



Is cosmic dust porous?

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Abstract

There is a long-standing discussion in the astrophysical/astrochemical community as to the structure and morphology of dust grains in various astrophysical environments (e.g., interstellar clouds, protostellar envelopes, protoplanetary and debris disks, and the atmospheres of exoplanets). Typical grain models assume a compact dust core which becomes covered in a thick ice mantle in cold dense environments. In contrast, less compact cores are likely to exhibit porosity, leading to a pronounced increase in surface area with concomitant much thinner ice films and higher accessibility to the bare grain surface. Several laboratory experimental and theoretical studies have shown that this type of dust structure can have a marked effect on several physico-chemical processes, including adsorption, desorption, mobility, and reactivity of chemical species. Porous grains are thus thought to likely play a particularly important and wide-ranging astrochemical role. Herein, we clarify what is meant by porosity in relation to grains and grain agglomerates, assess the likely astrochemical effects of porosity and ask whether a fractal/porous structural/morphological description of dust grains is appropriate from an astronomical perspective. We provide evidence for high porosity from laboratory experiments and computational simulations of grains and their growth in various astrophysical environments, and assess the observational constraints and perspectives on cosmic dust porosity. Overall, our paper discusses the effects of including porosity in dust models and the need to use such models for future astrophysical, astrochemical and astrobiological studies involving surface or solid-state processes.

Keywords Astrochemistry · Molecular processes · Solid state: refractory · (ISM:) dust · Extinction · (ISM:) evolution

Abbreviations

ADP	Agglomerated debris particles
AGB	Asymptotic giant branch
AFM	Atomic force microscopy
ALMA	Atacama Large Millimeter/submillimeter Array
BCCA	Ballistic Cluster–Cluster Aggregates
BE	Binding energy
CCA	Cluster–cluster aggregation
CDA	Cassini’s Cosmic Dust Analyzer
DDA	Discrete dipole approximation
DFT	Density functional theory
DHS	Distribution of hollow spheres
DoLP	Degree of linear polarization
EDX	Energy dispersive X-ray
EMA	Effective medium approximation
EPM	Electrostatic potential map
GRF	Gaussian Random Field
HST	Hubble Space Telescope
IDP	Interplanetary dust particles
IP	Interatomic potential
IR	Infrared
ISM	Interstellar medium
IUPAC	International Union of Pure and Applied Chemistry
JWST	James Webb Space Telescope
MCMC	Markov-Chain Monte Carlo
MD	Molecular dynamics
MLS	Multilayered spheres
MM	Molecular mechanics
MRN	Mathis, Rumpl, Nordsieck
NASA	National Aeronautics and Space Administration
PAHs	Polycyclic aromatic hydrocarbons
PBC	Periodic boundary conditions
PCA	Particle-cluster aggregation
PDR	Photon-dominated region
PSF	Point spread function
pSPF	Polarized intensity scattering phase function
RGD	Rayleigh–Gans–Debye
QM	Quantum mechanical
SPF	Scattering phase functions
SED	Spectral energy distribution
SEM	Scanning electron microscopy
TEM	Transmission electron microscopy
tSPF	Total intensity scattering phase function
UV	Ultraviolet
VLT	Very Large Telescope

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1 Introduction

1.1 General remarks

The properties of dust grains in various astrophysical environments, such as the envelopes of evolved stars, diffuse and dense interstellar clouds, protostellar envelopes, protoplanetary disks, debris disks, and the atmospheres of (exo)planets are the focus of much research for several obvious reasons. Dust grains: (i) are the building blocks of rocky planets, cores of gas giants, and minor bodies (comets, asteroids) in planetary systems; (ii) participate in the formation of planetary atmospheres; (iii) provide

surfaces for key chemical reactions defining astrochemical networks; (iv) can play a catalytic role in those reactions; and (v) influence the thermodynamic properties of astrophysical media.

A number of review papers discuss the role of dust grains in the aforementioned processes and we refer the reader to those papers for details (Henning and Salama 1998; Draine 2003; Blum and Wurm 2008; Henning 2010; Krivov 2010; Jones 2016; Johansen and Lambrechts 2017; Helling 2019; Öberg and Bergin 2021; Potapov and McCoustra 2021; Blum et al. 2022). However, despite of all these reviews (based on much research), there is a parameter of dust grains, which may play a crucial role in the processes mentioned above but which has never been discussed jointly from the observational, experimental, and theoretical points of view. This parameter is dust porosity.

There is considerable controversy over the porosity of cosmic dust grains and the astrophysical community is far from reaching a consensus. Clarification of this question, particularly an affirmative answer to the question “whether dust grains in astrophysical environments are porous?” would lead to re-evaluation of many previous results and approaches and would open new doors for future experimental, theoretical, and observational studies. That discussion must rightly rest, in part, in the field of materials science where porosity is not a loosely defined concept but a multiscale property of solid materials.

1.2 Definitions and key points

Porosity in a material is often defined as the ratio of the volume of voids/vacuum over the total volume. According to the International Union of Pure and Applied Chemistry (IUPAC): “The structure is defined by the distribution in space of the atoms or ions in the material part of the catalyst and, in particular, by the distribution at the surface. The texture is defined by the detailed geometry of the void space in the particles of catalyst. Porosity is a concept related to texture and refers to the pore space in a material.” Porous materials are classified into microporous ($d < 2$ nm), mesoporous ($2 \text{ nm} \leq d \leq 50$ nm), and macroporous ($d > 50$ nm), where d is the pore diameter (Burwell 1976). This leads us to consider two sources of porosity: the material itself (which we might call intrinsic porosity) and the morphology of the dust grain agglomerate (which we might call extrinsic porosity).

Thus, in speaking about cosmic dust porosity, we consider that dust grains in various astrophysical environments are not compact but consist of compact structural units and voids between these units and the fraction of the volume of voids over the total volume is high. Porous dust grains are also often described as fractal aggregates, which typically means that structural units of the aggregates are distributed in a 3D space with a dimension $\gamma < 3$, so that in a sphere of a radius r around a fixed unit there are $N \sim r^\gamma$ other units. There is no contradiction between these two definitions; however, porosity means the presence of “closed” voids between units (meaning the presence of an internal surface) and fractal structures can be completely “open” meaning absence of material in the lines of sight between the central unit and the edge of a grain aggregate (thus, only an external surface is present).

There are three important points of the high porosity view of cosmic dust grains. First, high porosity tends to lead to weak bonding between aggregated units and a corresponding fluffiness of the resultant grains, which should lead to more efficient growth/destruction of grain aggregates as compared to compact (strongly bound) grains. Secondly, high porosity implies the existence of a much larger surface area as compared to compact grains. A large surface area provides more sites for physico-chemical processes. Indeed, we should note that the catalytic formation of molecules on dust surfaces may be one of the most important astrochemical gas-grain interaction processes. For a definition of catalysis, we again refer to IUPAC: “Catalysis is the phenomenon in which a relatively small amount of a foreign material, called a catalyst, augments the rate of a chemical reaction without itself being consumed” (Burwell 1976). Thirdly, “closed” voids between grain units may provide efficient confinement, storage and shielding of reactants and reaction products that adsorb and form on the internal dust surface within pores.

1.3 Evolution of dust grains with respect to porosity

Various types of solids are considered as components of cosmic dust, with carbon- and silicate-based materials as major components and metallic oxides, carbides, sulfides, and metals themselves as minor components. In cold environments, refractory grains are mixed with molecular ices. The composition and origins of dust were recently discussed in a review paper and the reader can find details and relevant references therein (Potapov and McCoustra 2021).

In brief, primary, nm-sized dust grains form in circumstellar envelopes of evolved stars and expanding shells of supernovae, where they can reach sizes of up to tens of nm (Ventura et al. 2012; Gobrecht et al. 2016). Here, the first stage of fractal aggregation may take place leading to the formation of micropores. After formation, grains are pushed away from their parent stars, enter the ISM, travel through interstellar clouds, protostellar envelopes, and planet-forming disks, and finally act as building blocks of minor bodies, planets, and their atmospheres. Alternatively, star dust grains can be completely destroyed in the ISM and restart their evolution history there (Draine 2003). The journey from the ISM to planetary systems is accompanied by the growth of grains from nm-sized particles to mm-sized aggregates (Ossenkopf 1993; D’Alessio et al. 2001; Draine 2003) and there is much evidence for the fractal growth and appearance of meso- and macropores as discussed in the following sections.

Moreover, space weathering (by radiation fields, cosmic rays, shock waves) during the passage from source to sink has an impact on dust porosity, e.g., it might lead to pore deformation and collapse. Conversely, the efficiency of space-weathering processes is dependent on the physical properties of grains, such as grain size, surface roughness, and porosity (Bennett et al. 2013).

1.4 Dust grain models

There are several models describing the structure of dust grains in astrophysical environments. The still most popular model considers grains as a compact core of refractory

materials, which in cold dense environments (dense interstellar clouds, protostellar envelopes and protoplanetary disks beyond the snowline) is covered by a thick ice layer, which in the onion model is assumed to comprise an inner polar layer and an outer apolar layer (Ehrenfreund et al. 1998; Allamandola et al. 1999). In this model, a refractory dust core and ice are physically separated due to the thick ice coverage and dust has no or very limited influence on the physico-chemical processes on and within ice mantles. The compact refractory core itself might also have an onion-like structure with silicate materials in the center and a carbon-based accreted mantle (Li and Greenberg 1997; Jones et al. 2013a). Cold dense astrophysical environments attract a lot of attention due to the rich chemistry, known from detections of many organic molecules, including direct precursors of prebiotic species.

An alternative model considers a porous fractal dust core and a corresponding low ice coverage due to the dust/ice mixing and large dust surface area (Potapov et al. 2020). This concept is based on the results of various laboratory experiments and grain growth models demonstrating that dust grains in the interstellar medium (ISM) and planet-forming disks should be highly porous. These experiments and models are discussed in the following sections. In this alternative model, the dust surface should be available for physico-chemical processes in cold dense environments and may play an important (or in some cases crucial) role therein. The availability of the bare dust surface in cold environments was also shown in the experiments on H₂O agglomeration at low temperatures resulting in the presence of wet (water covered) and dry (bare dust) areas on the surface of dust (Rosu-Finsen et al. 2016; Marchione et al. 2019).

