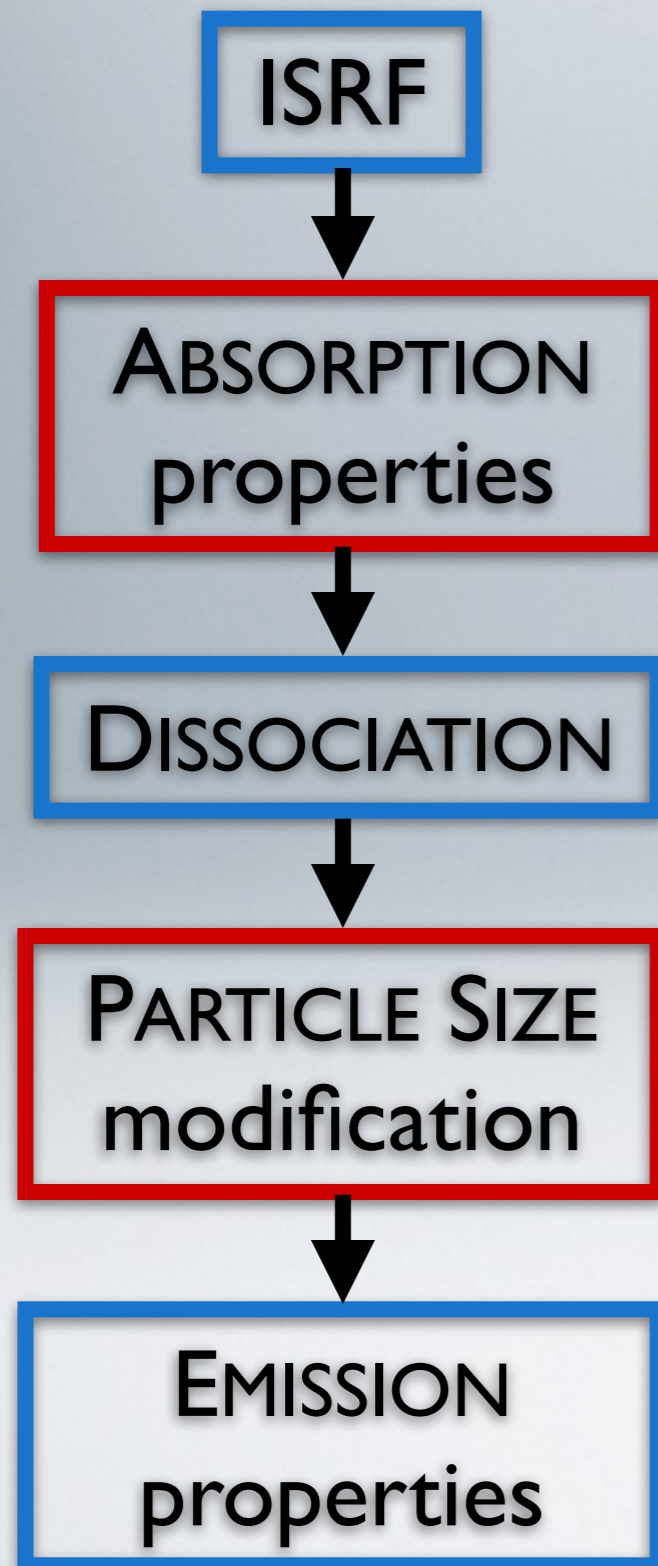
0.33 1 3 10 nm



a-C  
nanoparticles



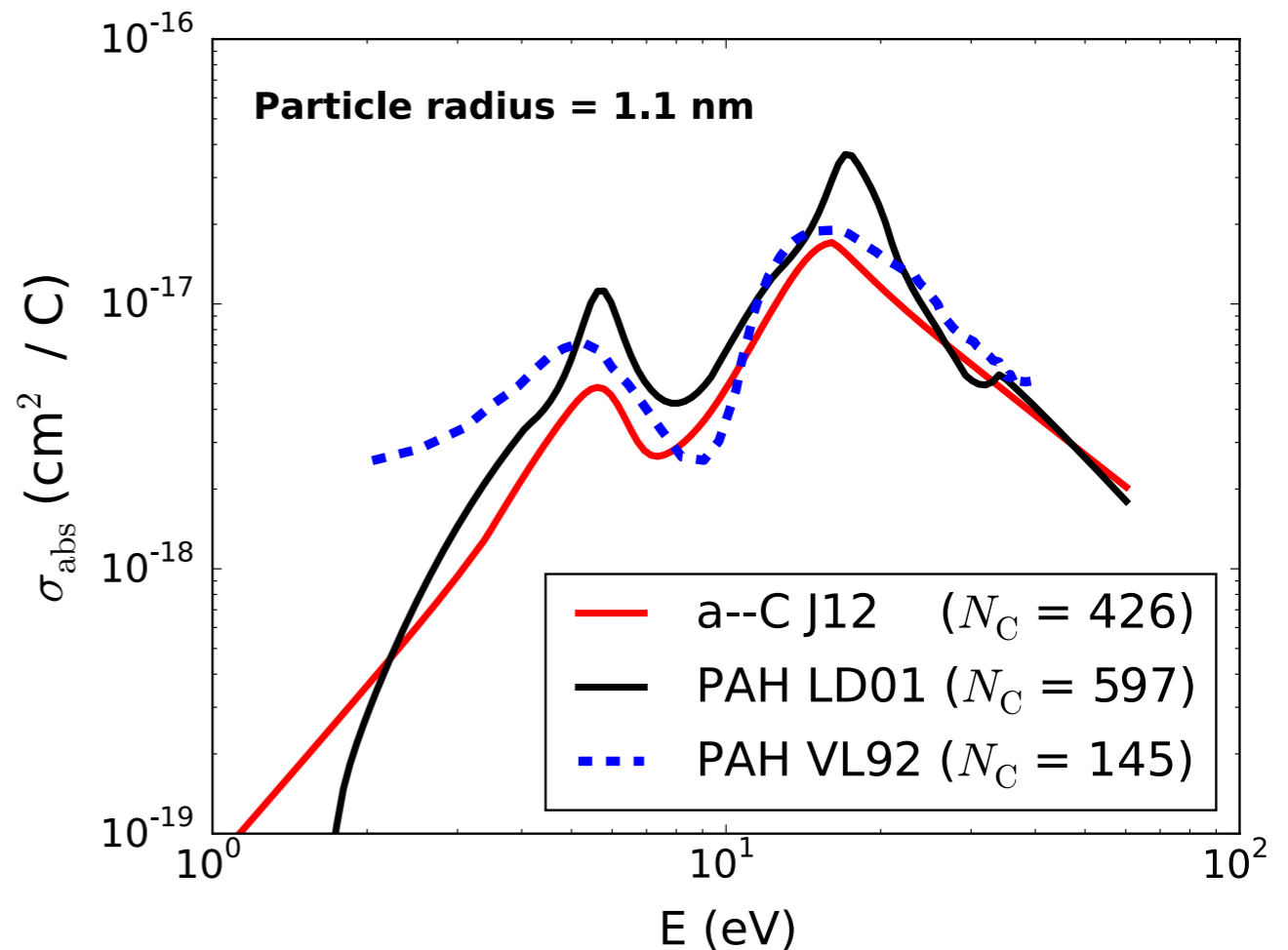
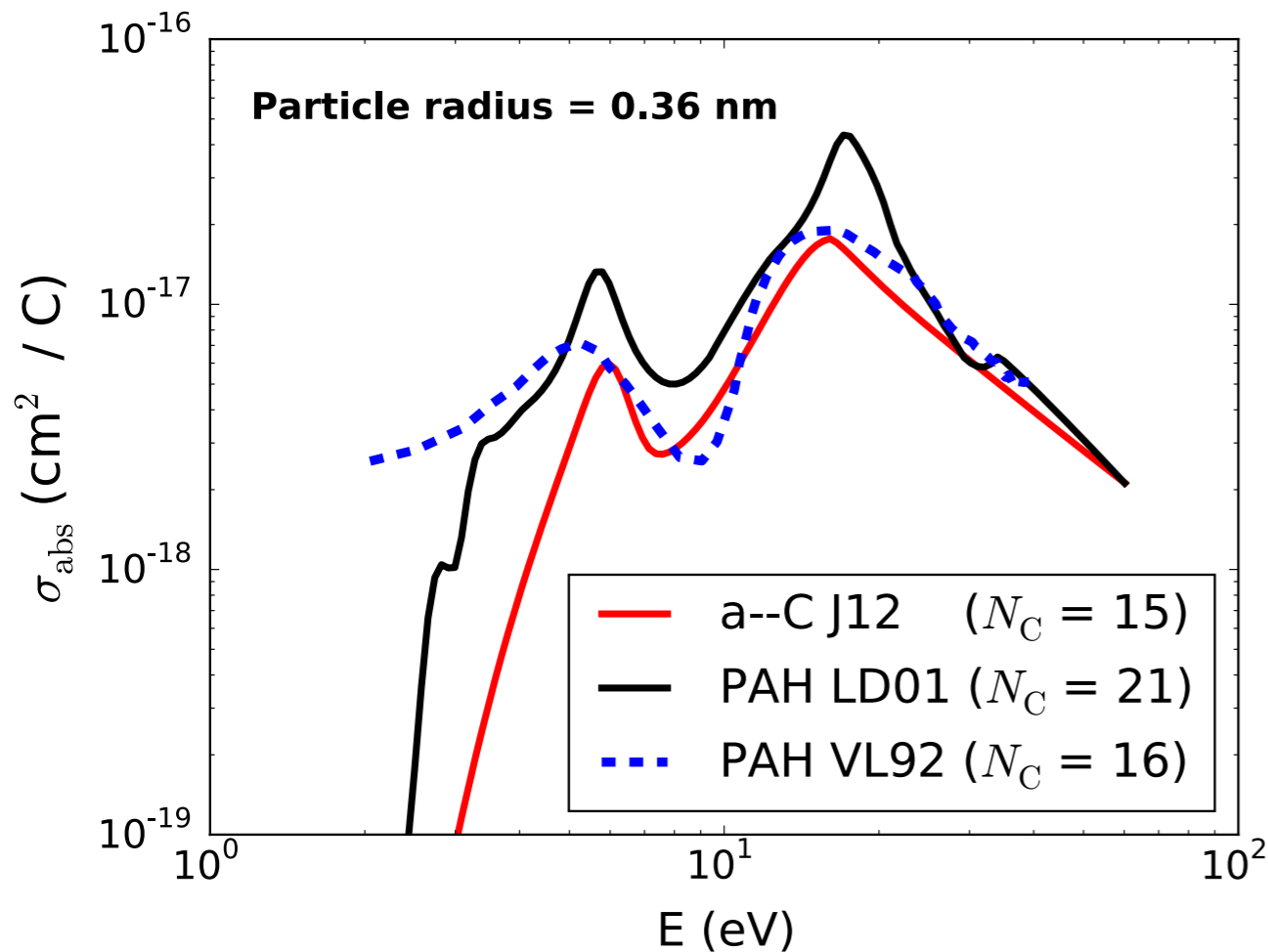
# Photo-processing



