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# MODELING GALACTIC EXTINCTION

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Abstract. We present a model for interstellar extinction dust, in which we assume a bimodal distribution of extinction carriers, a dispersion of core–mantle grains, supplemented by a collection of PAHs in free molecular form. We use state–of–the–art methods to calculate the extinction due to macroscopic dust particles, and the absorption cross–sections of PAHs in four different charge states. While successfull for most of observed Galactic extinction curves, in few cases the model cannot provide reliable results. Paradoxically, these failures appear to be very promising, suggesting that the whole body of dust extinction features might be described within the cycle of carbon in the interstellar medium.

## 1. Introduction

Since Robert Trumpler published in the thirties his study of the space distribution of the open clusters [1], interstellar dust studies have been steadily increasing. Nevertheless, after almost a century, the nature of interstellar dust remains elusive.

Dust is everywhere in space. Understanding the properties of interstellar dust particles is therefore essential for the interpretation of galactic spectra. An interstellar dust model is characterized by the abundance of the different elements locked up in the dust, and by the composition, morphology, and size of the consituents. Traditionally, interstellar dust has been identified with collections of grains, very small, submicronic, solids loosely populating the interstellar space. The grain dispersion is characterized by the size distribution of the individual particles (e.g., [2]). However, in the early eighties was realized that another kind of dust was present in space [3, 4], some form of molecular–size restricted aromatic carbon, such as single or stacked Polycyclic Aromatic Hydrocarbons (PAHs) [5].

It is now generally accepted that interstellar dust consists of amorphous silicates and carbonaceous materials. The former is inferred from the $9.7\,\mu$m Si$-$O stretching mode and $18\,\mu$m $\mathrm{O-Si-O}$ bending mode absorption features in interstellar regions, as well as the fact that the cosmically abundant heavy elements such as Si, Fe, Mg are highly depleted. Carbon is mainly inferred by the ubiquitous $3.4\,\mu$m C$-$H stretching vibrational band, and the fact that silicates alone are not able to provide enough extinction. The carbonaceous molecular component appears to be the carrier of 2175 Å bump, and to contribute significantly to the far–UV non–linear rise in extinction curves (see [6, 7] for a thorough description of the interstellar extinction curve), through two resonances, the $\pi^\star \leftarrow \pi$ and the $\sigma^\star \leftarrow \sigma$, ubiquitous in the absorption spectra of PAHs [8].

It is unclear at present whether the silicates and carbons form distinct populations of dust grains. The assumption most frequently adopted is that they are distinct and co–existing. On the basis of extensive laboratory evidence, Jones et al. [9] proposed that some of the carbonaceous material may be in the form of mantles on the surfaces of the silicate cores. Carbon atoms and ions are assumed to be deposited on dust grains, partially hydrogenated and retained on the surface. The newly deposited hydrogen–rich carbon is dominated by $sp^3$ bonding. Under the influence of the interstellar radiation field, this aliphatic carbon loses hydrogen and becomes more graphitic and aromatic, and is dominated by $sp^2$ bonding. Following such approach, we model dust grains as stratified spheres composed of hollow silicate cores coated with two carbonaceous layers, the inner layer of $sp^2$ carbon and the outer layer of $sp^3$ carbon. This population of grains is supplemented by a collection of free–flying PAH molecules, whose photo–absorption cross–sections have been made available by extensive quantum chemical calculations performed and validated by Malloci and co–workers (e.g., [10]). Reliable dust models may then be constructed joining quantum chemistry to light scattering tools [11].

We model extinction curves by means of a non–linear fitting procedure incorporating the stratified sphere description for the solid component and a linear combination of PAH spectra, to obtain the synthetic extinction curve to be compared with observations. The fitting problem is a typical ill–posed inversion problem, in which the grain size distribution and the inventory of the molecular component are the unknowns. The model is presented in the next Section, while results are shown in Section 3. Section 4 contains our conclusions.

## 2. The model

In this work we assume a bimodal distribution of extinction carriers, a dispersion of core–mantle grains, supplemented by a collection of PAHs in free molecular form.

A model grain is constructed assembling four concentric components: $(i)$ a cavity, whose volume is in fixed proportion for all core sizes, $(ii)$ the silicate shell, (iii) the $sp^2$ layer, and $(iv)$ the $sp^3$ external layer. The cavity and the silicate shell constitute the grain core, while the contiguous $sp^2$ and $sp^3$ layers constitute the mantle. The cavity has been introduced to simulate porosity. Details about the model can be found in [12, 13]. while Iatì et al. [14] present an accurate description of the method employed to compute the extinction and scattering cross–sections.

