Dust Modeling

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Why is dust important for IR and sub-mm astronomy?

1. Thermal emission from dust lies in the IR and sub-mm. A large fraction of the starlight generated in a galaxy is absorbed by dust and re-emitted.

2. Dust plays an important role in determining the physical conditions in the gas, affecting the emergent spectrum.

Two kinds of modeling:

1. "Dust modeling": efforts to understand the nature of dust, drawing on a variety of observational evidence and lab study of the optical properties of candidate grain materials. We want to know the composition, morphology, and size distribution.

2. "Dust physics": efforts to understand how dust interacts with its environment, especially the gas. This draws on results of (1) above, theory, and lab experiments.

The Latest Dust Models

(Weingartner & Draine 2001, ApJ, 548, 295; Li & Draine 2001, ApJ, 554, 778; Zubko, Dwek, & Arendt 2004, ApJS, 152, 211)

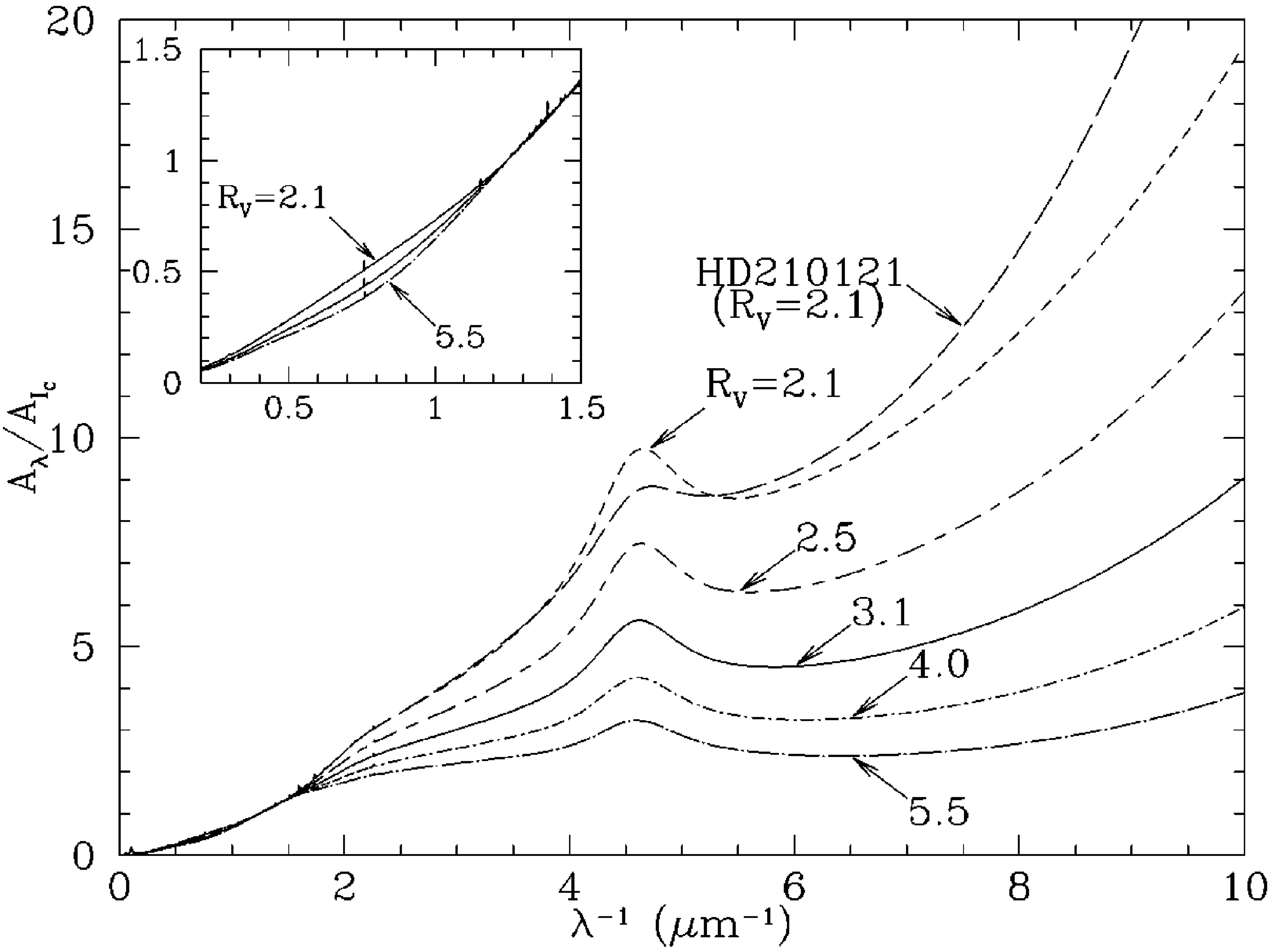
1. Adopt a set of compositions (motivated by spectral features in starlight extinction and thermal dust emission)

a) silicates: robustly indicated by 9.7 μm Si-O stretching mode and
18 μm O-Si-O bending mode