- Mathis, J. S., et al. 1983, A&A, 128, 212
- Galliano, F., et al. 2005, A&A, 434, 867

# Photo-absorption cross section

## Optical - UV

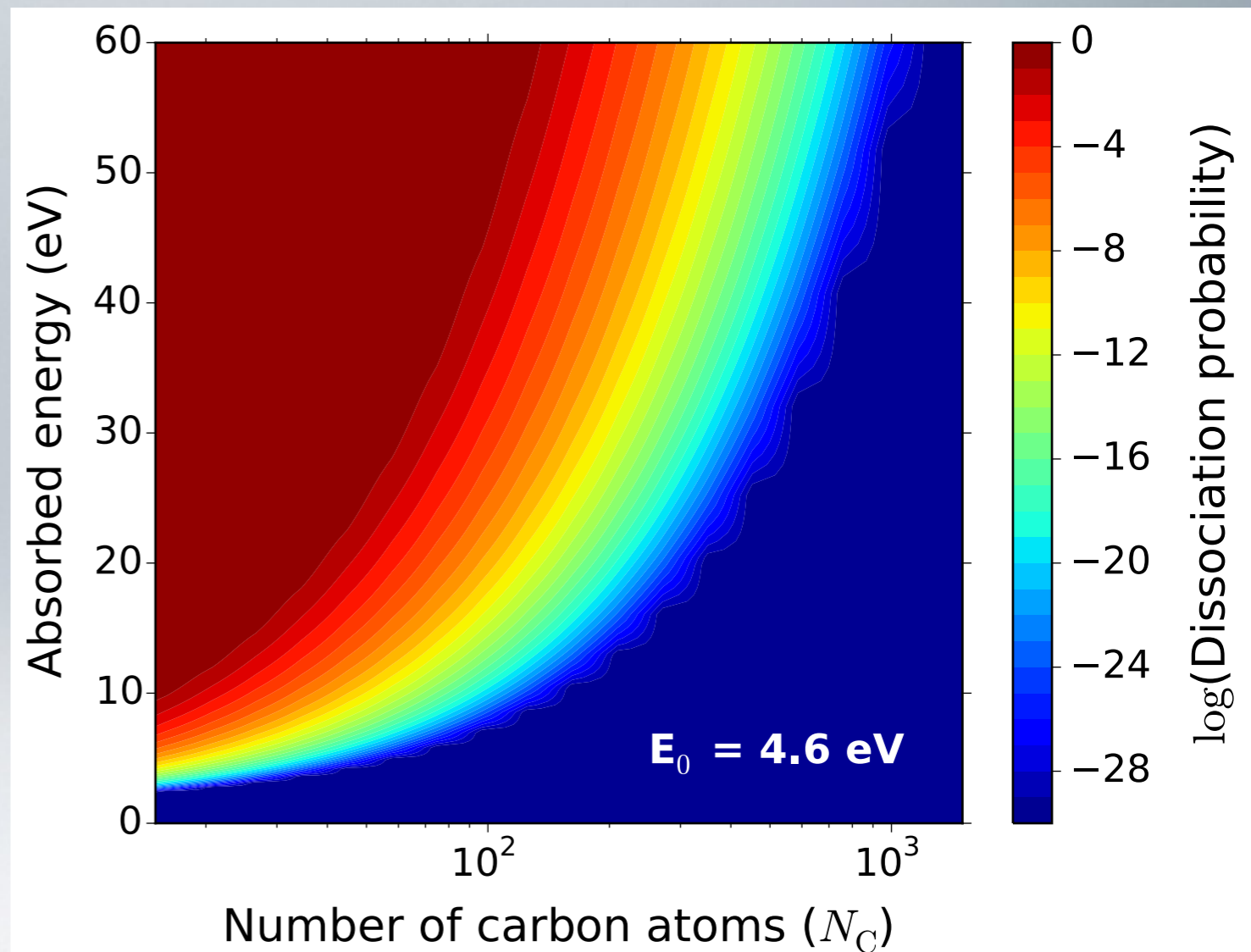


- Verstraete, L. & Léger, A. 1992, A&A, 266, 513
- Li, A. & Draine, B. T. 2001, ApJ, 554, 778
- Jones, A. P. 2012, A&A, 542, A98

*Micelotta, Jones & Juvela 2016, in prep.*

# Dissociation probability

- **STATISTICAL** fragmentation instead of IR emission
- All particles treated as **PAHs**
- Use of **FORMALISM** developed for **PAHs** to treat dissociation induced by **ELECTRON COLLISIONS** in shocks/hot gas (Micelotta et al. 2010a,b)