In less dense (diffuse interstellar clouds) and warmer (protostellar envelopes and protoplanetary disks inside the snowline and atmospheres of exoplanets) environments, the structure of dust is perhaps a little simpler. There is unlikely to be a layer of adsorbed volatiles and hence in such environments the bare refractory grain surface is exposed. This surface may be inorganic in nature and comprised of silicate minerals or may, over time, have accreted a layer of carbonaceous materials. In both instances, the materials will have been exposed to stellar and interstellar radiation fields for significant lengths of time.

2 Optical properties of porous dust particles

The problem of determining dust porosity in various astronomical environments relies on our understanding of the optical properties of porous dust particles, which describe how they absorb, scatter, and emit electromagnetic radiation. The purpose of this section is to provide an overview of their optical properties that are relevant for later discussion. In the following, we highlight four key behaviors in the optical properties of porous dust particles. The quantitative behavior of dust depends sensitively on the detailed morphology, size, and composition of the particles, and a complete discussion of the optical property is beyond the scope of this review. We limit our discussion to only qualitative behavior and aim to develop some basic intuition of the physical processes.

2.1 Qualitative behavior

2.1.1 Emission and absorption: cross section

Dust particles absorb incoming electromagnetic waves and re-emit via thermal emission. The magnitude of thermal emission and absorption of dust particles is given by their absorption cross section, C_{abs} , which has units of cm^2 . The incoming electric field induces polarization within a particle with polarizability α , which depends on the particle size, shape, and complex refractive index. A simple piecewise expression for C_{abs} for a spherical grain with a radius of a is (Bohren and Huffman 1983):

$$C_{\text{abs}} \simeq \begin{cases} k \text{Im}[\alpha] & (ka \ll 1), \\ \pi a^2 & (ka \gg 1). \end{cases} \quad (1)$$

Here, $k = 2\pi/\lambda$ is a wavenumber, λ is a wavelength measured in vacuum, and $\text{Im}[\dots]$ takes the imaginary part of a complex quantity α . For small grains such that $ka \ll 1$, C_{abs} is wavelength-dependent via k and α (Rayleigh limit), whereas for large grains it is wavelength-independent as C_{abs} is given by its geometrical cross section (geometrical optics limit).

First, we discuss the absorption property of porous dust particles. As such, we consider a fractal aggregate consisting of N spherical monomer grains, like Ballistic Cluster–Cluster Aggregates (BCCA; $\gamma \sim 2$) shown in Fig. 5. We assume that each monomer grain is optically soft ($|m - 1| \ll 1$) and has a small phase shift ($ka_0|m - 1| \ll 1$), where m is a complex refractive index and a_0 is the monomer radius. For $\gamma \lesssim 2$, geometrical overlapping of monomers along sight lines is negligible, and all monomers in the aggregate would be uniformly illuminated/excited by the external field so that absorption by each monomer may be treated as if it would be isolated. In other words, the aggregate is “transparent” under such conditions. Hence, the absorption cross section of each monomer would be approximated by $k\text{Im}[\alpha_0]$, where α_0 is the polarizability of each monomer grain without the presence of neighboring monomers. As a result, the total amount of absorption by the aggregate would be the sum of that by all monomers:

$$C_{\text{abs}}(\lambda) \simeq NC_{\text{abs},0}(\lambda) = Nk \text{Im}[\alpha_0] \quad (2)$$

where $C_{\text{abs},0}$ is the absorption cross section of a single monomer. The wavelength dependence of absorption/emission, or spectroscopic properties, of the aggregate is determined by that of each monomer grain. In other words, in a spectroscopic quantity, large porous aggregates may appear as small particles (e.g., Min et al. 2006a). As long as the transparent conditions are met, this equation may apply to whatever the aggregate size is.

The above approximation is called the Rayleigh–Gans–Debye (RGD) approximation (or equivalently 1st-order Born approximation), which only holds in the limit of a higher porosity and a lower refractive index (see Berry and Percival 1986; Sorensen 2001; Tazaki et al. 2016; Tazaki and Tanaka 2018, for more detailed conditions). If

those conditions are not met, each monomer would feel an electric field different from the external one due to shadowing by other monomers in the aggregate and/or electromagnetic interaction between neighboring monomers (Wright 1987; Bazell and Dwek 1990; Kozasa et al. 1992; Henning et al. 1995; Stognienko et al. 1995; Mackowski 1995, 2006; Köhler et al. 2011; Tazaki and Tanaka 2018; Lodge et al. 2024a). Despite its limited applicability, such a view is still useful to gain intuition on why large porous aggregates often exhibit spectroscopic properties similar to small particles.

This idea could also be applied to qualitatively assess the influence of dust porosity on solid state features. The information of the absorption features (i.e., enhanced absorption at a resonant wavelength of a solid material) is imprinted in the refractive index (and then polarizability). In the Rayleigh limit ($ka \ll 1$), the feature is clearly observable because C_{abs} directly reflects α , but would be weakened for large grains ($ka \gg 1$) because C_{abs} is independent of the wavelength (Eq. (1)). For large porous aggregates, we may still observe an absorption feature because their absorption property is governed by monomers' (or small particles') property (Eq. (2)). Qualitatively similar behavior has been reported by a number of numerical studies (Min et al. 2006a; Voshchinnikov and Henning 2008; Kolokolova et al. 2007; Vaidya and Gupta 2011; Kataoka et al. 2014; Gupta et al. 2016).

2.1.2 Emission and absorption: polarization

In the ISM, dust particles are often aligned with the interstellar magnetic field (Andersson et al. 2015). Aligned particles produce polarized light via dichroic extinction or dichroic emission. This occurs because they preferentially absorb or emit light polarized along specific directions, effectively acting as polarization filters or emitters.

A simple piecewise expression for the degree of linear polarization (DoLP) produced by an aligned spheroid is

$$\text{DoLP} = \frac{C_{\text{abs},\perp} - C_{\text{abs},\parallel}}{C_{\text{abs},\perp} + C_{\text{abs},\parallel}}, \quad (3)$$

$$\frac{C_{\text{abs},\perp}}{C_{\text{abs},\parallel}} \simeq \begin{cases} \frac{\text{Im}[\alpha_{\perp}]}{\text{Im}[\alpha_{\parallel}]} & (ka \ll 1), \\ 1 & (ka \gg 1), \end{cases} \quad (4)$$

where we have used $C_{\text{abs},j} = k \text{Im}[\alpha_j]$ for $ka \ll 1$ and $j = \perp, \parallel$ refers to the incident electric field polarized perpendicular or parallel to the grain's short axis, respectively. In this case, a is the radius for the longest axis of the spheroid. For spherical grains ($C_{\text{abs},\perp} = C_{\text{abs},\parallel}$), $\text{DoLP} = 0$. For spheroidal grains with $C_{\text{abs},\perp} \neq C_{\text{abs},\parallel}$, we observe a polarized light. Equation (4) captures an overall behavior of numerical results for DoLP reported in Cho and Lazarian (2007), although there may be a systematic error particularly for $ka \gg 1$ (Guillet et al. 2020). Figure 1 shows a DoLP in the $ka \ll 1$ regime for various sets of an aspect ratio and the real part of the refractive index. The real part of the refractive index plays a crucial role in determining DoLP; it essentially controls the extent to which the geometrical asymmetry of spheroid (long/short axis ratio) is converted into the polarization signal.

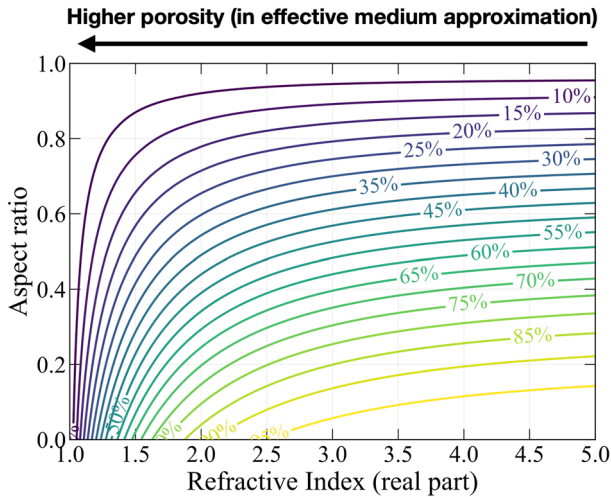


Fig. 1 Degree of linear polarization calculated using Eq. (4, $ka \ll 1$) for oblate spheroids with various axis ratios and the real part (n) of refractive index. The imaginary part (k) is assumed to be small such that $k \ll n - 1$



Fig. 2 A cartoon showing the concept of the spheroidal analog approximation of a porous aggregate

How does the porosity influence the DoLP by aligned particles? As with the previous case, let's consider porous dust aggregates. Porous aggregates may be approximated by a spheroid with an effective medium refractive index (Fig. 2). In fact, Draine (2025) recently demonstrated that the optical properties of irregular porous aggregates can be well approximated by spheroids using the EMT with the Bruggeman mixing rule. When the volume filling factor f (with porosity = $1 - f$) is small ($f \ll 1$), the Bruggeman mixing rule coincides with the Maxwell–Garnett (MG) mixing rule. Under the MG approximation, Kataoka et al. (2014) showed that $n_{\text{eff}} - 1 \propto f$, where n_{eff} is the real part of the effective refractive index of porous aggregates. If $f \rightarrow 0$, $n_{\text{eff}} \rightarrow 1$. This means that a higher porosity (lower f) leads to a lower effective real refractive index, which in turn leads to a lower degree of linear polarization (Fig. 1). Thus, porous grains are less efficient polarizers. The above trend has been confirmed by several numerical studies (Kirchschlager et al. 2019; Draine and Hensley 2021; Draine 2024b).