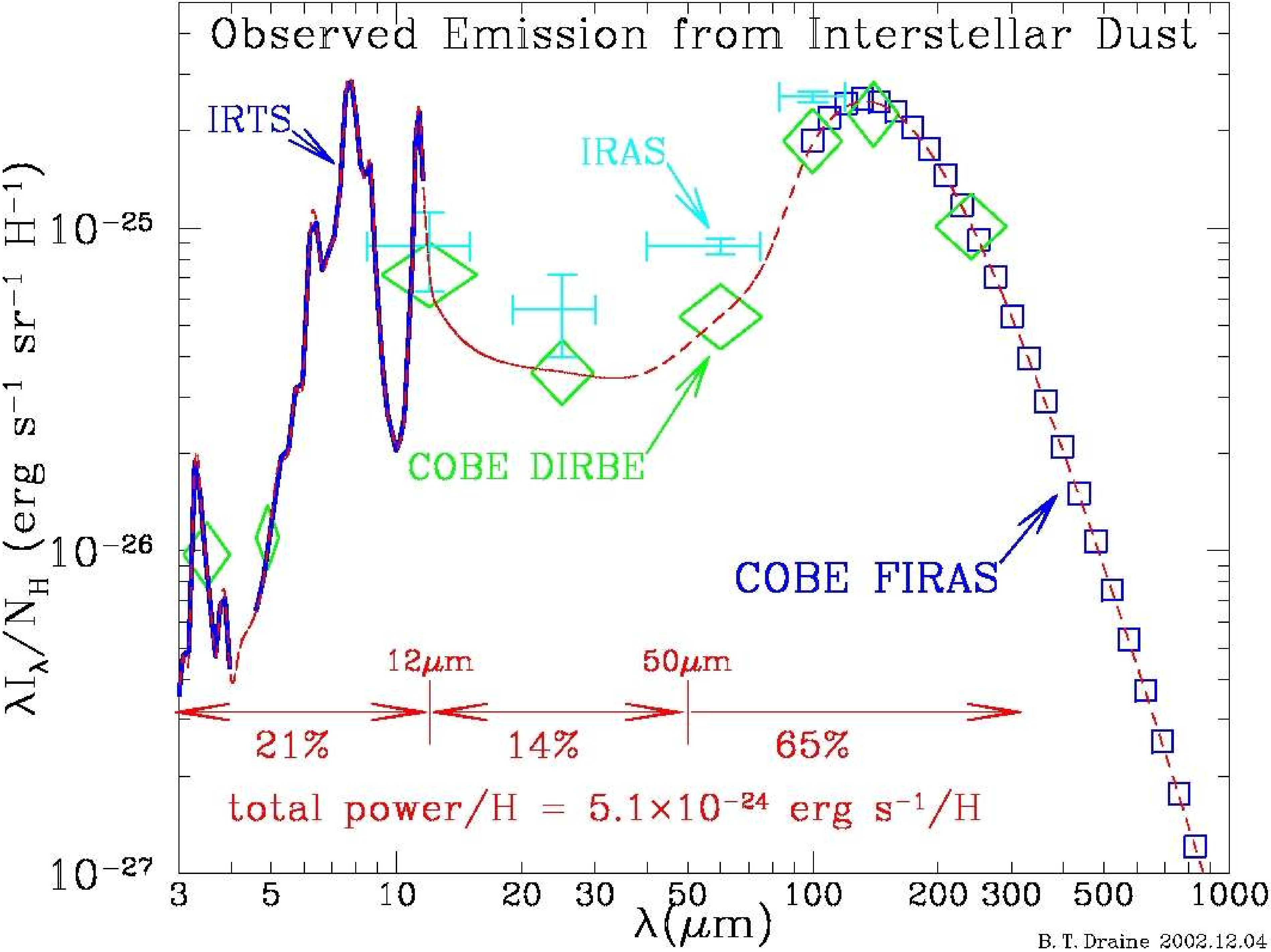
b) polycyclic aromatic hydrocarbons (PAHs): robustly indicated by emission features at 3.3, 6.2, 7.7, 8.6, and 11.3 μm

c) graphite: $\pi \rightarrow \pi^*$ transitions in aromatic C can yield the strong 2175 Å extinction feature. Graphite may be unnecessary since PAHs are present.

d) (hydrogenated) amorphous carbon



Draine 2003, ARAA, 41, 241: fig. 1



Draine, 2003: fig. 14

2. Construct grain size distributions for each composition so as to best fit extinction, emission, and abundance/depletion constraints. Adopt spheres or composite particles.

How reliable are "cosmic" abundances?

Element	AG89	GS98	AGS05	B stars	F&G stars
O	851	676	457	350	445
C	363	331	245	190	358
Mg	38.9	38.0	33.9	23.0	42.7
Si	35.5	36.3	32.4	18.8	39.9
Fe	32.4	31.6	28.2	28.5	27.9

AG89 = Anders & Grevesse 1989, Geochim. Cosmochim. Acta, 53, 197
GS98 = Grevesse & Sauval 1998, Space Sci. Rev., 85, 161
AGS05 = Asplund, Grevesse, & Sauval 2005, astro-ph/0410214
B, F&G stars from Sofia & Meyer 2001, ApJ, 554, L221

Numerous dust models satisfy the constraints employed.

3. Check the resulting model against other observational constraints.

a) Scattering of starlight off of grains (reflection nebulae, DGL)
b) X-ray halos

These additional constraints can be used to narrow the field of candidate models somewhat.