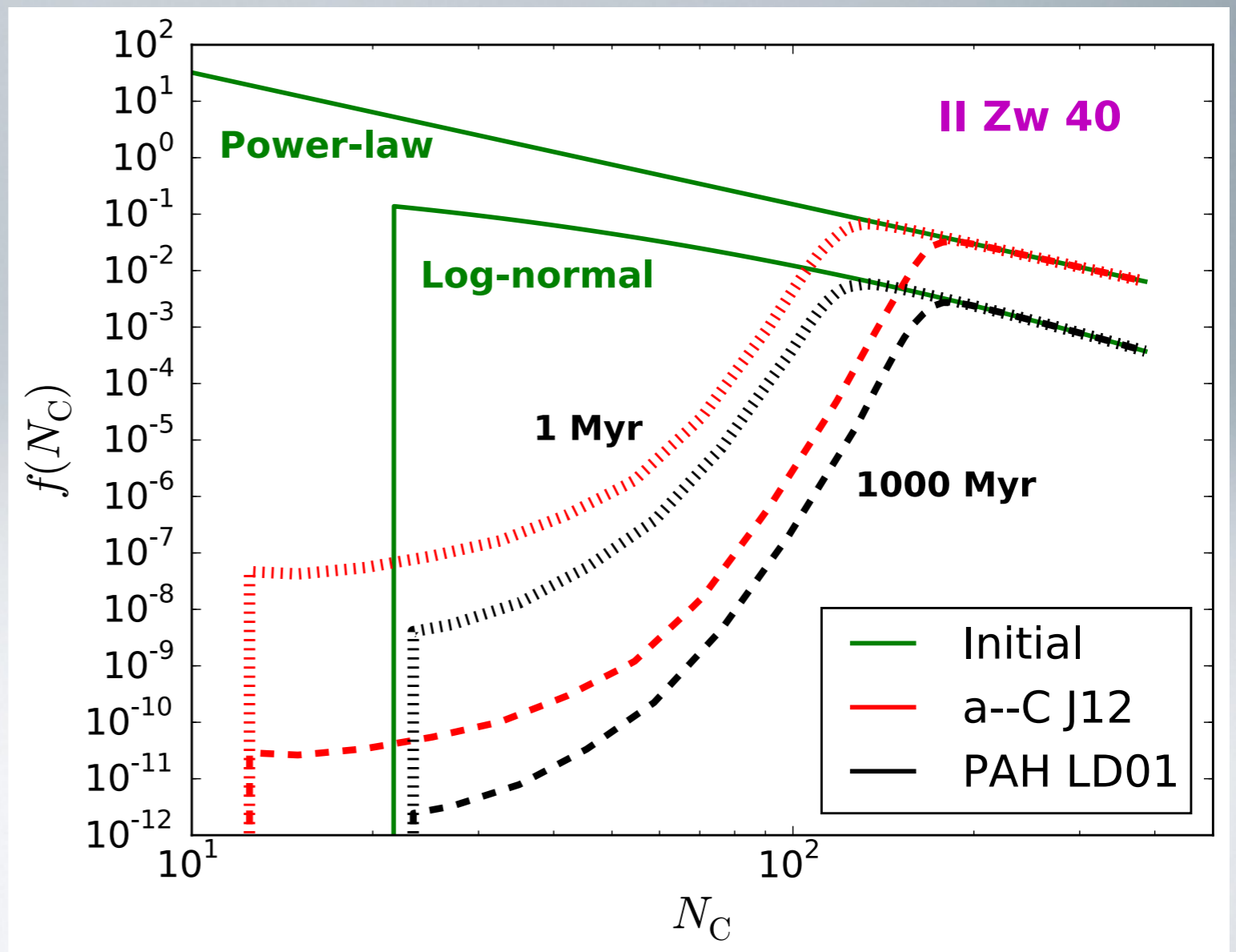


*Micelotta, Jones & Juvela 2016, in prep.*

# Modified size distributions

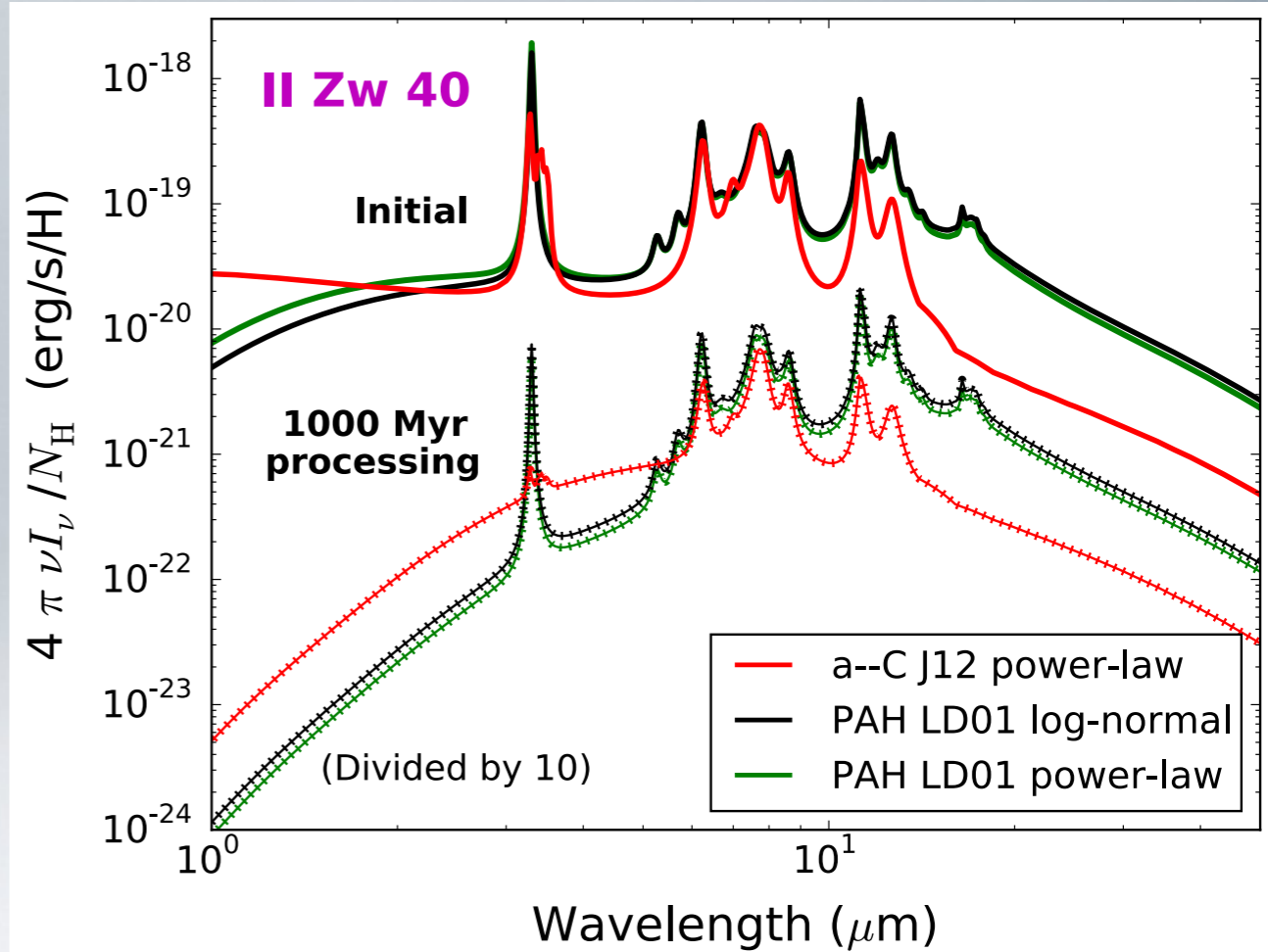
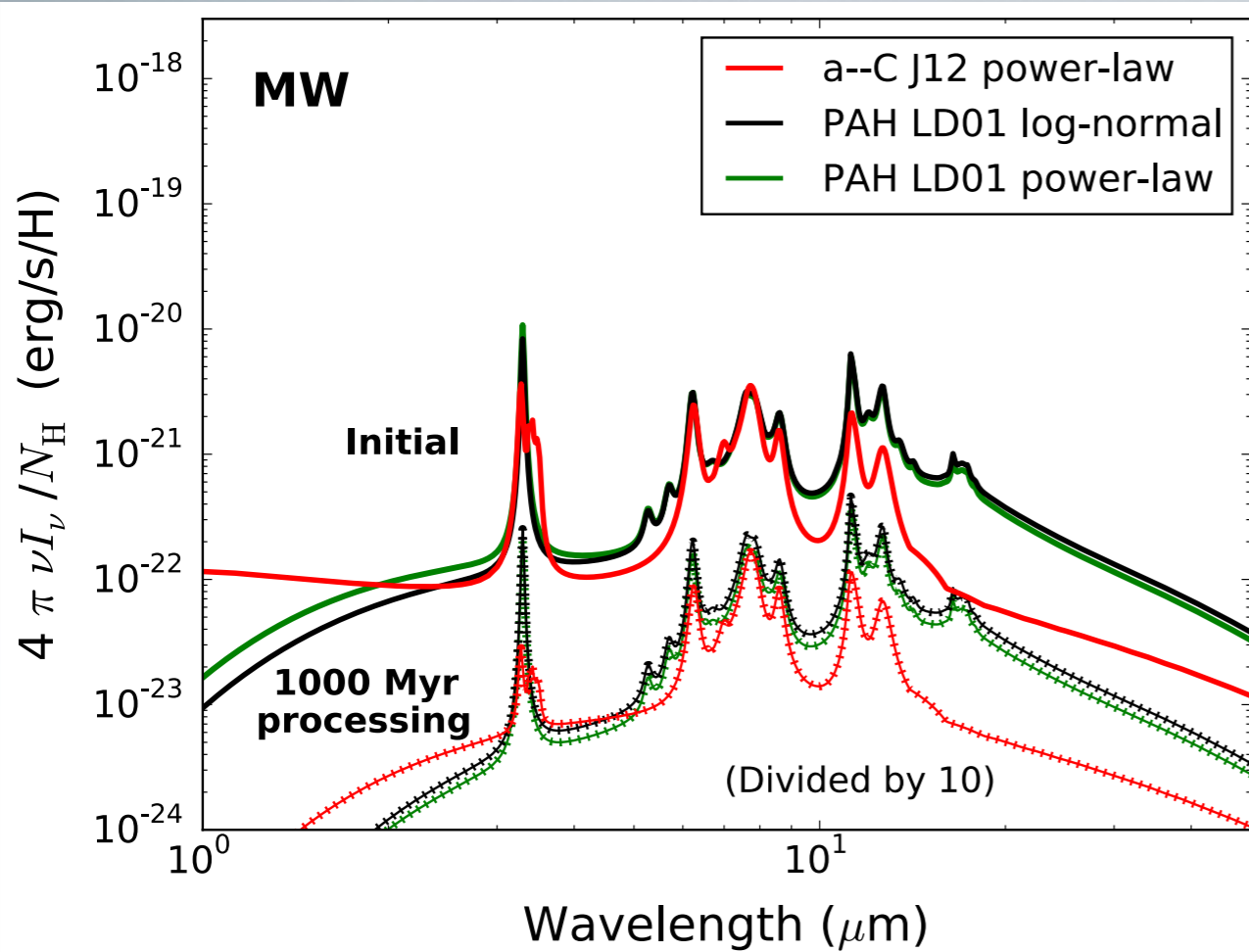
The effect of photo-dissociation & initial grain size distribution