Figure 1 also highlights a parameter degeneracy between assumptions about intrinsic dust composition (i.e., the refractive index n before introducing porosity) and the

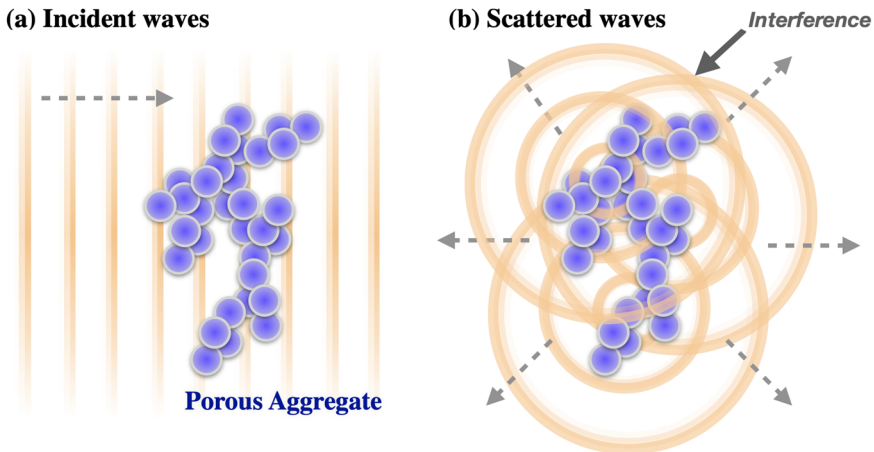


Fig. 3 Plane wave incidents on porous aggregates of spherical monomer grains **(a)** and scattered waves from them **(b)**

grain aspect ratio. Also, the observed polarization fraction depends on an efficiency of grain alignment, which should also be dependent on dust porosity (Herranen et al. 2021).

2.1.3 Scattering: cross section and phase functions

Light scattering has received considerable attention in the context of dust porosity because it directly encodes morphological information about porous dust aggregates, such as their size and internal structure (e.g., porosity).

We begin with the simplest case, that is the scattering cross section of a spherical particle, which may be expressed by:

$$C_{\text{sca}} \simeq \begin{cases} \frac{k^4}{6\pi} |\alpha|^2 & (ka \ll 1), \\ \pi a^2 & (ka \gg 1), \end{cases} \quad (5)$$

where the first case corresponds to the Rayleigh scattering limit and the second to the geometrical optics limit (Bohren and Huffman 1983).

As in Sect. 2.1.1, we follow the RGD approximation to qualitatively explore how porosity affects light scattering. In the RGD framework, the scattering cross section is given by (Berry and Percival 1986; Sorensen 2001):

$$C_{\text{sca}}(\lambda) = N^2 C_{\text{sca},0}(\lambda) \cdot F_s(\lambda), \quad (6)$$

where $C_{\text{sca},0}$ is the scattering cross section of an individual monomer, and F_s is a function factor that encapsulates the spatial configuration of the monomers (i.e., porosity). Physically, interference of scattered waves play important role in determining scattering properties (see Fig. 3), and F_s describes the degree of coherence among scattered

waves. When all scattered waves interfere constructively, we have $F_s = 1$. When part of scattered waves undergoes destructive interference, we have $F_s < 1$. For a fractal aggregate, we have a simple scaling law (Berry and Percival 1986; Sorensen 2001; Tazaki and Tanaka 2018)

$$F_s \sim \begin{cases} 1 & (ka_{\text{agg}} \ll 1), \\ (ka_{\text{agg}})^{-\gamma} & (ka_0 \ll 1 \ll ka_{\text{agg}}), \\ 1/N & (ka_0 \gg 1), \end{cases} \quad (7)$$

where a_0 and a_{agg} are the radii of the monomer and aggregate, respectively, and γ is the fractal dimension. The progression from the first to the third regime may be considered as wavelength dependence: the first case ($ka_{\text{agg}} \ll 1$) corresponds to the long-wavelength limit, while the third case ($ka_0 \gg 1$) corresponds to the short-wavelength limit. Therefore, by measuring wavelength dependence of scattered light, such as colors, one may constrain a_{agg} , γ , and a_0 .

The wavelength dependence of scattered light (color) is one of important diagnostics of dust properties, and it is often explained by the single scattering albedo of dust particles, defined by

$$\omega(\lambda) = \frac{C_{\text{sca}}(\lambda)}{C_{\text{sca}}(\lambda) + C_{\text{abs}}(\lambda)}. \quad (8)$$

Using Eqs. (1) and (5), one can anticipate $\omega \propto k^3 \propto \lambda^{-3}$ for small grains (Rayleigh scattering) and $\omega \sim 0.5$ for large grains (geometrical optics). Note that in Rayleigh scattering we have used $C_{\text{sca}} \ll C_{\text{abs}}$ and assumed that the wavelength dependence of polarizability is negligible. Rayleigh scattering gives a bluish color, whereas geometrical optics gives a gray color.

The single scattering albedo may not accurately represent the color of observed scattered light, particularly when a grain scatters light anisotropically. This is because the single scattering albedo, ω , is defined based on C_{sca} , which represents the total energy scattered into *all* directions. In contrast, observations often sample scattered light at specific scattering angles. As a result, when scattering is anisotropic, the wavelength dependence of the observed scattered light does not necessarily match that of ω . To address this, Mulders et al. (2013) introduced the concept of the effective scattering albedo, ω_{eff} , which is defined by integrating scattered light only over the observable range of scattering angles. This quantity is illustrated in Fig. 4. The difference between ω and ω_{eff} increases as scattering becomes more anisotropic. For small grains ($ka \ll 1$), since Rayleigh scattering is nearly isotropic, we have $\omega \approx \omega_{\text{eff}}$. In contrast, for large grains ($ka \gg 1$), anisotropic scattering causes ω_{eff} to be significantly lower than ω . In such cases, contrary to the gray scattered light implied by ω , the color of scattered light may appear reddish, as shown in Fig. 4 (see also Min et al. 2016).

What about scattered light colors of porous aggregates? We can discuss the single scattering albedo of the aggregate using Eqs. (2), (6), and (7) by ignoring the wavelength dependence of polarizability. When the aggregates are small ($ka_{\text{agg}} \ll 1$), scattering obeys Rayleigh scattering, producing blue scattered light. If aggregates are large, but each monomer is still smaller than the wavelength ($ka_0 \ll 1 \ll ka_{\text{agg}}$), the

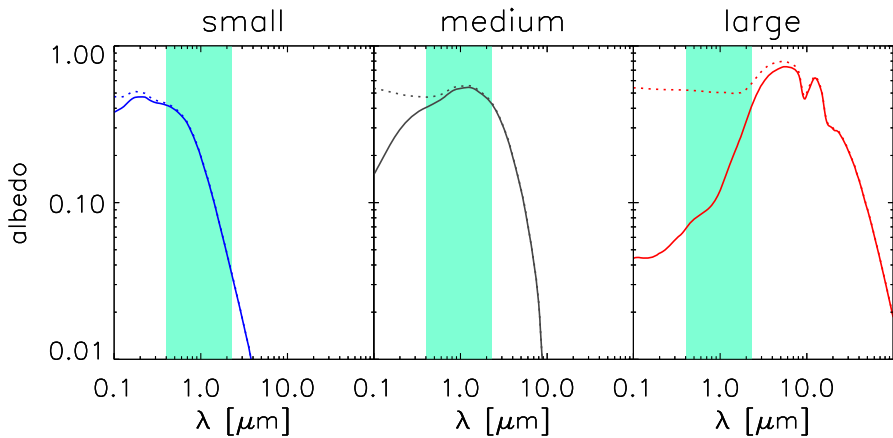


Fig. 4 The effective albedo ω_{eff} (solid lines) and the single scattering albedo ω (dashed lines). In the former, scattered light flux is integrated from 34° to 126° , while it is integrated for all scattering directions (i.e., from 0° to 180°) in the latter. Left, middle, and right panels represent the results for a grain size of $0.08 \mu\text{m}$, $0.25 \mu\text{m}$, and $2.5 \mu\text{m}$, respectively. The green area represents the range of wavelengths covered by the HST scattered light images of the protoplanetary disk around a young star HD 100546. Image reproduced with permission from Mulders et al. (2013), copyright by ESO

albedo is

$$\omega = \frac{C_{\text{sca}}}{C_{\text{sca}} + C_{\text{abs}}} \simeq N F_s(\lambda) \frac{C_{\text{sca},0}}{C_{\text{abs},0}} \propto \lambda^{\gamma-3}, \quad (9)$$

where we have used $C_{\text{sca}} \ll C_{\text{abs}}$ and $C_{\text{sca},0}/C_{\text{abs},0} \propto \lambda^{-3}$ as each monomer obeys Rayleigh scattering. For $\gamma \sim 2$ (i.e., BCCAs), the albedo follows $\propto \lambda^{-1}$. This means that even if aggregates are large compared to the wavelength, low-dimension fractal aggregates may appear bluish in scattered light. Finally, if the wavelength is shorter than the size of the monomers ($ka_0 \gg 1$), we obtain $\omega \sim \omega_0$, meaning that aggregates would exhibit a similar scattered light color to that of each monomer.

Another important diagnostic of dust porosity is the scattering phase function (SPF), which describes the angular dependence of scattering. Within the RGD approximation, the elements of the scattering matrix are expressed as (Sorensen 2001; Tazaki et al. 2016):

$$S_{ij}(\theta) \simeq N^2 S_{ij}^{\text{mono}}(\theta) \cdot \mathcal{S}(q), \quad (10)$$

where $q = 2k \sin(\theta/2)$, θ is the scattering angle, and $\mathcal{S}(q)$ is the structure factor, characterizing the interference pattern of scattered waves due to the internal monomer arrangement. For a fractal aggregate, we have simple relations:

$$\mathcal{S}(q) \sim \begin{cases} 1 & (qa_{\text{agg}} \ll 1), \\ (qa_{\text{agg}})^{-\gamma} & (qa_0 \ll 1 \ll qa_{\text{agg}}), \\ 1/N & (qa_0 \gg 1). \end{cases} \quad (11)$$

Since q depends on both the wavenumber k and the scattering angle θ , the transition from the first to the third regime (for fixed k) may be considered as the angular depen-

dence of scattering. The first case corresponds to forward scattering, while the third case corresponds to large-angle (e.g., backward) scattering. Therefore, by measuring the intensity of scattered light as a function of scattering angle, one may constrain a_{agg} , γ , and a_0 .

Figure 5 shows some examples of total intensity scattering phase function (tSPF; proportional to S_{11}) and/or polarized intensity scattering phase function (pSPF; proportional to $-S_{12}$) computed by the discrete dipole approximation (for irregular grains) and the T matrix method (for aggregates) taken from the AggScatVIR database (Tazaki et al. 2023a). Scattering becomes progressively anisotropic with increasing particle radius regardless of particle morphology; however, the detailed angular dependence of the SPF differs for different particle morphologies.