Other observations

a) Polarization of starlight

b) Photoluminescence (eg., ERE)

c) Grains in the solar system

i) Presolar grains in meteorites and IDPs; not generally representative of interstellar grains

ii) Ulysses and Galileo impact detectors: greater-than-expected abundance of large grains, to 1 μm (Frisch et al. 1999, ApJ, 525, 492).

iii) Stardust: return to Earth in Jan, 2006. Hopefully comet grains will be intact. Info on composition and size of interstellar grains.

iv) Radar meteors: Extrasolar meteors have been detected with Arecibo and AMOR. Probes very large grains (several μm and larger).

d) X-ray absorption edges: Detailed edge structure depends on the material in which the atom resides; could reveal grain composition in detail (e.g., which type of silicate). Lab data for candidate grain materials is needed! (Lee & Ravel 2005, ApJ, 622, 970: recent work at the National Synchrotron Light Source and Advanced Photon Source) X-ray absorption yields total abundance of an element, in both gas and dust.

Additional Dust Modeling Issues

1. We need lab measurements of dielectric functions for candidate grain materials across the entire spectrum, and for interstellar temperatures.

2. Constraining the mix of PAH molecules (size, structure, ionization, hydrogenation). Much recent progress in IR spectroscopy (Hudgins & Allamandola 2004, in "Astrophysics of Dust", ASP Conf. Ser. 309, 665). We also need UV spectroscopy! Can PAHs account for the 2175 Å feature?

3. Grain evolution in the ISM: coagulation, shattering, and vaporization in grain-grain collisions; accretion

Grain Charging

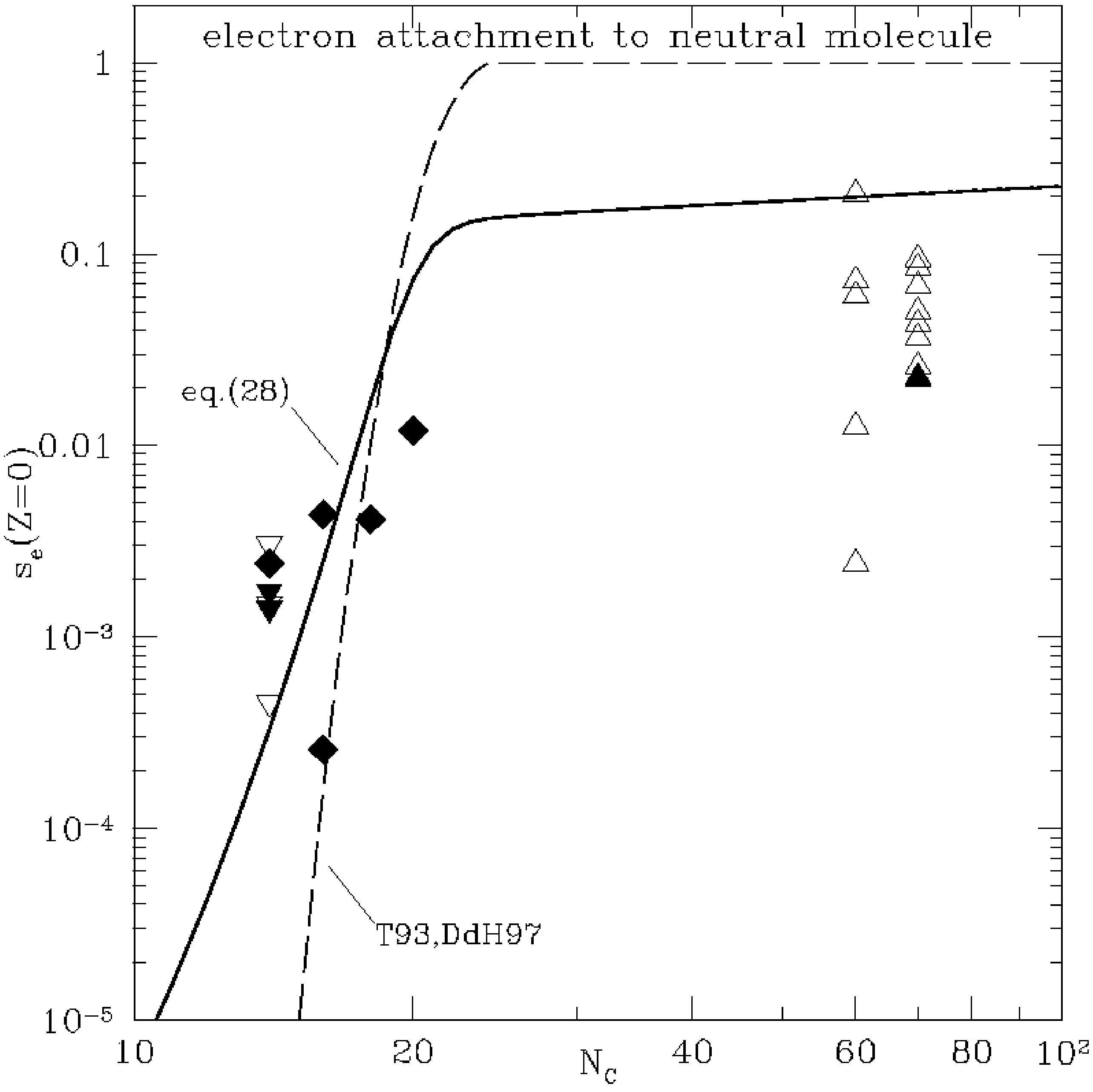
(modeled by Weingartner & Draine 2001, ApJS, 134, 263; van Hoof et al. 2004, MNRAS, 350, 1330; incorporated in CLOUDY)

In H I regions, collisions with gas-phase electrons balances photoemission. Gas heating is dominated by the smallest grains (PAHs).