**EACH KIND**  
of particle with its  
“**NATIVE**”  
initial distribution



# Infrared emission

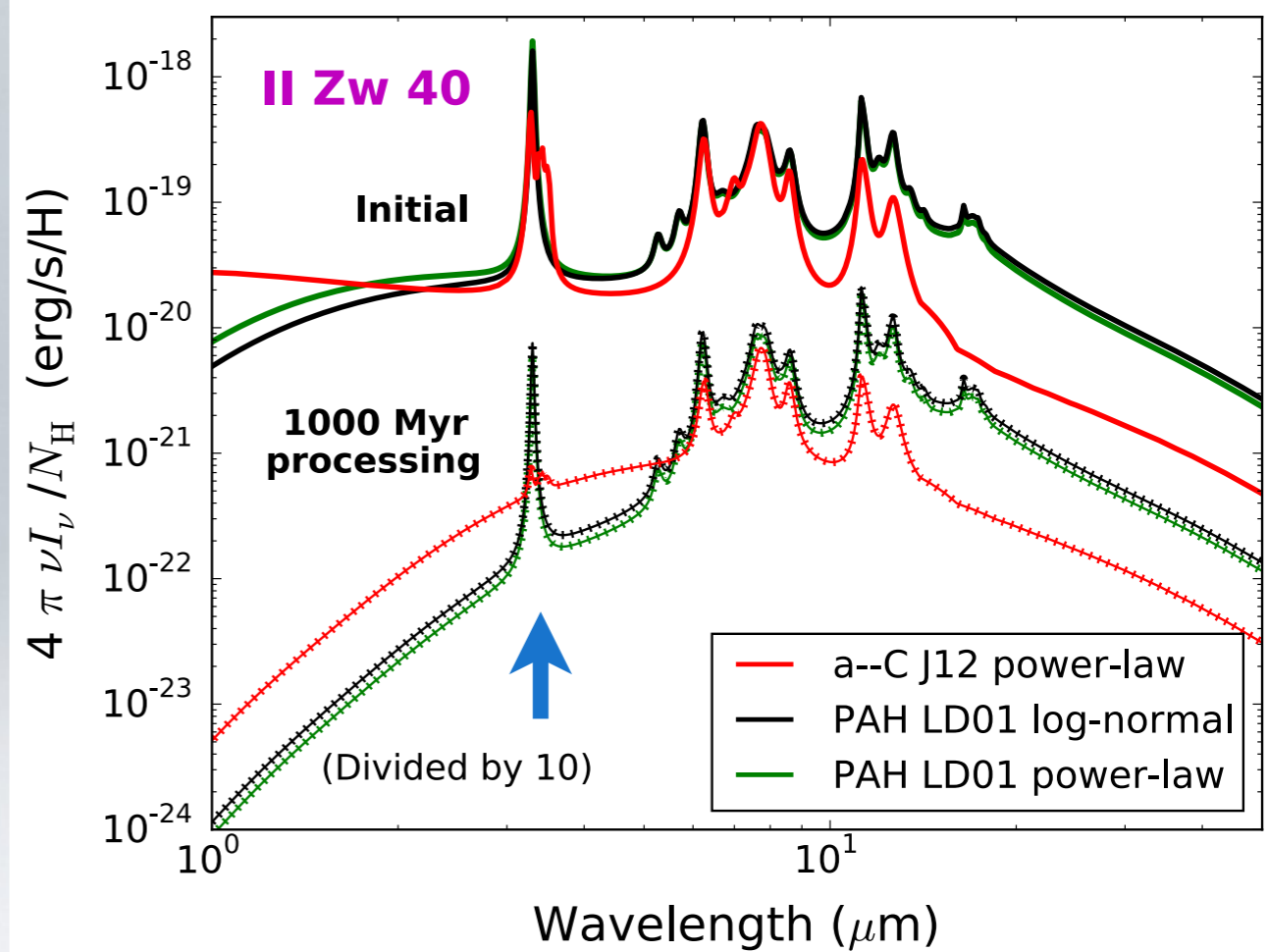
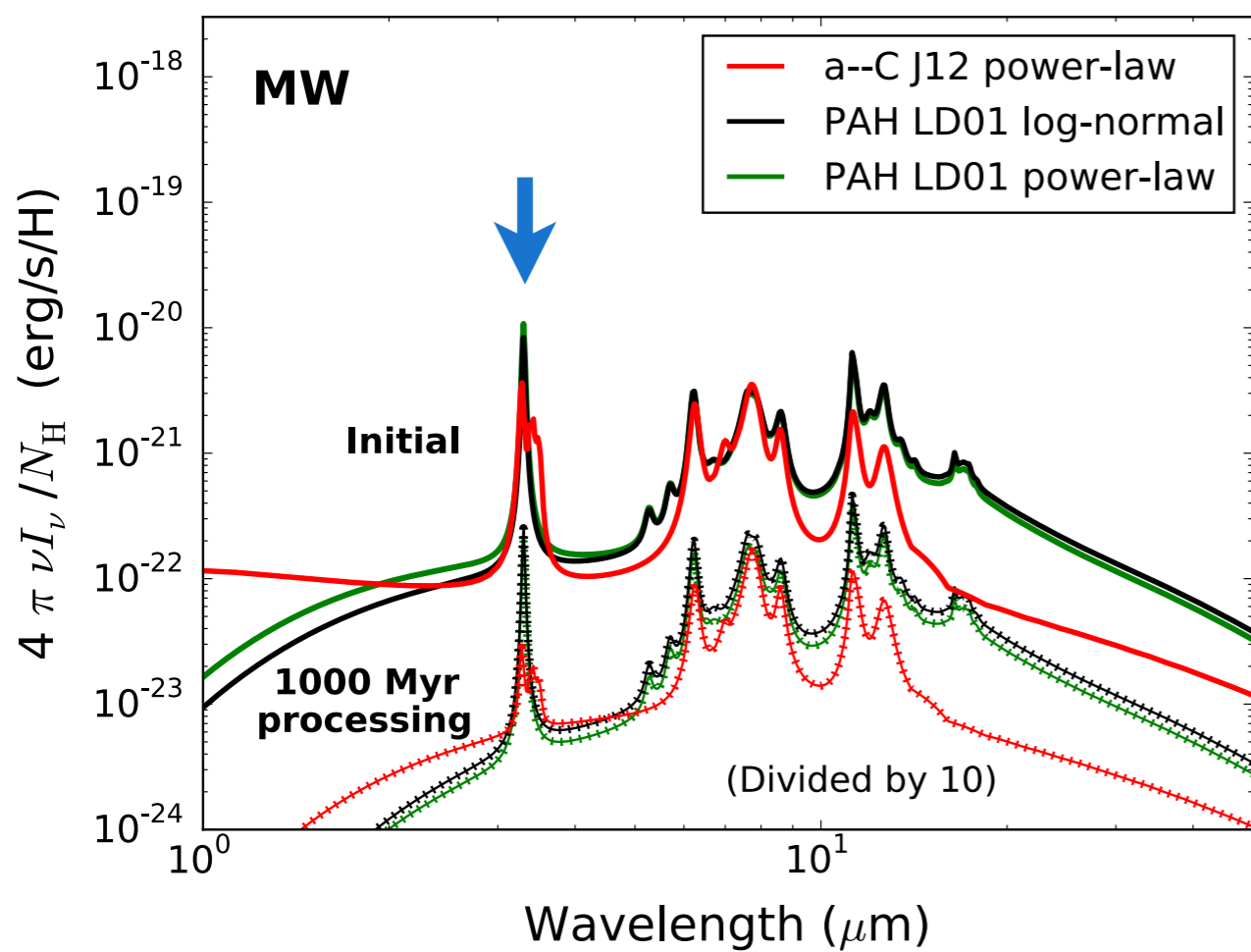
From photo-processed species and size distributions



DustEM implementation (Compiègne et al. 2011)

# Infrared emission

From photo-processed species and size distributions



**Note the SUPPRESSION of the 3.3 - 3.4  $\mu\text{m}$  complex in NANOPARTICLES emission**

# Conclusions & Perspectives

- **Energetic processing** has multiple implications and needs **detailed analysis**.
- **Analytical models important** for astrophysics.
- **Interconnection PAHs - fullerenes - nanoparticles**.
- **Theory & Experiments & Observations**.
- **New experimental facilities + telescopes (JWST)**.



# Collaborators

- X. Tielens (STRW Leiden)
- A. Jones (IAS Orsay)
- M. Juvela (University of Helsinki)
- E. Peeters, J. Cami, G. Fanchini (U. of Western Ontario)
- J. Bernard-Salas (Open University)
- H. Zettergren, H. Cederquist, H. Schmidt (Stockholm University)

**Thank you!**

Stopping power  $\leftarrow \frac{dE}{dR} = N S_n(E) \rightarrow$  Nuclear stopping cross section

$\downarrow$   
Atomic number density

Cross section  $C_m E^{-m} T^{-1-m} dT \quad 0 \lesssim T \lesssim T_m$

$S_n(E) = \int_{T_0}^{T_m} d\sigma(E, T) \cdot T \rightarrow$  Transferred energy

$V(r) \propto r^{-1/m}$

$= 4\pi a_U Z_1 Z_2 e^2 \frac{M_1}{M_1 + M_2} s_n^U(\varepsilon) \left[ 1 - \left( \frac{E_{0n}}{E} \right)^{1-m} \right]$

$\downarrow$   
**ZBL Universal screening length**

$\downarrow$   
**ZBL Universal reduced stopping cross section**

Micelotta et al.  
2010a, A&A,  
510, A36

$\left\{ \begin{array}{l} \text{--- } S_n^0(E) \text{ NO threshold} \text{ ---} \\ \text{--- } \text{Threshold effect} \text{ ---} \end{array} \right.$

## Total cross section

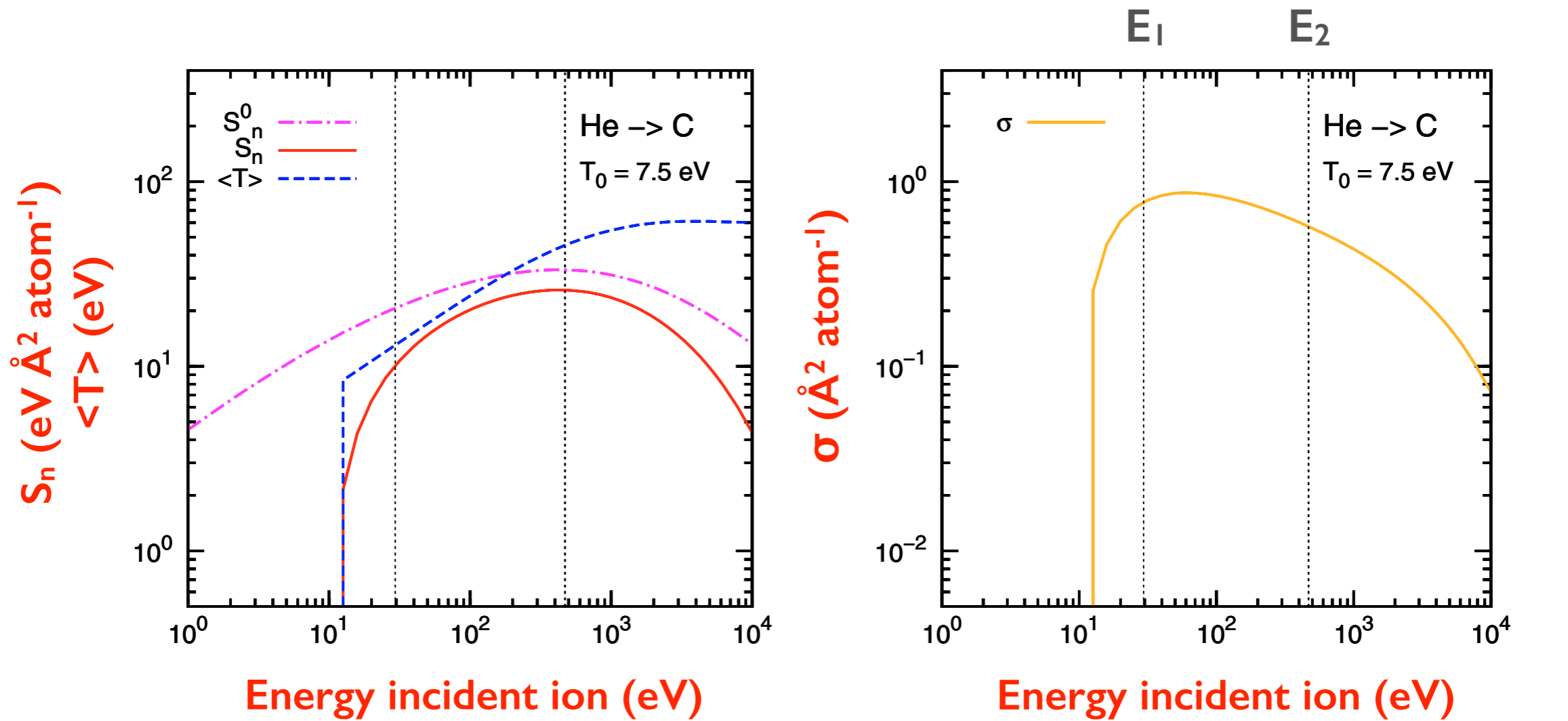
$$\begin{aligned} \sigma(E) &= \int_{T_0}^{T_m} d\sigma(E, T) \\ &= 4\pi a_U Z_1 Z_2 e^2 \frac{M_1}{M_1 + M_2} s_n^U(\varepsilon) \frac{1-m}{m} \frac{1}{\gamma E} \left[ \left( \frac{E_{0n}}{E} \right)^{-m} - 1 \right] \end{aligned}$$