2.1.4 Scattering: polarization

Finally, we discuss scattering polarization by dust grains. We start again from the simplest case, that is, a single spherical grain. A simple piecewise expression for the DoLP of scattered light by spherical grains is (e.g., Tazaki et al. 2021):

$$\text{DoLP} \simeq \begin{cases} \frac{(1-\cos^2 \theta)}{(1+\cos^2 \theta)} & (ka \ll 1), \\ \text{often low} & (ka \gg 1, ka\text{Im}[m-1] \ll 1), \\ \frac{R_{\perp}-R_{\parallel}}{R_{\perp}+R_{\parallel}} & (ka \gg 1, ka\text{Im}[m-1] \gg 1), \end{cases} \quad (12)$$

where $R_{\perp}$ and $R_{\parallel}$ are the Fresnel reflectances for the electric field vectors perpendicular and parallel to the plane of incidence. The first case corresponds to Rayleigh scattering. Since the cosine factor vanishes at $\theta = 90^\circ$, Rayleigh scattering produces a 100% DoLP at this angle. The second and third cases ($ka \gg 1$) correspond to geometrical optics, and former and latter are transparent and opaque particle cases, respectively. For the transparent case, DoLP is often (but not always¹) lower than that of Rayleigh scattering. For the opaque case, $R_{\parallel}$ vanishes at $\theta = \pi - 2\Theta_B$, where $\Theta_B = \tan^{-1}(n)$ is the so-called Brewster angle and scattering at this angle is referred to as Brewster scattering. Thus, the Brewster angle gives a 100% DoLP. Compared to Rayleigh scattering which is peaking at 90° , Brewster scattering peaks at scattering angles smaller than 90° for $n \geq 1$.

Figure 5 shows the DoLP of numerical dust particles. The DoLP of irregular grains (the lower left panel) shows the increasing grain radius lowers DoLPs. This is due to a transition from Rayleigh scattering ($ka \ll 1$) to the second case ($ka \gg 1, ka\text{Im}[m-1] \ll 1$). Those grains are not opaque enough to enter the third regime ($ka \gg 1, ka\text{Im}[m-1] \gg 1$) and therefore we do not see a high polarization due to Brewster scattering.

What about scattering polarization of porous aggregates? In light of the RGD approximation, we can calculate the DoLP of scattered light by Eq. (10). The DoLP for

¹ One such an example is light scattering by a water droplet in the atmosphere causing rainbow. A DoLP of rainbow is larger than that of Rayleigh scattering. This is because internal reflection of light within a droplet occurs close to Brewster angle.

unpolarized incident light is given by the ratio of the two scattering matrix elements, and we obtain

$$\text{DoLP} \equiv -\frac{S_{12}}{S_{11}} = -\frac{S_{12,\text{mono}}}{S_{11,\text{mono}}} \quad (13)$$

indicating that the polarization properties of large aggregates are governed by the monomer characteristics. If monomers are single-sized and spherical, their polarization characteristics follow Eq. (12). For example, if monomers are small ($ka \ll 1$), porous aggregates will show a polarization similar to $(1 - \cos^2 \theta)/(1 + \cos^2 \theta)$. In contrast, if monomers are large and transparent ($ka \gg 1$, $ka\text{Im}[m - 1] \ll 1$), DoLP from porous aggregates becomes low because monomers are not efficient polarizers anymore. These behavior has been well confirmed by numerical studies (West 1991; Kozasa et al. 1993; Lumme et al. 1997; Petrova et al. 2000, 2004; Kimura 2001; Kimura et al. 2006; Bertini et al. 2007; Shen et al. 2009; Kolokolova and Kimura 2010; Tazaki et al. 2016; Halder et al. 2018; Tazaki and Dominik 2022) and laboratory studies (Zerull et al. 1993; Gustafson and Kolokolova 1999; Volten et al. 2007; Tobon Valencia et al. 2022; Gómez Martín et al. 2024). Figure 5 shows the DoLP of fractal aggregates made of Rayleigh-scattering monomers (rightmost column). The results show that DoLPs remain essentially similar to Rayleigh scattering despite the fact that aggregate sizes are much larger than the wavelength.

2.1.5 Short summary

The qualitative behavior discussed above can be summarized as follows.

1. Emission and absorption by large porous aggregates behave similarly to those of their constituent monomers.
2. Porous aggregates are less efficient polarizers for dichroic extinction and emission.
3. Scattered light from large porous aggregates differs from that of compact spherical grains of the same size, and carries information about the aggregate size and internal structure.
4. Scattering polarization from large porous aggregates resembles that of their constituent monomers.

The above concepts have been applied to constrain dust porosity in various astrophysical environments, as we will discuss in Sect. 3. For example, the detection of a certain level of dichroic polarization can place an upper limit on dust porosity knowing grain composition, since higher porosity tends to reduce the DoLP. This approach has been applied to polarization arising from grain alignment in both the interstellar medium (Sect. 3.2) and protoplanetary disks (Sect. 3.3). Analyses of SPFs have also been used to constrain size and morphology of fractal aggregates in planet-forming disks (Sect. 3.3).

2.2 Toward further quantification: approximations, numerical and experimental approaches

In Sect. 2.1, we summarized only qualitative behavior. The discussion was incomplete in the sense that we limited our discussion mostly to porous dust aggregates for

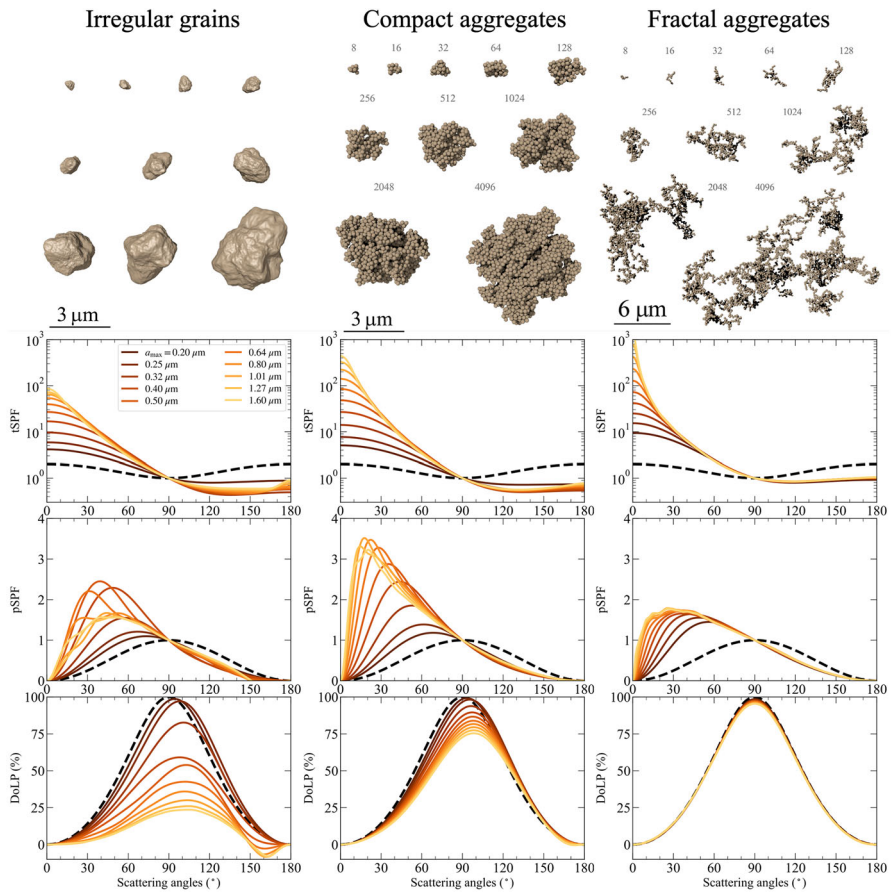


Fig. 5 Numerical models of non-porous irregular grains (left column), low-porosity compact aggregates (a Ballistic Aggregate model called BAM2 originally proposed in Shen et al. 2008) (middle column), high-porosity fractal aggregates with a fractal dimension of 1.9 (or Ballistic Cluster–Cluster Aggregates) (right column). The panels show tSPF (top), pSPF (middle), and DoLP (bottom) at a wavelength of $1.04\ \mu\text{m}$. All models have a refractive index of $1.49 + 0.0108i$. Numbers shown next to each aggregate represent the number of monomers, where each monomer has a radius of $0.1\ \mu\text{m}$. Note that tSPF is shown in logarithmic scale, whereas pSPF is in linear scale. Assuming particle size distribution obeying $a^{-3.5}$ ($0.2\ \mu\text{m} \leq a \leq a_{\text{max}}$) with a being the mass-equivalent sphere radius, the scattering properties averaged over the size distribution are shown. Note that the mass-equivalent sphere radius represents a radius of a sphere that has the same mass of each non-spherical particle, and therefore, an apparent size of each particle could be much larger than this value. Dashed lines represent the Rayleigh scattering solution, which is similar to the scattering properties of each individual monomer of aggregates. These calculation results are taken from the AggScatVIR database (Tazaki and Dominik 2022; Tazaki et al. 2023b)

which the RGD approximation is valid. We summarize some major approaches to find quantitative optical properties of porous dust grains.

Calculating the optical properties of non-spherical grains is not an easy task as numerical approach is usually required, i.e., solving Maxwell's equations given non-spherical particle boundary conditions. There are various numerical techniques that can

accurately calculate the optical properties of non-spherical grains, such as the T -matrix method and the discrete dipole approximation (DDA; see, e.g., for a comprehensive textbook by Mishchenko et al. 2000). A number of numerical simulations have been performed to understand the optical properties of porous dust grains in astronomical context (e.g., Wright 1987; Kozasa et al. 1992, 1993; Stognienko et al. 1995; Kimura 2001; Kimura et al. 2006; Lasue and Levasseur-Regourd 2006; Shen et al. 2008, 2009; Kolokolova and Kimura 2010; Köhler et al. 2011; Kirchschrager and Wolf 2014; Min et al. 2016; Tazaki et al. 2016; Tazaki and Tanaka 2018; Tazaki and Dominik 2022; Tazaki et al. 2023b; Halder et al. 2018; Lodge et al. 2024b; Draine 2024a,b, 2025). For readers interested in light scattering by cometary dust, we refer to Kimura et al. (2016).