Collisional charging rate:

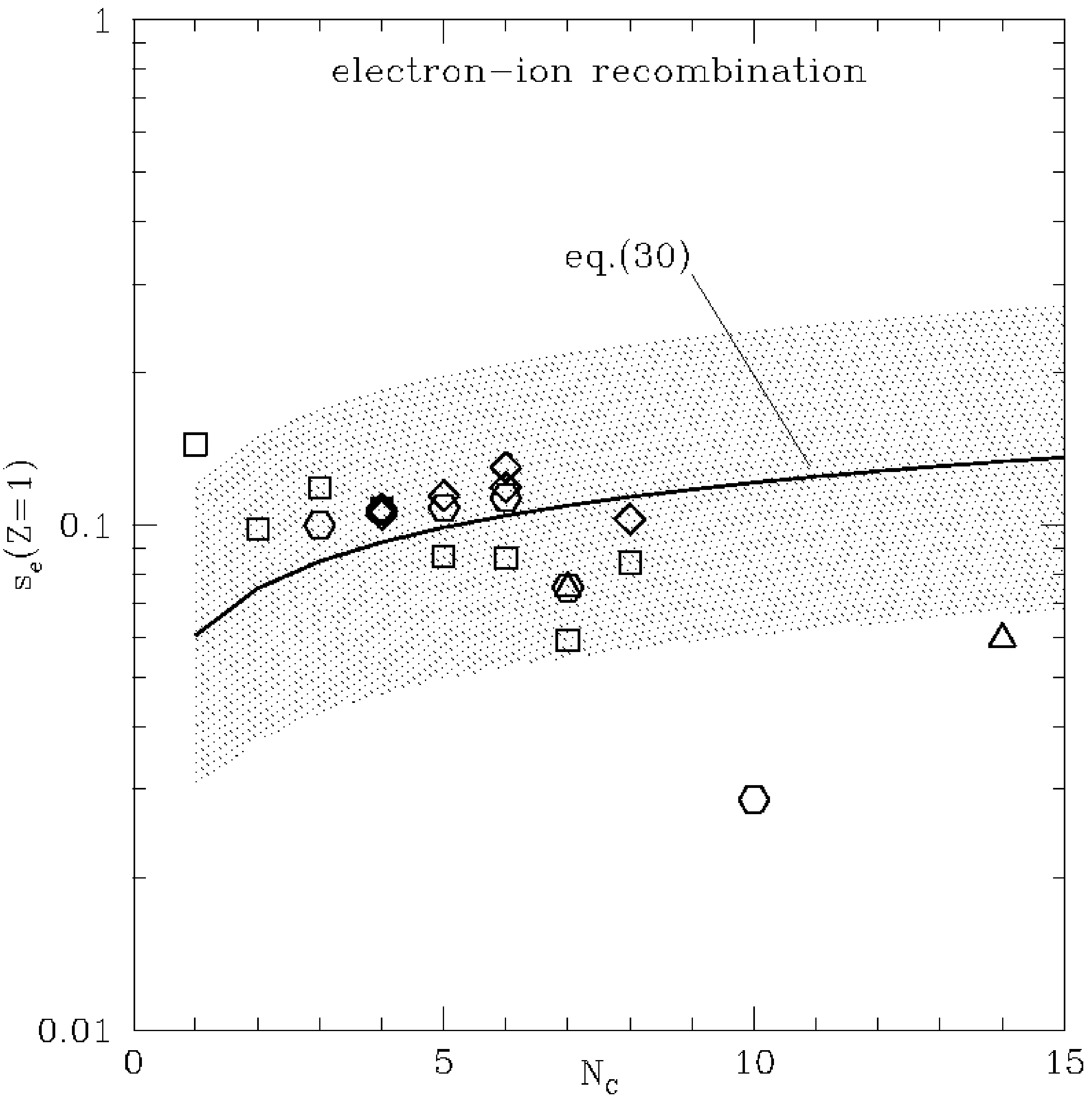
$$J_e(Z) = n_e s_e(Z) \left(\frac{8kT}{\pi m_e}\right)^{1/2} \pi a^2 \tilde{J}(\tau, \xi) \qquad \text{with} \qquad \tau \equiv akT/e^2 \quad \text{and} \quad \xi \equiv -Z$$

$\tilde{J}$ accounts for Coulomb focusing in the case of a conducting sphere (Draine & Sutin 1987, ApJ, 320, 803) and s_e is the probability that the electron sticks to the grain.



We adopt physically-motivated expressions for s_e, with parameters chosen to best reproduce the limited experimental data available for carbonaceous molecules. More data are needed! (Also for larger grains and other materials.)