┌  $S_n^0(E)$  NO threshold ─┐

$$\langle T(E) \rangle = \frac{S_n(E)}{\sigma(E)} = \langle T(E) \rangle = \frac{m}{1-m} \gamma \frac{E^{1-m} - E_{0n}^{1-m}}{E_{0n}^{-m} - E^{-m}}$$

Average  
transferred  
energy

**Micelotta et al. 2010a, A&A, 510, A36**



Micelotta et al. 2010a, A&A, 510, A36

$$T_e(\vartheta) = 27.2116 \int_{-R/\sin \vartheta}^{R/\sin \vartheta} v \gamma(r_s) ds$$

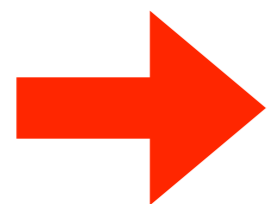
**Transferred energy  
electronic interaction**

$$S(E) = \frac{h \log(1 + a E)}{f E^g + b E^d + c E^e}$$

**Fit to stopping power  
electrons interaction**

$$T_{\text{eff}} \simeq 2000 \left( \frac{T_e(\text{eV})}{N_C} \right)^{0.4} \left( 1 - 0.2 \frac{E_0(\text{eV})}{T_e(\text{eV})} \right)$$

**Effective  
temperature  
after energy  
transfer**



$$P(n_{\text{max}}) = \frac{k_0 \exp[-E_0/k T_{\text{av}}]}{k_{\text{IR}}/(n_{\text{max}} + 1)}$$

**Dissociation  
probability**

# Stopping of high-energy ions

**E = 5 MeV/nuc. - 10 GeV** → **Electronic** interaction **only**

## Bethe - Bloch equation

$$\begin{aligned}
 \kappa &\equiv 4\pi r_0^2 m_e c^2 \\
 S &= \frac{\kappa Z_2}{\beta^2} Z_1^2 \left\{ \left[ f(\beta) - \frac{C}{Z_2} - \ln \langle I \rangle - \frac{\delta}{2} \right] \right. \\
 &\quad \left. + Z_1 L_1(\text{Barkas}) + Z_1^2 L_2(\text{Bloch}) \right\}
 \end{aligned}$$

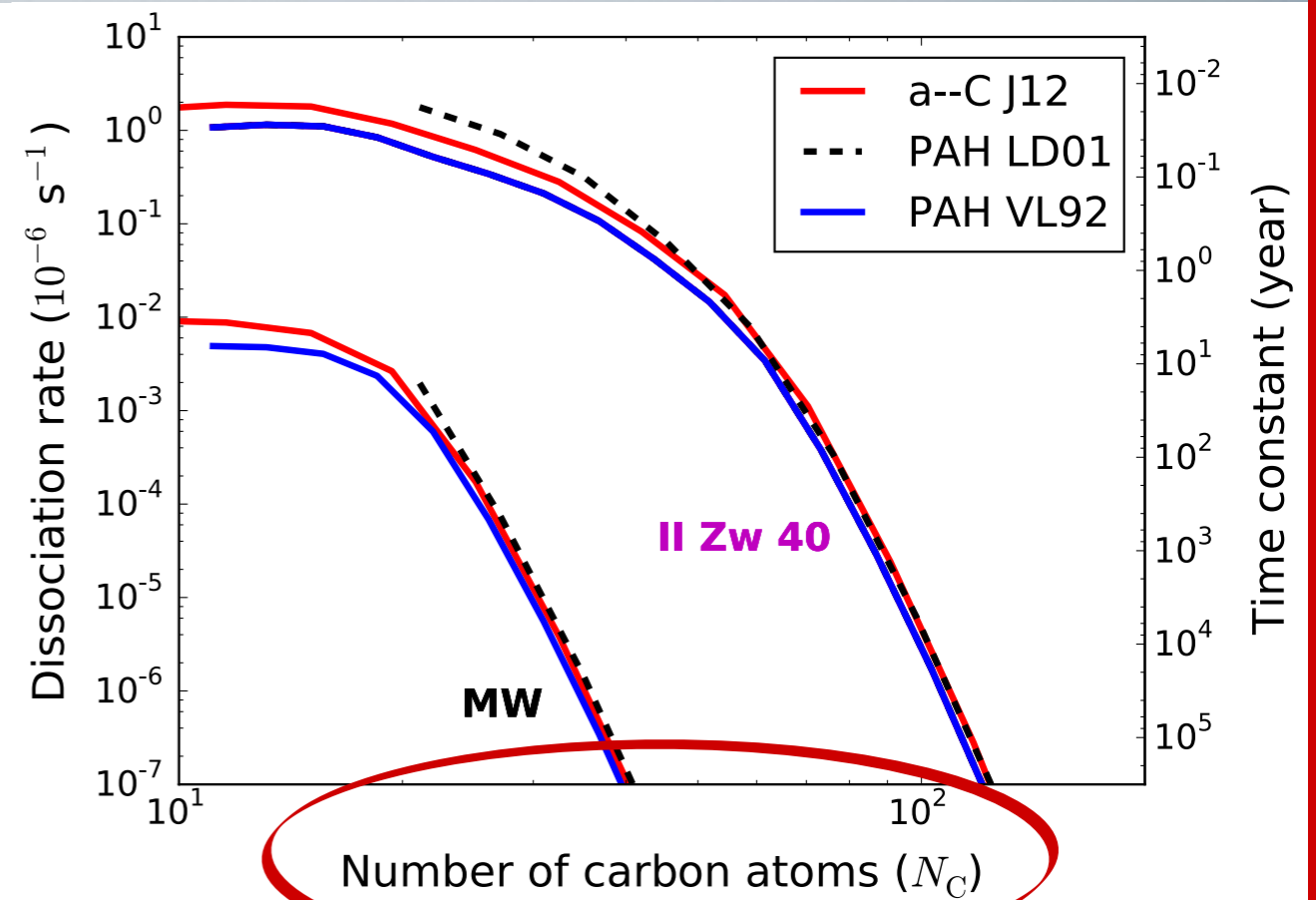
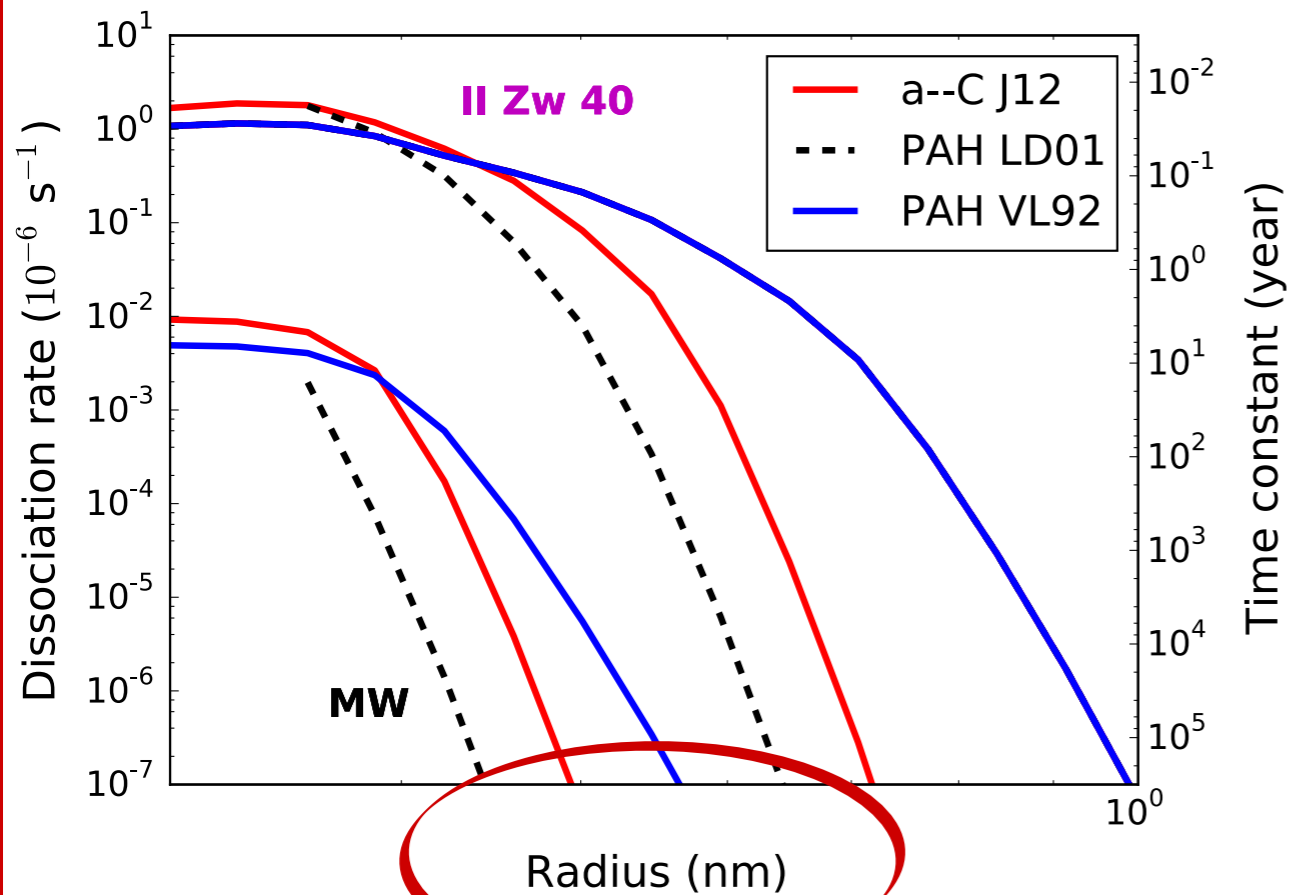
Annotations:
 

- Stopping power** (red arrow) points to  $S$ .
- Shell correction** (blue arrow) points to  $\frac{C}{Z_2}$ .
- Mean ionisation** (blue arrow) points to  $\ln \langle I \rangle$ .
- Density effect** (blue arrow) points to  $\frac{\delta}{2}$ .