Although the above numerical methods provide accurate results, they are still computationally demanding. To ease the computational cost, various approximate methods have been adopted in observational modeling of cosmic dust. The most common way to calculate the optical properties of porous dust grains is to use the Mie theory (van de Hulst 1957; Bohren and Huffman 1983) together with the effective medium approximation, where one defines an effective refractive index of a mixture of different materials (including vacuum) assuming a mixing rule prescription. There are two popular prescriptions for the mixing rule: Maxwell–Garnett and Bruggeman mixing rules (Bohren and Huffman 1983; Chýlek et al. 2000), although other prescriptions are also used (Ossenkopf 1991; Ossenkopf and Henning 1994; Henning and Stognienko 1996; Voshchinnikov and Mathis 1999; Min et al. 2008). The Mie theory with the EMA may reproduce optical properties of some types of porous grains, such as spherical grains with small vacuum inclusions (Wolff et al. 1998; Voshchinnikov et al. 2005, 2007); however, its validity for arbitrary-shaped porous dust particles is by no means trivial. For example, Tazaki et al. (2016) highlighted that the EMA leads to significant errors in scattering properties when applied to fractal dust aggregates with a fractal dimension of $\gamma \sim 2$. There have been proposed alternative methods that offer better accuracy than the Mie theory with EMA, while remaining computationally tractable, such as the Distribution of Hollow Spheres (DHS) (Min et al. 2003, 2005, 2016), the multilayered spheres (MLS) (Voshchinnikov et al. 2005), the mean-field approximation (Berry and Percival 1986; Botet et al. 1997; Rannou et al. 1997; Tazaki and Tanaka 2018; Tazaki 2021; Lodge et al. 2024b; Rannou et al. 2024), the spheroid analog approximation for compact dust aggregates (Draine 2025).

Laboratory experiments are another important approach to study optical properties of non-spherical grains (Greenberg et al. 1961; Zerull et al. 1993; Gustafson and Kolokolova 1999; Kolokolova and Gustafson 2001; Hadamcik et al. 2002, 2006, 2007; Volten et al. 2007; Muñoz et al. 2012, 2020, 2021; Tobon Valencia et al. 2022, 2024; Gómez Martín et al. 2024; Renard et al. 2024). These studies not only provide benchmarks of numerical simulations, but are also useful to study the optical properties of larger particles that are often computationally demanding.

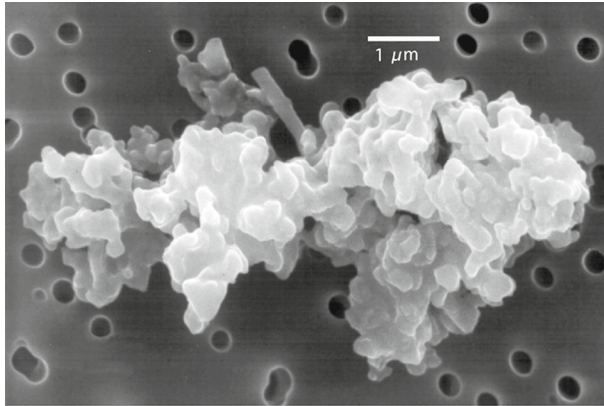


Fig. 6 Scanning electron microscope image of an interplanetary dust particle with nearly chondritic composition. Credit: D. Brownlee and E. Jessberger, adapted from Jessberger et al. (2001). Available with a Creative Commons Attribution 2.5 License

3 Observations

3.1 Dust porosity in the solar system

In the following sub-sections we focus on the properties of dust particles in the ISM and planet-forming disks as inferred via remote observation. However, materials in the Solar System provide an opportunity to explore the properties of solids more directly, and in some instances we can even touch extraterrestrial particles by hand. An example of a highly-porous interplanetary dust particle (IDP) is shown in Fig. 6 and the reader can find many similar examples in the NASA catalog (Warren et al. 1997). The image shows a non-spherical aggregate with several clear areas of vacuum. The size of this particular IDP is of order $10\ \mu\text{m}$; IDP sizes span from $1\ \mu\text{m}$ to $1\ \text{mm}$ (Jessberger et al. 2001). Analysis of dust scattering at mid-infrared wavelengths with Spitzer (Pagani et al. 2010) and high precision JWST spectroscopic observations of ice absorption profiles (Dartois et al. 2024) demonstrate that grains grow to $\sim 1\ \mu\text{m}$ in the dense ($n > 10^4\ \text{cm}^{-3}$) interstellar medium. As such the typical IDPs (with size $> 1\ \mu\text{m}$) clearly are representative of modest aggregate growth in the ISM and more substantive growth within the solar nebular disk.

Another example is the cometary particles from comet 81P/Wild 2 captured by the Stardust mission. The sizes and morphologies of these particles are diverse, varying from tens of nanometers to hundreds of micrometers and from dense grains of about $3\ \text{g cm}^{-3}$ to fluffy aggregates with densities of $0.3\ \text{g cm}^{-3}$ (Hörz et al. 2006). Seven candidate interstellar particles are identified with compact particles having smaller sizes, of a few hundred nm, in contrast to the low-density particles having sizes of $> 1\ \mu\text{m}$ (Westphal et al. 2014). The easiest way to understand these structures is to assume that interstellar dust particles in this size range consist of materials with low density and high porosity (Westphal et al. 2014). We note that Silsbee and Draine (2016) suggest that at least 2 of these particles are likely not interstellar in origin.

Analysis of radar observations of comet Hyakutake (Harmon et al. 1997) are consistent with these results as they indicate a backscatter from porous grains (0.3 g cm^{-3}) with the grain size distribution ranging from $1 \text{ }\mu\text{m}$ to 1 cm in the coma of the comet. Simulations of the Ulysses interstellar dust measurements in the Solar System has led to a similar result, a decrease of the density of dust particles with an increase of their radius (Sterken et al. 2015). Fluffy grain aggregates with the fractal dimensions of 1.5 and 2.9 were considered by the modeling of the light scattering properties of the cometary dust (Lasue and Levasseur-Regourd 2006). The conclusion based on these results is that cometary dust constitutes of fluffy particles that originate from fractal aggregation of sub-micron sized grains (see also Kimura et al. 2016). Analysis of in situ data from Cassini's Cosmic Dust Analyzer (CDA) suggests the detection of interstellar dust particles in the Saturnian system (Altobelli et al. 2016). These particles are mainly compact small particles in the size regime of less than a few hundred nanometers observed by the CDA.

Analysis of the results from the Rosetta mission reveal the detailed properties of the comet 67P/Churyumov–Gerasimenko and its dust particles (see e.g., Blum et al. 2022). Some of dust particles collected by the Rosetta are reminiscent of the CP (Chondritic porous)-IDP (see Güttler et al. 2019, for a summary of particle morphology). It was found that dust particles collected in the coma of 67P can be divided in two families: compact and fractal particles. For the compact family, Fulle et al. (2016) estimated the porosity of the compact dust particles detected by the GIADA instrument on board the Rosetta spacecraft and found it to be $\sim 48\% \pm 8\%$. For the fractal family, particles are found to have (extrinsic) porosity of more than 99% (Fulle et al. 2015; Bentley et al. 2016; Mannel et al. 2016, 2019). Fractal aggregates are likely to be formed in the early phase of dust coagulation (thus, they are directly linked to interstellar dust) (Fulle and Blum 2017, and references therein), as seen in near-IR disk observations (Tazaki et al. 2023b).

3.2 Dust porosity in the diffuse and dense ISM

Dust has been known to be present in the diffuse interstellar medium since the pioneering work of Trumpler (1930). Much of our understanding of dust extinction and properties arose as new windows with the spectrum of light were opened up within the ultraviolet (UV) through the infrared (IR) and into the far-infrared/submillimeter. The most prominent effect of dust is the wavelength-dependent extinction of starlight which is known as the extinction curve. A sample of the extinction curve is shown in Fig. 7. Notable aspects in the optical/UV (top panel) are the significantly stronger effects of extinction towards shorter UV wavelengths and the prominent “bump” at $0.2175 \text{ }\mu\text{m}$ that is believed to arise from a carbonaceous component within the population (Stecher and Donn 1965; Fitzpatrick and Massa 1986). In Fig. 7 this is associated with polycyclic aromatic hydrocarbons or PAHs (Joblin et al. 1992; Hensley and Draine 2023); but alternate suggestions exist (Jones et al. 2013b). A central determination is that interstellar dust has a size distribution that follows a $\text{size}^{-3.5}$ power law distribution with maximum sizes of $\simeq 0.2 \text{ }\mu\text{m}$ (or larger) with most of the mass found in large grains and the surface area carried by small grains (Mathis et al. 1977; Draine

and Lee 1984). Sight lines towards dense regions show a shift in the extinction curve (Fitzpatrick et al. 2019) that relates to greater extinction per H atom beyond $0.3\ \mu\text{m}$ (Draine 2003); this is believed to be the result of grain growth by coagulation and accretion in the denser regions of the ISM.

In the infrared the overall trend is a decrease in extinction with increasing wavelength and towards even longer wavelengths the energy absorbed by grains is released via a continuous emission spectrum peaking near $100\text{--}200\ \mu\text{m}$ (Dwek et al. 1997). Prominent features in this regime are the excess absorption seen in bands associated with silicates near 10 and $18\ \mu\text{m}$. Dust emission is widely used as a tracer of both the dust and the gas mass within dense ($n > 1000\ \text{cm}^{-3}$) regions of the galaxy (Hildebrand 1983).

Another important observational constraint associated with interstellar grains is that both the absorption and emission are partially polarized (Davis Jr and Greenstein 1951; Hildebrand et al. 2000; Andersson et al. 2015). In the UV/optical the peak polarization (linear) is of order a few percent near $0.55\ \mu\text{m}$ (Serkowski et al. 1975). A defining characteristic of the polarization is that while extinction rises from the visible to the UV, the polarization percentage peaks in the visible with a monotonic decline towards both shorter and longer wavelengths (Serkowski et al. 1975; Anderson et al. 1996). The presence of polarization peaking in the visible part of the spectrum suggests that interstellar grains are not spherical, with typical sizes of $\sim 0.1\ \mu\text{m}$, and that they are aligned with the galactic/local magnetic field (Davis Jr and Greenstein 1951; Andersson et al. 2015; Draine 2011). A final point is that dust grains are also responsible for the scattering of starlight which is a major contributor to the overall extinction (Whittet 2022).

Given these observational constraints, a wide range of detailed models with different assumptions with respect to grain composition and population(s), optical properties/methodology, presence/absence of ices have been constructed (Draine and Lee 1984; Greenberg and Hage 1990; Ossenkopf and Henning 1994; Weingartner and Draine 2001; Jones et al. 2013b; Hensley and Draine 2023, to name just a few). These contributions, as well as the full import of dust within astrophysics are nicely summarized in the formative reviews of interstellar dust by Mathis (1990), Draine (2003), Whittet (2022) and Henning (2010). Here we will focus on the question of porosity and the potential evidence of its presence.