Weingartner & Draine 2001: fig. 6



Weingartner & Draine 2001: fig. 7

Photoelectrons are ejected at a rate

$$J_{\rm pe} = \pi a^2 \int_{\nu_{\rm pet}}^{\nu_{\rm max}} d\nu Y Q_{\rm abs} \frac{c u_\nu}{h\nu} + \int_{\nu_{\rm pdt}}^{\nu_{\rm max}} d\nu \sigma_{\rm pdt} \frac{c u_\nu}{h\nu}$$

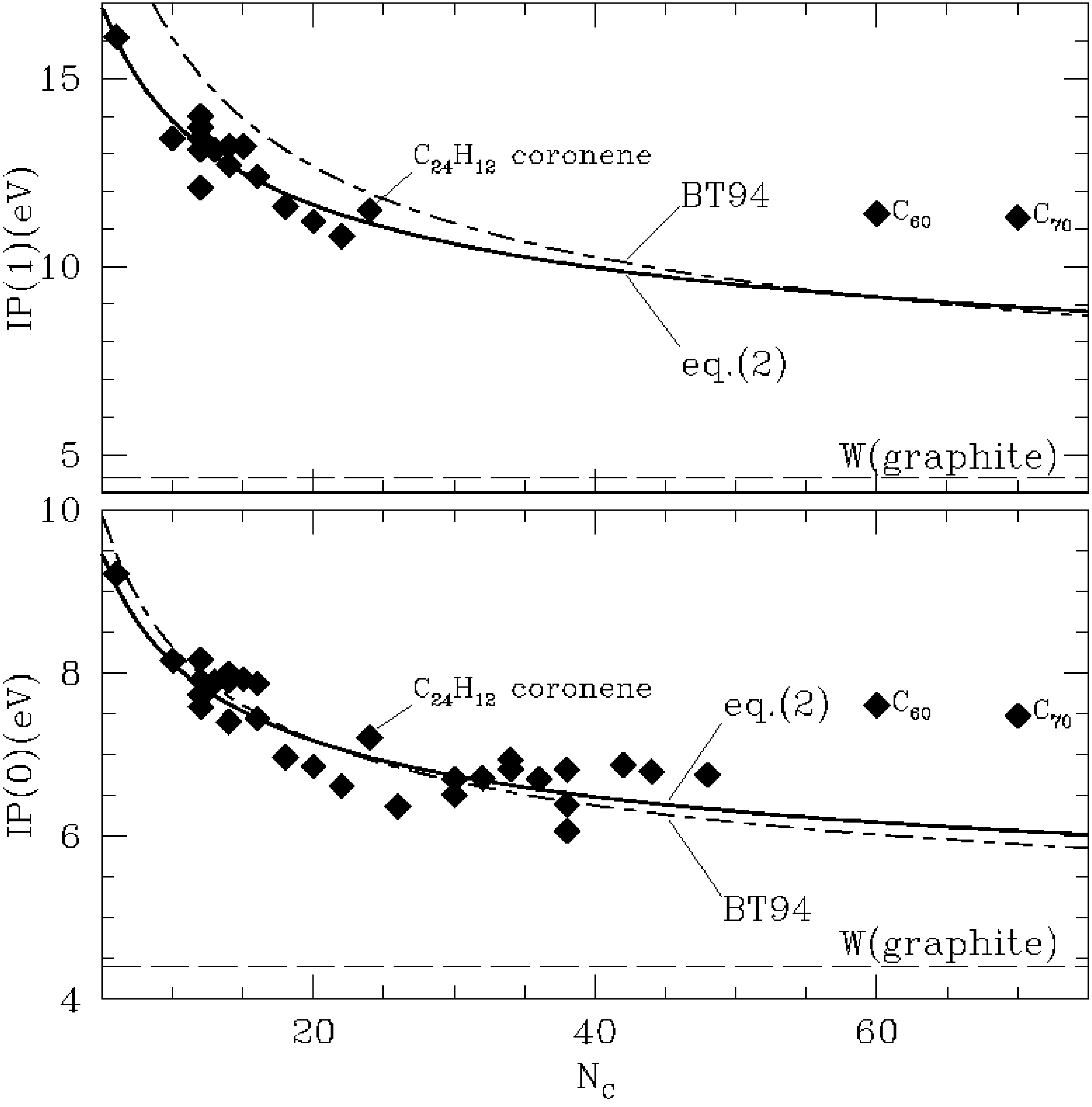
$h\nu_{\rm pet}$ = the threshold photon energy for photoemission