Ziegler et al. 1999

# Photo-dissociation rate

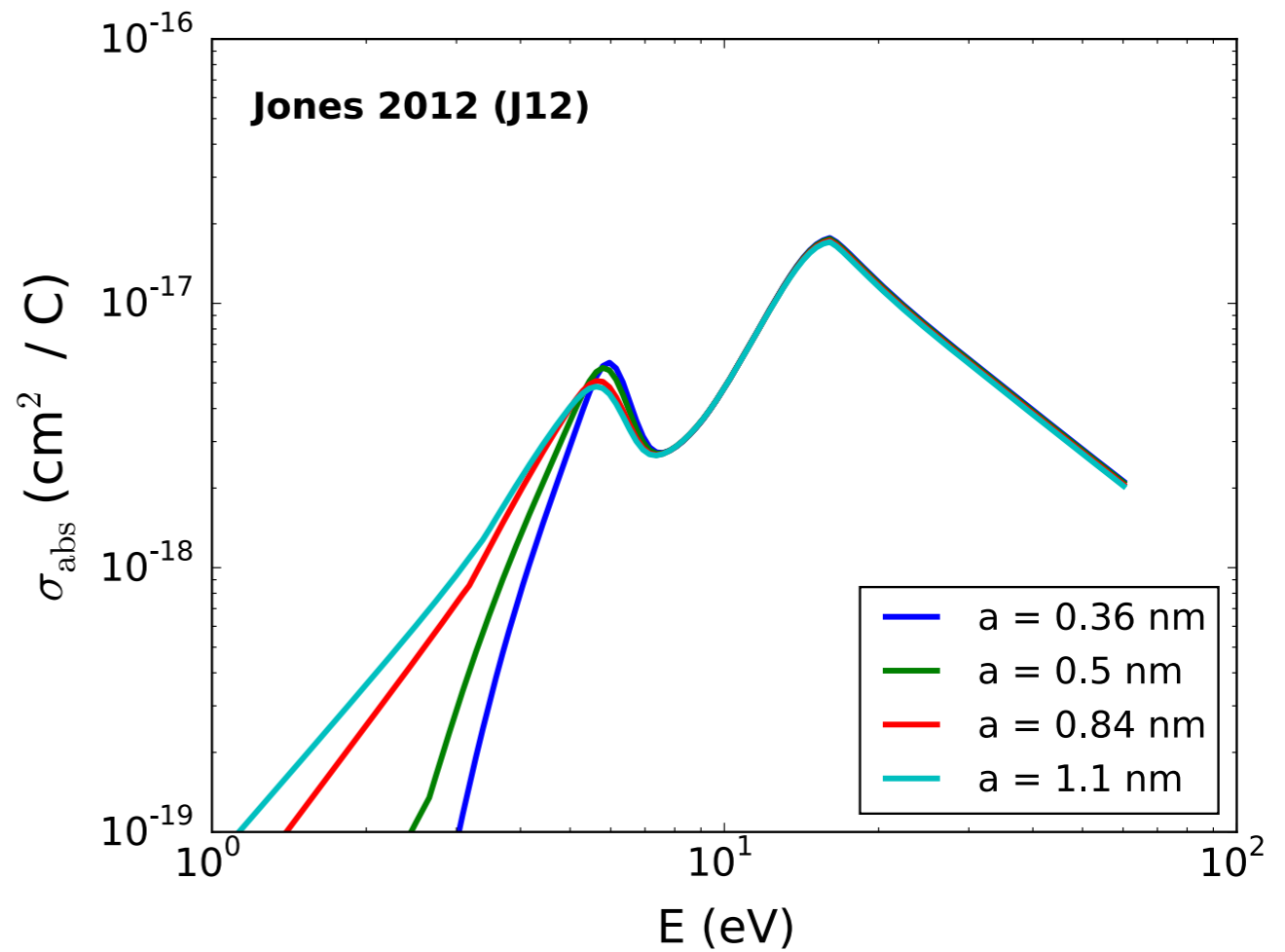
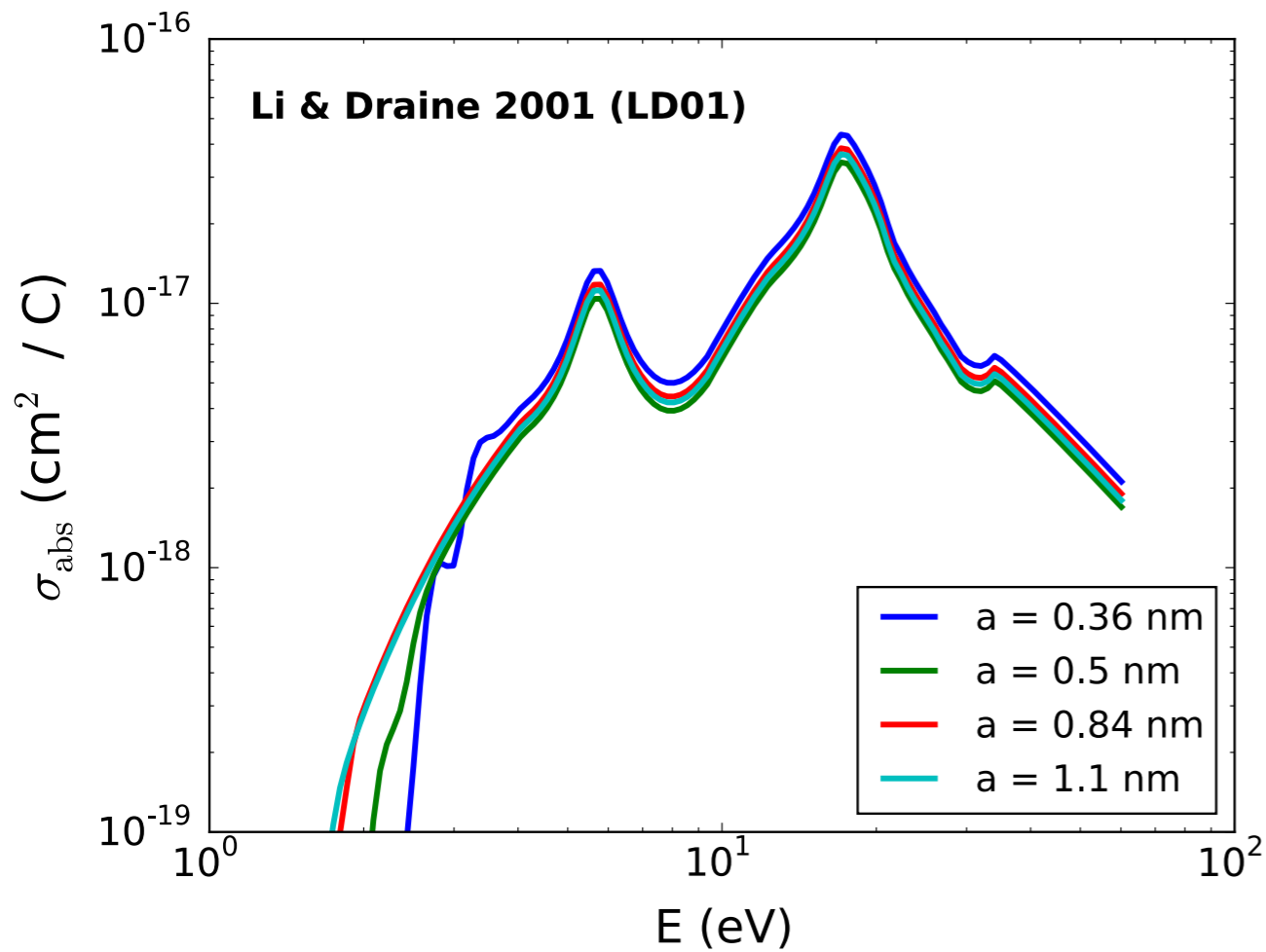
Following Vis-UV absorption