Many of the early papers within the field explored the question of dust porosity either as a central aspect (Mathis and Whiffen 1989; Hage and Greenberg 1990) or as an important open question (Draine and Lee 1984). There were several aspects that drove this exploration. First and foremost imaging studies of chondritic interplanetary dust particles (IDP), which are believed to originate from comets (MacKinnon and Rietmeijer 1987), find structures that are highly porous and fragile (Bradley and Brownlee 1986). These aggregate-like structures would be consistent with low velocity coagulation of lower mass particles ($v \lesssim 1\ \text{cm/s}$ for mass $< 10^{-6}\ \text{g}$) as seen in laboratory experiments and might be expected to form inside denser regions of the interstellar medium (Tielens 1989; Güttler et al. 2019). An example of one such image is shown in Fig. 6.

Cosmic elemental abundances and the interstellar extinction curve present another possible driver towards a need for porous grains; this issue is particularly acute for car-

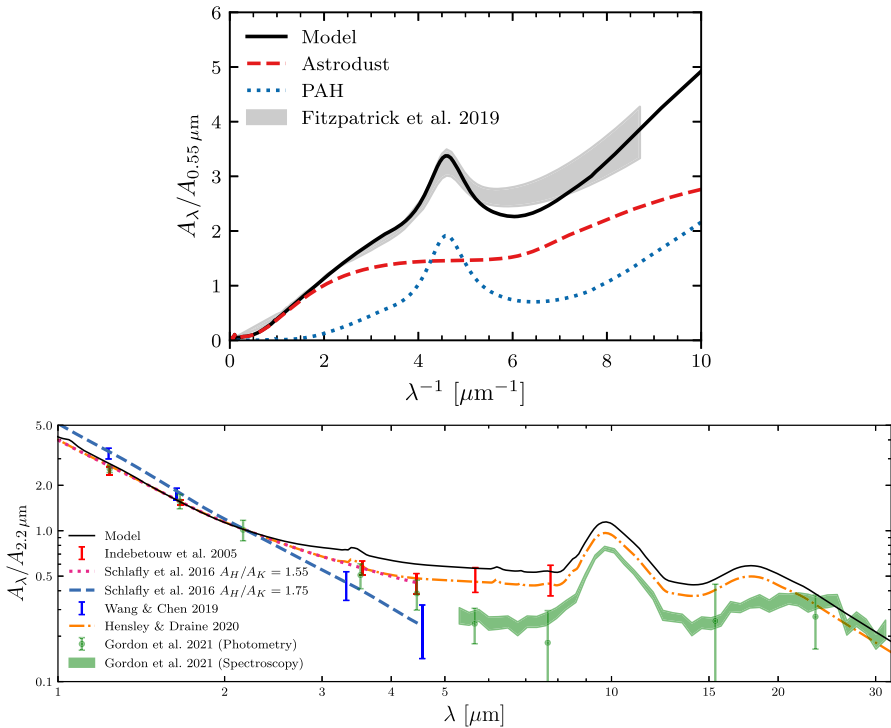


Fig. 7 Plot of the interstellar grain extinction curve as compiled and modeled by Hensley and Draine (2023). (Top Panel): Extinction (A in magnitudes) normalized to $0.55\ \mu\text{m}$ plotted as a function of inverse wavelength. The gray shaded area is the average galactic extinction curve (from observations) taken from Fitzpatrick et al. (2019). The black line is the model fit which is broken down into contributions from Astro dust (red; composite grains containing silicates and other materials including hydrocarbons) and polycyclic aromatic hydrocarbons (blue; PAHs). (Bottom panel): Extinction curve in the infrared normalized to $2.2\ \mu\text{m}$. Observed values of the extinction are as noted in the figure with references noted here (Indebetouw et al. 2005; Schlafly et al. 2016, 2017; Wang and Chen 2019; Hensley and Draine 2020; Gordon et al. 2021) and the model fit is shown as the black curve. Images reproduced with permission from Hensley and Draine (2023), copyright by the author(s)

bon. Models of interstellar extinction adopt an assumed size distribution of grains with an assumed composition. The composition of interstellar grains is estimated through observations of ultraviolet gas absorption lines of atoms and molecules towards stellar sources that lie behind low to modest extinction diffuse gas clouds; one such example is ζ Oph (Savage and Sembach 1996). These measurements give an estimate of the total column and in many instances absolute abundances relative to hydrogen. Using a standard for cosmic abundances, such as the Sun, the amount missing from the gas is attributed to the solids or the interstellar grains. Initial models of grains adopted the solar standard, but the local ISM cosmic carbon abundance appears to be sub-solar within young B stars (Nieva and Przybilla 2012). We note that this is not uniformly the case and measurements towards older populations (F, G, K) find abundances closer to solar (see Hensley and Draine 2021). Regardless, the observed fraction of carbon gas in particular provides a tension between some models which require more material

than cosmically available to be present in the grain population to match extinction (Mathis 1996). Dust grains dominate the extinction at wavelengths where their size is nearly equivalent ($\lambda \sim 2\pi \times \text{size}$). With strong extinction near $\sim 0.1 \mu\text{m}$ (see Fig. 7) this implies sizes near $0.1 \mu\text{m}$, close to the maximum size of the MRN distribution. Large fluffy grains with areas of vacuum offer a way to retain the observed extinction with less material. However, areas of vacuum can also affect the optical and scattering properties of materials as they interact with radiation (Jones 1988; Voshchinnikov et al. 2006; Draine 2003). This interaction relates to the composite polarizability of individual atoms within the substrate and hence polarizability voids within a given volume can affect both scattering and absorption at some modest level (Voshchinnikov et al. 2006). An additional motivation for large fluffy grains was argued to be needed to account for the X-ray scattering halos surrounding point sources such as Nova V1974 Cygni (Mathis et al. 1995). Overall, the issue of cosmic abundances and scattering within X-ray halos as a motivation for porous grains, appears to be of less importance in more modern simulations (Smith and Dwek 1998; Draine and Tan 2003; Li 2005; Hensley and Draine 2021). For an X-ray scattering halo for GX13+1, dust porosity has been constrained to be less than 55% (Heng and Draine 2009). At present, models for the diffuse ISM with an assumed porosity of 20% can match the observational constraints in terms of the overall extinction as a function of wavelength, polarization, scattering and dust emission (Hensley and Draine 2023).

Looking at the denser regions of the ISM there is a generic expectation of grain growth to be consistent with changes in the extinction curve at optical/UV (Fitzpatrick et al. 2019) and infrared wavelengths (McClure 2009). Detailed models of grain evolution suggest the formation of aggregates which can have porosities ~ 30 – 80% (Ossenkopf 1993; Ossenkopf and Henning 1994; Ormel et al. 2009). However, it should be noted that models exist that match the observational constraints yet have little to no porosity (Ysard et al. 2019). More generically dust grain aggregates in the ISM (with vacuums and without) have an increased far-infrared/mm wavelength opacity coefficient (Ossenkopf and Henning 1994; Ormel et al. 2011; Köhler et al. 2012) relative to the models of the diffuse ISM. Observations of dust extinction at near infrared wavelengths and the mm/sub-mm continuum emission along the same line of sight towards molecular clouds find agreement with this prediction (Kramer et al. 2003). Thus, grain growth in the dense ISM is present, as is clear from the JWST spectroscopic observations (Dartois et al. 2024), and this growth may foster an increase in grain porosity.

The strongest limits on porosity at present is dust polarization and, to a lesser extent, the overall dust temperature. In the latter case models of fluffy grains with high porosity ($>80\%$) appear to have increased opacities and subsequently become too cold to match the equilibrium temperature of large grains in the diffuse ISM (Mathis 1990; Dwek 1997). Furthermore, these grains may be difficult to construct (Jones 1988). In terms of dust polarization in Fig. 8 we show the allowed solutions for ISM grain models by Draine and Hensley (2021), whether prolate or oblate, as constrained by starlight polarization and the polarized emission at submillimeter wavelengths. Based on these models oblate shapes are preferred and porosity is limited to ≤ 0.75 . Additional work (Draine 2024b) discusses the formation of aggregates and their observational proper-

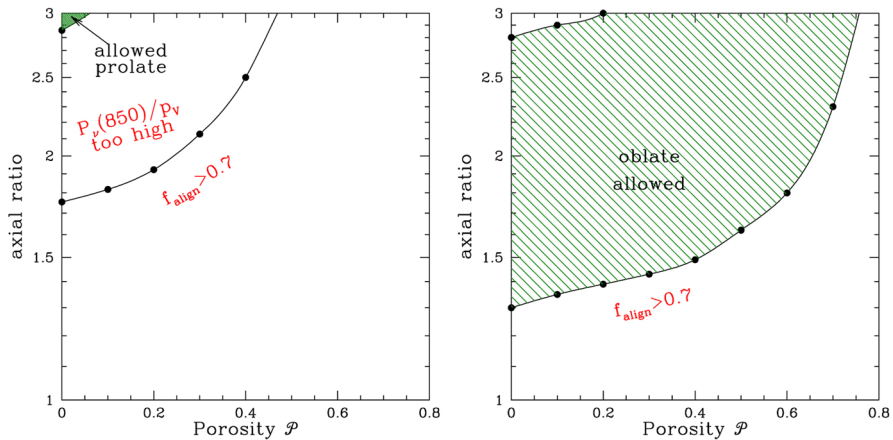


Fig. 8 Summary figure of the allowed solutions of ISM grain models with variable porosity when compared to the monochromatic polarized 850 μm intensity normalized per unit V-band polarization in the diffuse ISM. Models are shown for both prolate and oblate spheroids. The green shaded regions show the allowed axial ratios which are limited for prolate spheroids to the upper left corner. Image reproduced with permission from Draine and Hensley (2021), copyright by AAS

ties. These models also suggest porous grains form with either extreme elongation or flattening; if this is not the case then they must have reduced values of porosity.

Overall growth models suggest that porosity is likely fostered as grains grow. However, if porous grains are present in the diffuse ISM then some external process may need to be present to reduce their porosity, unless the process of growth itself (i.e. collisions) leads to compactness. This sets the stage for the next phase—the disk—where significant grain growth is fostered inside the dust-rich midplanes. Here the question of porosity powered by this growth becomes even more central.