$h\nu_{\rm max}$ = the maximum energy in the radiation field

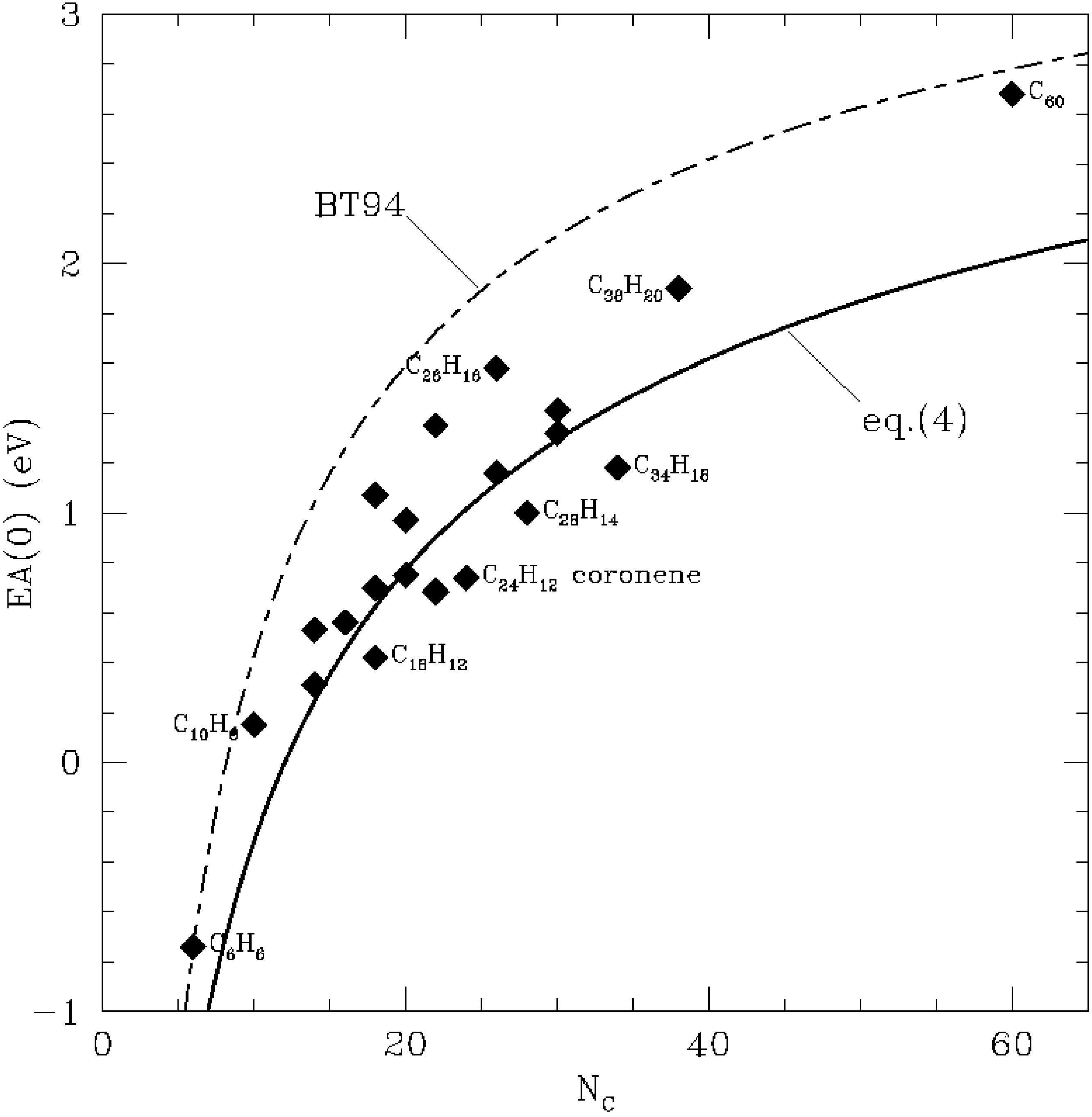
Y = the photoelectric yield (i.e., the probability that an electron is ejected following the absorption of a photon)

The second term is only present for negatively charged grains and accounts for the photodetachment of the excess electrons, which may lie above the valence band.

For a bulk solid, $h\nu_{\rm pet}$ = the work function. For smaller grains, we must also include the Coulomb and image (i.e., polarization) potentials and, for very small grains, quantum effects.