**vs.**

# Photo-absorption cross section II

Optical - UV

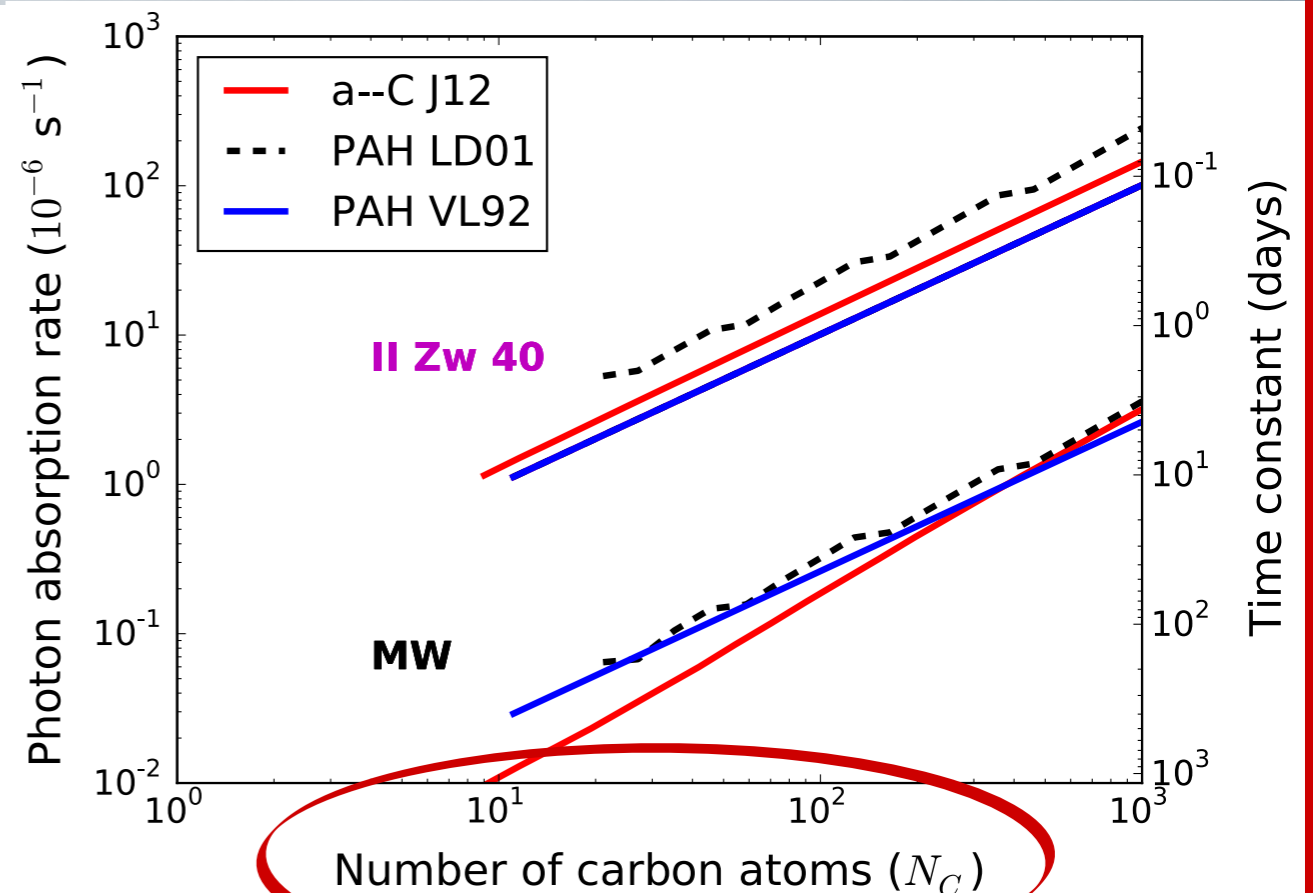
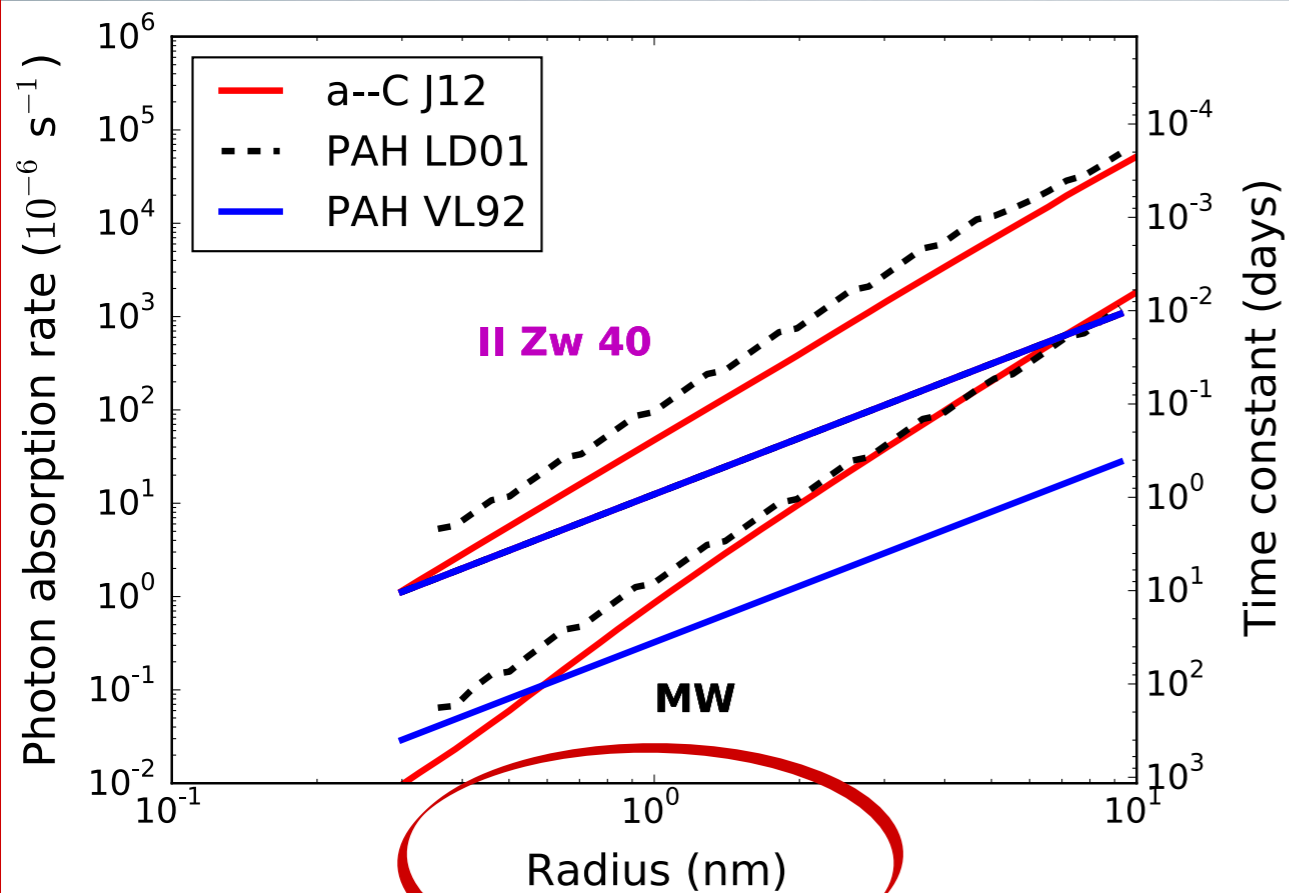


- Li, A. & Draine, B. T. 2001, ApJ, 554, 778
- Jones, A. P. 2012, A&A, 542, A98



# Photon absorption rate

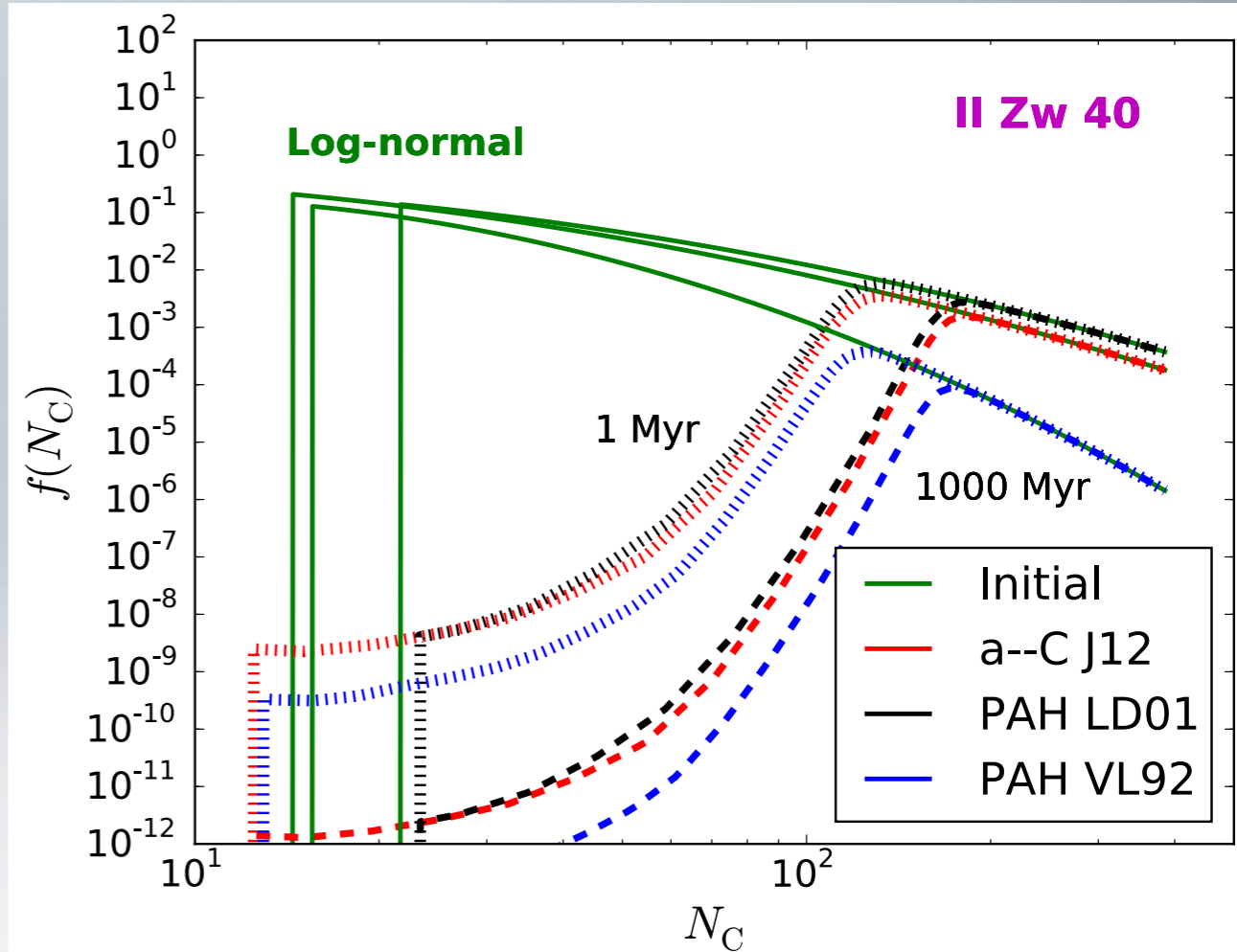
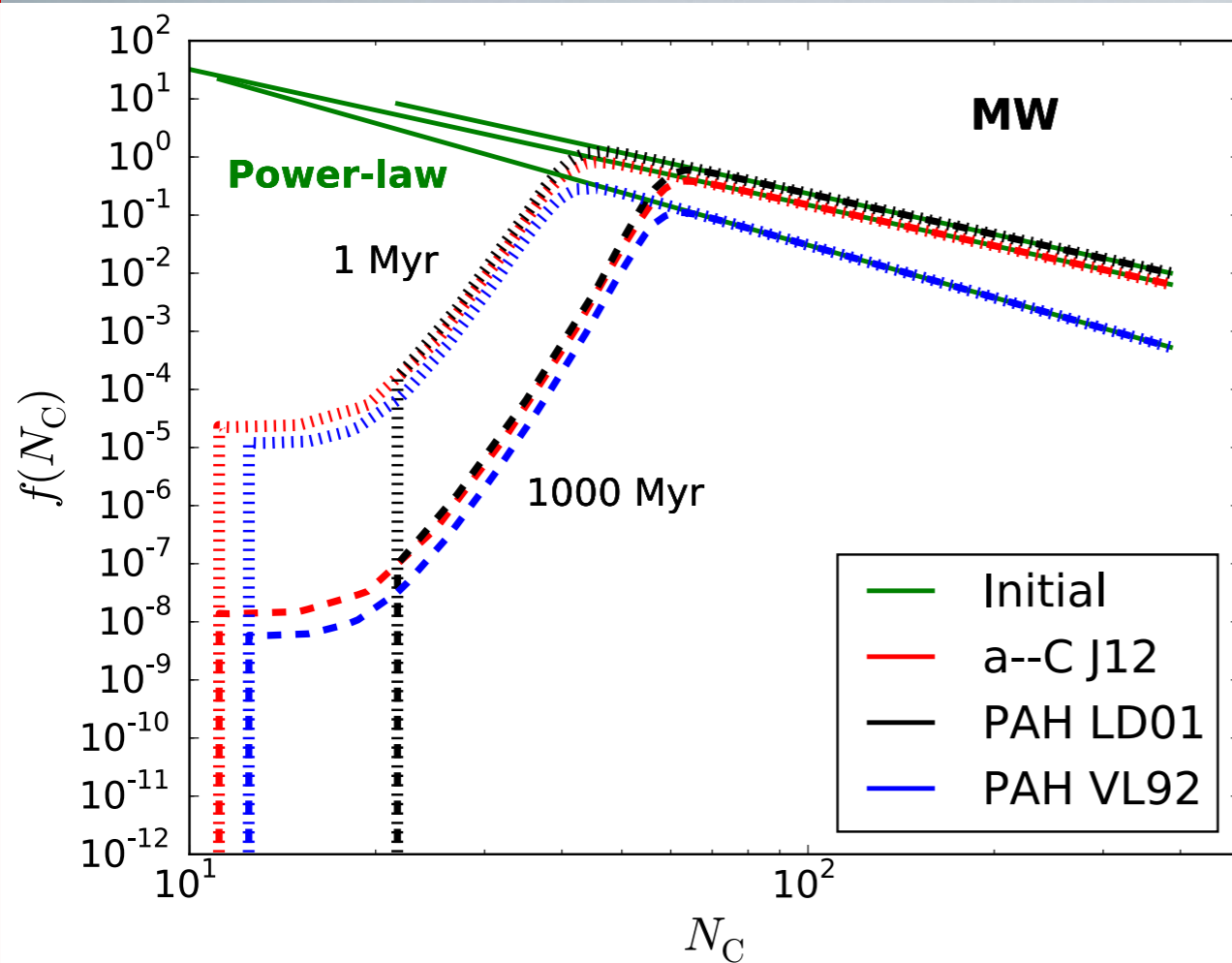
Optical - UV