3.3 Dust porosity in planet-forming disks

In planet-forming disks, dust grains undergo coagulation by mutual collisions and then form a cluster of grains called dust aggregates. The intergrain voids are the source of (extrinsic) porosity. Porosity has been a major subject in this field because it directly affects how dust grains grow in the disks, eventually affecting the formation of planetesimals (see reviews by Johansen et al. 2014; Blum 2018). Once planetesimals are formed, they collide and produce smaller fragments in disks, like IDPs in the Solar System.

Recent disk observations start to show some clues on dust porosity in disks. However, no consensus on observational constraints on dust porosity has been reached. This is partly because of incoherent modeling methods/techniques among different studies (e.g., light scattering calculations) used to infer dust porosity. Also, the number of protoplanetary disks analyzed in this context is still limited. In this section, we aim to summarize the current status—rather inconclusive though—of dust porosity in planet-forming disks. Interpretation of multiwavelength observations of planet-forming disks

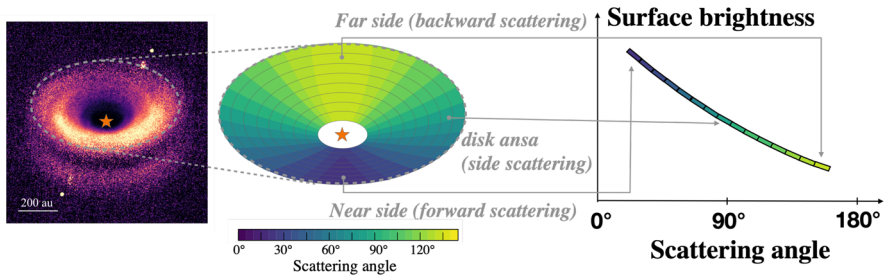


Fig. 9 Basic concept of scattered light mapping to extract an SPF from an observed scattered-light image

depends on whether the disk is optically thin or not. Hence, we discuss two evolutionary stages of planet-forming disks separately: protoplanetary disks (Sect. 3.3.1) and debris disks (Sect. 3.3.2), where the latter is older and is optically thin at all wavelengths, and the former is not.

3.3.1 Protoplanetary disks

Dust porosity in protoplanetary disks has been inferred from modeling of the following observational results:

- Optical/near-infrared (IR) scattered light observations (e.g., HST, VLT, Subaru, Gemini),
- Mid-IR spectroscopy (e.g., Spitzer, JWST),
- Millimeter(mm)-wave thermal and scattered radiation (e.g., ALMA).

One of the major challenges here is that the disk is optically thick at most of the wavelengths at which we observe. The immediate consequence is that different wavelengths trace dust particles in different regions of the disk (disk surface for IR vs. closer to the midplane for mm). Since dust particles in different regions may have different sizes and porosity (see Sect. 4.2), we cannot directly combine multiwavelength observables to determine a single dust model. Dust properties (e.g., porosity) should be modeled each observing wavelength separately.

Optical/near-IR scattered light observations.

In this wavelength region, we probe relatively small grains (typically around $\sim 1 \mu\text{m}$) floating in atmospheric regions of a protoplanetary disk. Those grains are directly illuminated by the central radiation source, such as a star or thermal radiation from the innermost regions, and the grains scatter the incoming light toward the observer.

As explained in Sects. 2.1.3 and 2.1.4, the information of dust properties (including porosity) is imprinted in the SPF, the DoLP, and scattered light colors. By conducting observations, we obtain a scattered light image of a protoplanetary disk with each pixel in the image containing total intensity, polarized intensity, or DoLP. By comparing disk images taken at different wavelengths, we can also derive scattered light colors. How do we measure the SPF? The most common way is to use a technique called scattered light mapping (Fig. 9), where we compute scattering angles at each location of the disk surface and then map the observed surface brightness as a function of the scattering

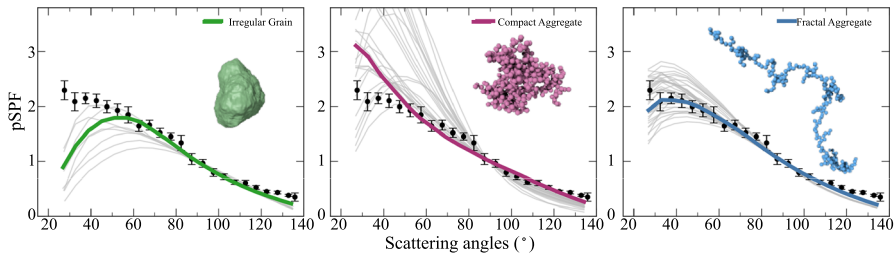


Fig. 10 Polarized scattering phase function (pSPF) extracted for the disk around IM Lup (black points with error bars) and radiative transfer models for irregular grains (left), compact aggregates (middle), and fractal aggregates (right). Thin gray lines in each panel correspond the results obtained for changing aggregate/monomer sizes, porosity, and composition, and the thick solid lines represent the best fit among them for each class of particle morphology. Particle images shown in each panel is the dust model used in the best-fitting model. See Tazaki et al. (2023b) for more detailed information

angle (e.g., Stolker et al. 2016; Roumesy et al. 2025). Although scattered light mapping is only applicable to axisymmetric disks, there have been measurements for several protoplanetary disks so far (McCabe et al. 2002; Avenhaus et al. 2014; Takami et al. 2014; Ginski et al. 2016; Stolker et al. 2016; Ginski et al. 2023; Chen et al. 2024; Roumesy et al. 2025).

Pinte et al. (2008) modeled disk-scattered light of IM Lup using the Mie theory with EMA and found that it is either explained by a dust porosity of 80% or ice-rich non-porous grains based on the asymmetry parameter (the first cosine moment of a tSPFs). Perrin et al. (2009) and Dykes et al. (2024) studied the disk-scattered light around AB Aur using the Mie theory with EMA and found a dust porosity of 55% and 60–80%, respectively, based on the observed DoLP. Chen et al. (2024) modeled SPFs, DoLP and color information toward the disk around HD 34700 A using the Mie theory/DHS with EMA and obtained a dust porosity of 40%. Taken at face value, those studies favor dust grains with some amount of porosity; however, it is worth keeping in mind that those values may be affected by what grain size distribution is assumed (e.g., Chen et al. 2024). Canovas et al. (2013) reported VLT/NACO observations for HD 142527 in the H band and found that the DoLP was relatively low. Based on this result, they argued that the dust grains in the disk surface are likely compact and not highly porous. However, this interpretation needs to be taken with care because a low DoLP could be due to the size effect of monomers within highly porous aggregates (Tazaki and Dominik 2022) (Sect. 2.1.4). Mulders et al. (2013) focused on disk-scattered light color around HD 100546. The color is found to be reddish, requiring grains a few microns in size (see also Sect. 2.1.3). Along with a dynamical argument, the authors pointed out the possibility that the grains may be porous to the order of 99% with sub-micron-sized monomers, though the scattering properties of the aggregates were not considered. According to the RGD light scattering theory (see Sect. 2.1.3, Eq. (9)), aggregates with a porosity $> 99\%$ (likely having a low fractal dimension; $\gamma < 3$) will produce bluish scattered light (Tazaki et al. 2019a). Therefore, it remains unclear whether fluffy aggregates of sub-micron-sized monomers explain the observed reddish colors.

The above studies have used the Mie theory or DHS with EMA to constrain dust porosity. Another line of research is to model disk-scattered light using a more sophisticated light scattering models. Tazaki et al. (2023b) studied disk-scattered light around IM Lup with T -matrix light scattering simulations of fractal dust aggregates ($1.1 \leq \gamma \leq 3$). They found that fractal aggregates can naturally explain the observed pSPF, as shown in Fig. 10. Fractal aggregates suggested in their modeling have a characteristic radius greater than $\sim 2 \mu\text{m}$ and $\gamma \lesssim 2$ and with a monomer radius of $0.2 \mu\text{m}$. The inferred aggregate structure suggests that they form via Brownian motion, as suggested by laboratory and numerical experiments (see Sect. 4.2). Fractal dust aggregates in the IM Lup disk imply that cometary fractal aggregates might have formed in the early-stage planet-forming disks (Sect. 3.1).

Looking ahead, two major challenges remain in constraining dust porosity from disk-scattered light observations. First, the systematic uncertainty in inferred porosity is still poorly understood due to the diversity of modeling approaches and the lack of a robust diagnostic signature. A key limitation is perhaps the non-uniqueness of model solutions: extensive exploration of parameter space is needed to assess degeneracies, but such surveys are often computationally prohibitive. This is because accurate modeling requires not only detailed light-scattering calculations, but also radiative transfer simulations, as SPFs and DoLPs are significantly affected by multiple scattering and limb brightening effects (Tazaki et al. 2023b; Takami et al. 2013; Ma and Schmid 2022). These challenges underscore the need for more accurate and computationally efficient modeling techniques. Second, it is essential to collect as much observational information as possible, including SPFs, DoLPs, and color indices. Fortunately, recent advances in observational facilities, instrumentation, and data reduction techniques have made it increasingly feasible to obtain accurate and quantitative measurements of scattered light. For instance, pSPFs have been obtained for about 10 protoplanetary disks, revealing two distinct behavioral categories that may correspond to different dust populations (Ginski et al. 2023; Roumesy et al. 2025). Similarly, measurements of the DoLP are rapidly increasing, owing to the improved stability and quality of reference differential imaging (RDI) observations (Hunziker et al. 2021; Tschudi and Schmid 2021; Ren et al. 2023a; Chen et al. 2024). Color measurements are also becoming more common (Fukagawa et al. 2010; Mulders et al. 2013; Zhong et al. 2024; Avenhaus et al. 2018; Ginski et al. 2024; Ma et al. 2024a,b). However, several caveats must be considered when interpreting these observations. Surface brightness and color analyses can be affected by temporal variability if multi-wavelength images are taken at different epochs (Watson et al. 2007; Rich et al. 2019; Ma et al. 2024a). Additionally, different wavelengths may trace different surface heights in the disk, introducing further complexity in interpreting color trends (Duchêne et al. 2004; Pinte et al. 2007). In some cases, disk surface brightness may be influenced by shadowing from the inner disk (Acke et al. 2009; Garufi et al. 2022), meaning that observed faintness does not necessarily reflect the scattering properties or reflectivity of the dust grains if this is the case.

Mid-IR spectroscopy.