Weingartner & Draine 2001: fig. 2



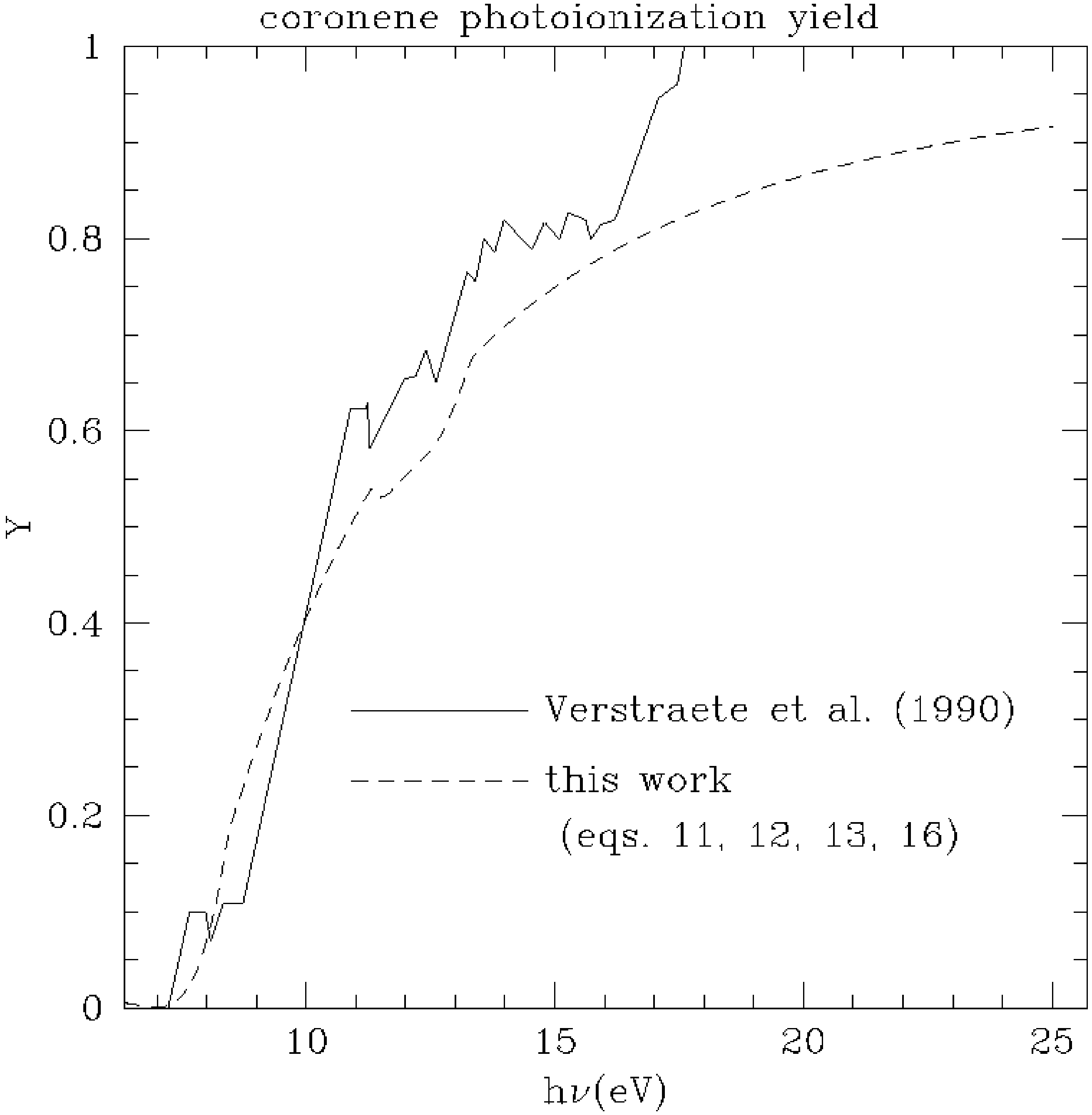
Weingartner & Draine 2001: fig. 3

The yield Y for small grains differs from that for bulk material:

1. For positively charged grains, not all electrons have sufficient energy to escape the potential well. We assume a parabolic energy dist. for the photoelectrons. Better characterization is needed, esp. for PAHs.

2. Small-grain yield enhancement because typical distance from point of electron excitation to surface is smaller (and photon attenuation length exceeds electron escape length). We adopt the simple model of Watson (1973, J. Opt. Soc. Am., 63, 164). A series of experiments in the 1980s on silver spheres with $27\ \text{Å} < a < 54\ \text{Å}$ found much larger yield enhancements. Experiments on sub-micron grains are desperately needed!

For carbonaceous grains, we base the frequency-dependent yield on the measured photoionization yield of coronene ($C_{24}H_{12}$; Verstraete et al. 1990, A&A, 237, 436). As a result, the bulk yield substantially exceeds the measured yield of graphite (Feuerbacher & Fitton 1972, J. Appl. Phys., 43, 1563).