vs.

# Modified size distributions I

## The effect of photo-dissociation

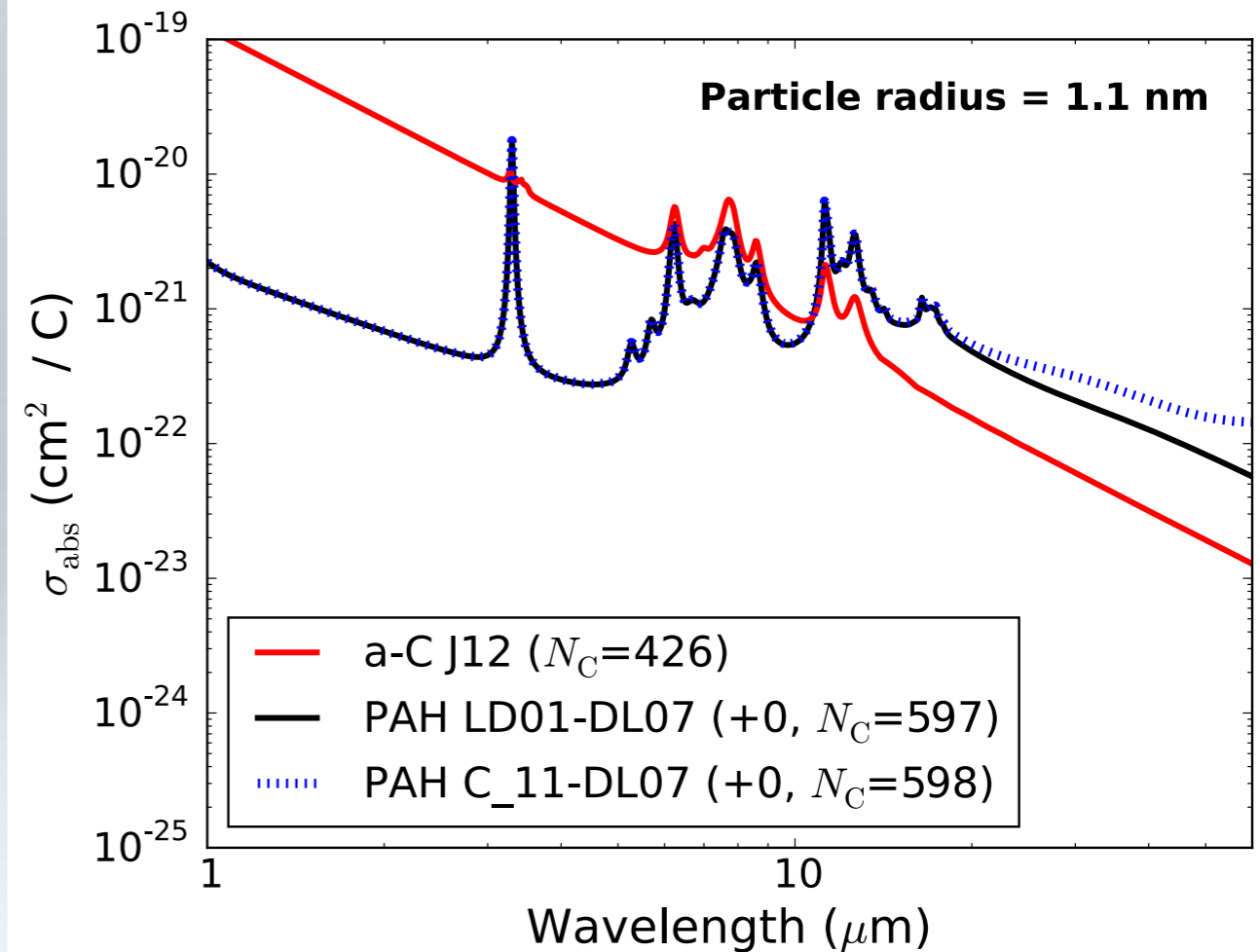
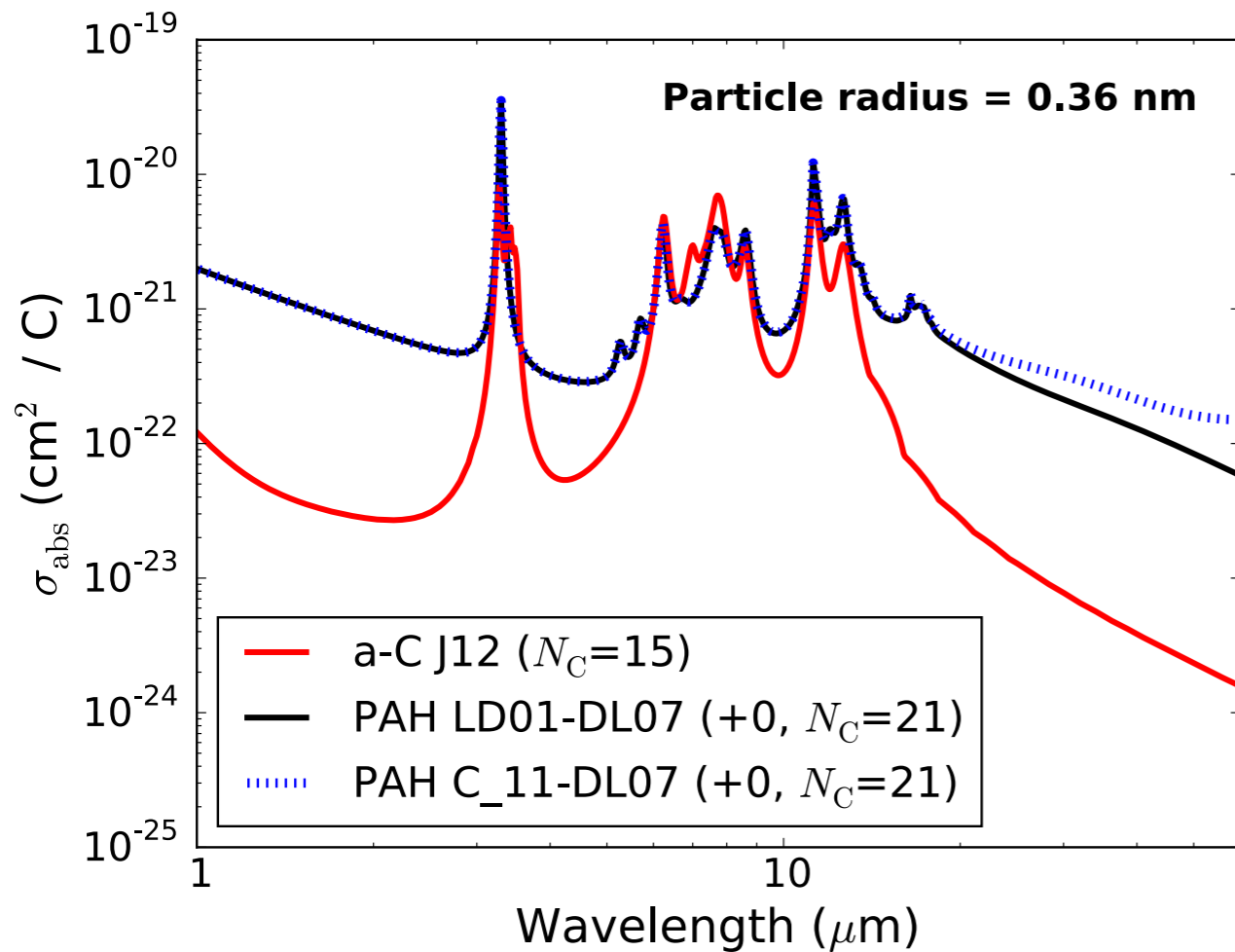


**Power-law for all:**  
the "native" distribution of  
nanoparticles - J12

**Log-normal for all:**  
the "native" distribution of  
astronomical PAHs - LD01

# Photo-absorption cross section III

## Infrared



- Verstraete, L. & Léger, A. 1992, A&A, 266, 513 — Compiègne, M., et al. 2011, A&A, 525, A103
- Li, A. & Draine, B. T. 2001, ApJ, 554, 778 — Draine, B. T. & Li, A. 2007, ApJ, 657, 810
- Jones, A. P. 2012, A&A, 542, A98