To model the absorption due to the molecular component we exploit the database of spectral properties of PAHs computed by Malloci et al. [10], including about 70 molecules in the size range $10 - 66$ C atoms, and in the charge states 0, $\pm 1$, and $+2$[1]. We include only fully hydrogenated unsubstituted PAHs. The presence of dehydrogenated PAHs, as proposed by Duley [15], is dismissed on the base of accurate theoretical studies of the electronic spectra of dehydrogenated PAHs [16]. State–of–the–art techniques in the framework of the density functional theory (DFT) have been exploited to obtain the electronic ground–state geometries, together with time–dependent DFT to evaluate the electronic excited–state properties (see [10] for details).

[1] http://astrochemistry.ca.astro.it/database/

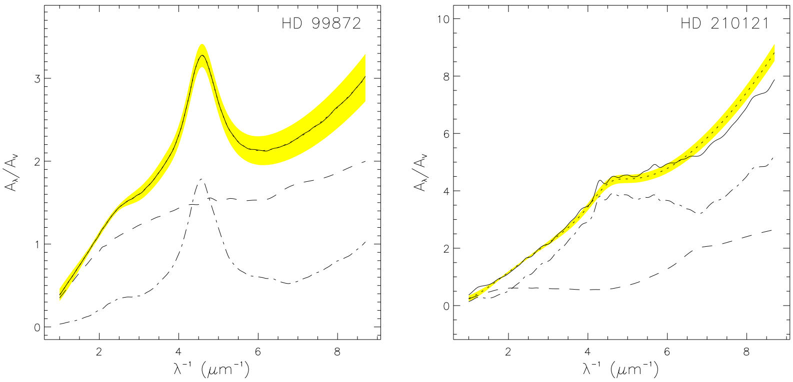


**Figure 1.** Results of the fitting technique applied to the extinction curve towards HD 99872 (left panel) and HD 210121 (right panel). The dark–gray shaded region shows the $1\sigma$ variance about the observed curves. Solid line: total synthetic extinction, dashed line: grain contribution, dot–dashed line: PAH aborption.

The retrieval procedure is based on the Levemberg–Marquardt method (e.g., [17]).

## 3. Results

The present model has been successfully applied to five Galactic extinction curves taken from the sample of Fitzpatrick and Massa [6] by Cecchi–Pestellini et al. [11]. Comparison with the selected observed extinction curves showed quantitatively that it is practically possible to match an extinction curve very accurately using a mixture of even a relatively small sample of real PAHs. A few tens of species provide enough chemical diversity to very effectively wash out spectral features of individual species in the UV, resulting in a very smooth extinction curve.

Such an approach, that is more physical with respect to use an unrealistic single spectrum of a not–well defined average astronomical PAH collection (e.g., [18, 14]), has the effect of introducing a ludicrous number of free parameters, i.e. the column density of each species included in the linear combination. However, even if the mixture of PAHs results severely underdetermined, meaning that there is no uniquely defined composition of PAHs required to produce a given observed interstellar extinction curve, some collective properties of the mixture are well–determined, e.g., the charge per carbon atom, which relates to the relative intensity between the 2175 Å bump and the non–linear far–UV rise (see [11]).

In this work we extend the computation to the whole sample of extinction curves observed by Fitzpatrick and Massa [6], with excellent results (see Fig. 1, left panel). Interestingly, we find that for a small number of peculiar lines of sight the fitting technique fails remarkably (Fig 1, right panel). Such lines of sight exhibit extinction profiles where the 2175 Å bump is weak or even totally missing, while showing a marked UV rise. Such cases are impossible to interpret in terms of the photo–absorption properties of free–flying PAHs, and some other component consisting of (probably carbonaceous) very small (nanometer sized) particles must be responsible for the extinction. Possible candidates might be nanodiamonds [19] or hyperhydrogenated $sp^3$ bonding carriers.

## 4. Conclusions

In this work we present a model of interstellar dust in which, for the first time in literature, PAH molecules are included individually, with their optical properties derived computationally with a state–of–the–art method. Together with the molecular component we include a population of grains, whose scattering properties are derived exploiting a flexible and fast technique, that provides results with an arbitrary degree of accuracy [20].

While such a brute force approach to the contribution of PAHs to interstellar extinction is probably not the best way for a comprehensive modelling of dust absorption and emission, it shows that the currently available global models (e.g., [18]) lose some important information with their necessary simplification of PAH absorption, for example disregarding the impact of charge on far–UV extinction. We are currently implementing in the procedure physical constraints, such as e.g., the link among ionization stages, in order to reduce the degree of arbitrariety, and the number of free parameters.

Failures in the fitting technique suggest that carbon might be recycled from $sp^2$ to $sp^3$ in the dynamical interstellar medium.

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