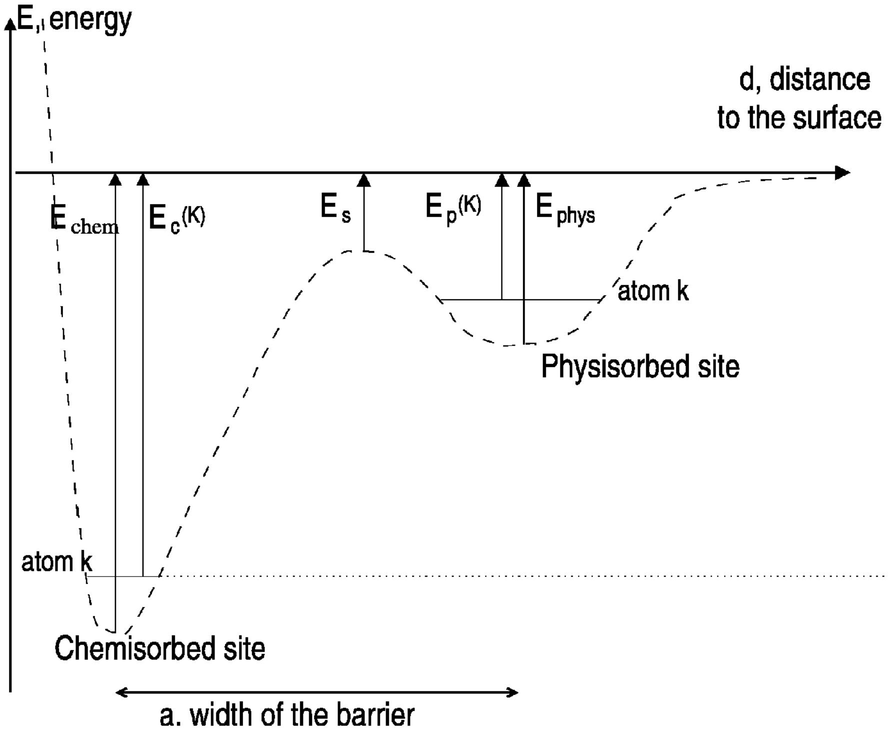


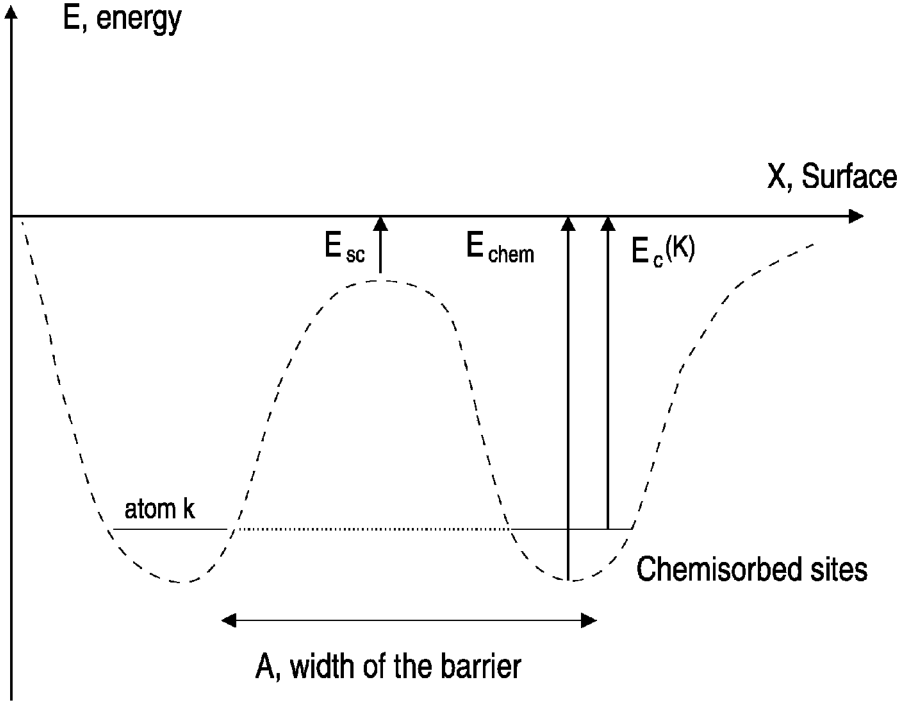
Weingartner & Draine 2001: fig. 4

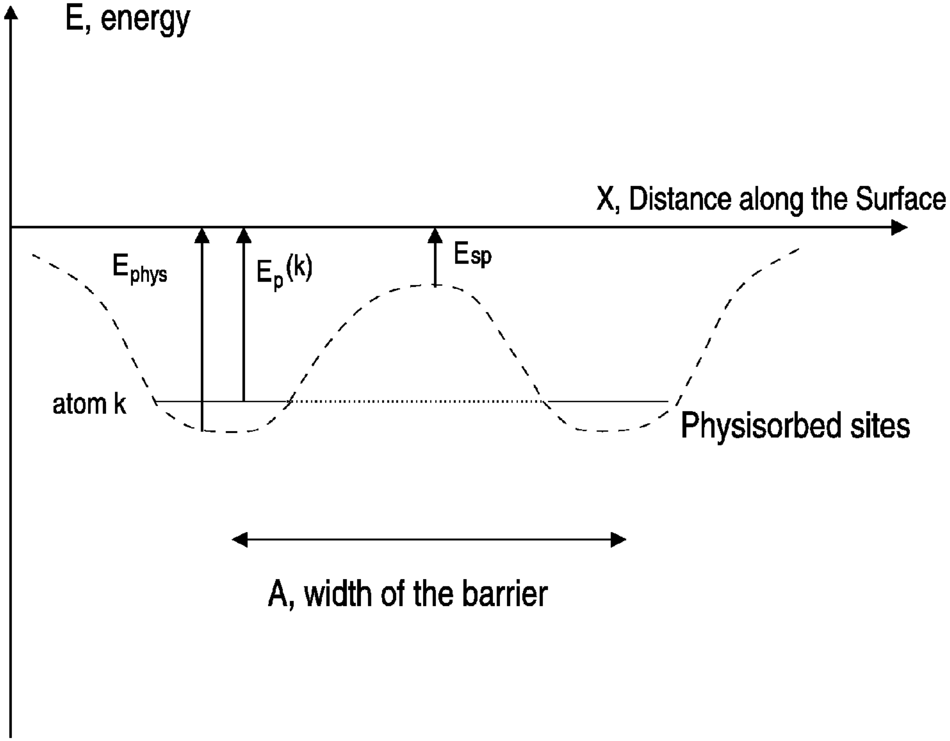
For silicate yield, we adopt the result of Feuerbacher et al. (1972, Geochim. Cosmochim. Acta Suppl. 2, 3, 2655) for a powdered sample of lunar dust.

H_2 formation on grains

There has been much recent experimental progress (Pirronello et al. 2004, in "Astrophysics of Dust", ASP Conf. Ser. 309, 529). But the lab conditions are still far from interstellar; extrapolation to the interstellar case is not straightforward. We need better lab characterization of surface binding sites.







Cazaux & Tielens (2004, ApJ, 604, 222): figs. 1, 2, 3

My wish list from the lab

1. X-ray absorption edges for elements in candidate grain materials

2. Optical properties of candidate grain materials

3. PAHs: optical, UV spectroscopy; sticking coefficients of electrons and ions; ionization potentials; photoionization yields

4. Sub-micron grains in traps: sticking coefficients, ionization potentials, photoelectric yields, surface chemistry

5. Characterization of surface binding sites

6. Photoluminescence from ultra-small grains

7. Grain-grain collisions