In this wavelength region, we can observe thermal emission most dominantly from lukewarm grains ($\sim 300 \text{ K}$), which are located at a radial distance of $\lesssim 10 \text{ au}$. In

particular, the mid-IR domain is rich in solid-state features of various minerals, providing another way to constrain dust properties, including porosity. One of the most well-studied mid-IR features would be the $10\text{ }\mu\text{m}$ silicate feature (see e.g., a review by Henning 2010).

Voshchinnikov and Henning (2008) studied the effect of porosity on the $10\text{ }\mu\text{m}$ silicate feature using the MLS (e.g., Voshchinnikov et al. 2005). They fitted the observed silicate feature from $\lambda = 8\text{ }\mu\text{m}$ to $12\text{ }\mu\text{m}$ for 47 sources (30 T-Tauri stars and 17 Herbig Ae/Be stars) observed with the Spitzer Space Telescope (Schegerer et al. 2006; van Boekel et al. 2005; Sargent et al. 2006; Sicilia-Aguilar et al. 2007) by assuming small grains that are in the Rayleigh domain. The derived porosity for 47 sources varies from $\approx 39\%$ to $\approx 98\%$ with an average value of $64 \pm 15\%$. Recently, Jang et al. (2024) studied mid-IR spectra for PDS 70 with JWST using a porous irregular grain model generated via the Gaussian Random Field (GRF) algorithm (Min et al. 2007). They computed the optical properties of those grains with DDA and found that the porous-GRF model reproduces the observed mid-IR spectra better than DHS and laboratory spectra by Tamanai et al. (2006, 2009).

Although there are studies favoring the presence of porous grains based on mid-IR spectra, the detailed structure of dust grains, such as fractal dimension and the monomer size, still remains unclear. Furthermore, it is worth keeping in mind that the absorption property of grains in the Rayleigh regime is sensitive to the particle shape (Bohren and Huffman 1983; Min et al. 2006b; Mutschke et al. 2009). In other words, the failure of spherical-grain models (like the Mie theory) should not be interpreted as (indirect) evidence for porous grains; the failure may simply be attributable to asphericity of grains.

Millimeter-wave thermal and scattered radiation. In this wavelength region we observe thermal emission from cold (sub)millimeter-sized grains in a region close to the disk midplane. There are two main approaches to constrain dust porosity. One is to use mm-wave polarization and the other one is to perform multi-band analysis (i.e., the spectral index), or the combination of both. The strongest constraint on porosity at present appears to be from mm-wave polarization, as described below.

Thanks to its sensitivity and spatial resolution, ALMA opened up a new window to observe mm-wave polarization of disks. It is suggested at least two polarization mechanisms are needed to explain the observed polarization patterns (Stephens et al. 2017). One is self-scattering (Kataoka et al. 2015; Yang et al. 2016), which can naturally explain polarization patterns uniformly oriented parallel to the disk minor axis (e.g., Hull et al. 2018; Dent et al. 2019). Another one is polarized thermal emission from aligned grains (Cho and Lazarian 2007; Bertrang et al. 2017; Tazaki et al. 2017; Guillet et al. 2020; Thang et al. 2024; Kataoka et al. 2019; Lin et al. 2024b), although the detailed alignment process/direction remains being debated (Andersson et al. 2015; Yang et al. 2019). These two mechanisms are not exclusive each other and may work simultaneously (Mori and Kataoka 2021; Stephens et al. 2023; Lin et al. 2024a).

Theoretical studies have suggested that a less-porous dust origin is favorable for the mm-wave polarizations, regardless of whether it is due to scattering (Tazaki et al. 2019b; Brunngräber and Wolf 2021) or alignment (Kirchschlager et al. 2019). This has been supported by subsequent, more detailed observational modeling (Zhang et al.

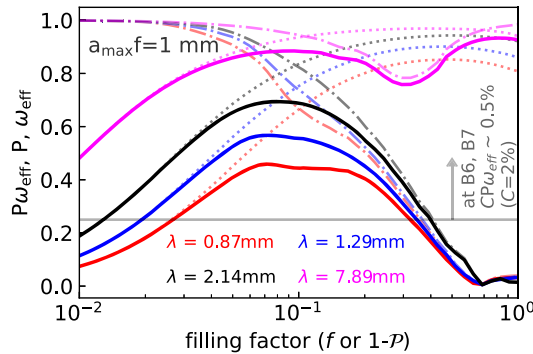


Fig. 11 The scattering polarization efficiency at millimeter wavelength. P is the degree of polarization (dot-dashed), and ω_{eff} is the (effective) scattering albedo (dotted). Their product $P\omega_{\text{eff}}$ (solid lines) gives an efficiency of scattering polarization, which only exceeds the required level to explain the observations at a porosity of 70–97% in the HL Tau disk. Image reproduced with permission from Zhang et al. (2023), copyright by the author(s)

2023; Ueda et al. 2024). Zhang et al. (2023) studied the multi-band fluxes and polarization observations of the HL Tau disk by using the Mie theory with EMA. They estimated the viable porosity range to be 70–97% (Fig. 11), and a porosity > 99% is unlikely. Ueda et al. (2024) constructed a dust evolution model in a self-gravitating disk using a dust evolution code DustPy (Stammler and Birnstiel 2022) and applied it to the mm-wave observations for the IM Lup disk. The model favors grains with 80% porosity for the IM Lup disk. Kirchschlager et al. (2019) studied mm-wave polarized thermal radiation from aligned grains for the disk around HD 142527 and found that a grain porosity of $\leq 70\%$ is needed unless the grain’s axis ratio is extremely large. Ohashi et al. (2023) studied the dust porosity in the DG Tau disk; however, the observations are found to be explained by both non-porous and porous (80%) models, and hence, the porosity for this source remains not well constrained.

Another approach for constraining porosity is multi-band mm-wave flux analysis. If disks are optically thin, we may constrain dust porosity from the spectral index of mm-wave flux (Miyake and Nakagawa 1993; Natta et al. 2004; Draine 2006; Testi et al. 2014; Cuzzi et al. 2014; Kataoka et al. 2014). However, there is growing evidence for disks being (at least marginally) optically thick at mm wavelengths (e.g., Chung et al. 2024), making the porosity constraint not straightforward as anticipated for the optically thin case. For a higher optical thickness, the effect of scattering also affects the observed emission (Birnstiel et al. 2018; Zhu et al. 2019; Liu 2019; Sierra and Lizano 2020; Ueda et al. 2020). To find a dust property, simultaneous fitting of multi-band data from mm to cm-wave by taking into account scattering has been performed (e.g., Carrasco-González et al. 2019; Sierra et al. 2021; Macías et al. 2021; Ueda et al. 2022; Guidi et al. 2022; Ohashi et al. 2023; Zhang et al. 2023). Guidi et al. (2022) performed multi-band analysis for HD 163296 with five wavelengths and found that low-porosity grains (with 25% porosity) better reproduce the data compared to high-porosity grains (with 80% porosity). More recently, Yoshida et al. (2025) proposed a novel approach to breaking the degeneracy between dust temperature and dust scattering albedo in the

TW Hya disk using CO line emission. They derived a dust porosity of $< 96\%$ and a power-law index of the size distribution > -4.1 . These porosity range is consistent with what has been inferred from mm-wave polarization measurements.

Overall, observations of mm-wave polarization and multi-band analysis thus far point to a dust porosity of approximately 90% or less, ruling out extreme porosity greater than 99%. The less-porous particles in disks might be linked to cometary particles found in the comet 67P/Churyumov–Gerasimenko with the GIADA instrument, which have a porosity of $\sim 48\% \pm 8\%$ (see Sect. 3.1), although dust evolution models in disks still do not fully explain how these less-porous particles were formed (see Sect. 4.2).

It is worth keeping in mind in the above modeling studies that grain's optical properties are still mostly modeled using the Mie theory or DHS with the EMA. There are some studies claiming potential issues with using the Mie theory. For example, Kirchschlager and Bertrang (2020) demonstrated that non-porous spheroid grains show scattering polarization behavior different from the mass-equivalent counterpart of the Mie theory. Lin et al. (2023) also pointed out that the scattering properties of laboratory non-porous grains show qualitatively different polarization properties from the Mie theory's prediction. Further careful studies on light scattering properties and its application to the actual disk observations are mandatory to push forward our understanding of dust porosity in disks.

3.3.2 Debris disks

Debris disks are circumstellar disks found around (pre)main sequence stars. Although these disks are placed in a later evolutionary stage of protoplanetary disks, they are not simply the leftover of protoplanetary disks. Dust grains (and sometimes gas) in debris disks are likely of secondary origin (i.e., those replenished by collisions of planetesimals), as primordial grains are short-lived due to orbital decay via Poynting Robertson drag or blown out by radiation pressure (Burns et al. 1979). Therefore, dust properties in those disks are likely different from those found in protoplanetary disks and are perhaps more similar to those seen in the Solar System, e.g., IDP (Fig. 6). Hence, studies of debris disks offer a unique opportunity to investigate how the Solar System is different from other extrasolar systems.

Determining the dust porosity in debris disks poses fewer challenges than for protoplanetary disks, because they are optically thin at all wavelengths and disk geometry is constrained relatively well compared to protoplanetary disks. Nevertheless, there have been several challenges in observational modeling of debris disks. For example, dust properties inferred from SED fitting are often in conflict with those inferred from scattered light observations [HD 181327: Lebreton et al. (2012), HD 207129: Krist et al. (2010), HD 32297: Rodigas et al. (2014), HR 4796A: Rodigas et al. (2015)], although a more flexible assumption in the refractive index (and then dust composition) may reconcile this issue (Rodigas et al. 2015; Ballering et al. 2016). Furthermore, even if we only aim to model scattered light observations, different fitting outcomes are sometimes obtained depending on which of total or polarimetric observational data are used (Arriaga et al. 2020; Duchêne et al. 2020). The issue may imply limitations of simple light scattering models used, such as the Mie theory. For example, Olofsson

et al. (2022) found pSPF extracted for HD 32297 could be well explained by a light scattering model of fractal aggregates (MMF; Tazaki and Tanaka 2018), whereas not when the Mie theory or DHS is used. In this way, observations have been challenging our understanding of the optical properties of dust particles in debris disks. In the following, we will highlight studies on dust porosity for a few well-studied debris disks: HR 4796 A (A0 star, 10 ± 3 Myr old; Bell et al. 2015), AU Mic (M star, 22 ± 3 Myr; Mamajek and Bell 2014), and β Pic (A6 star, ~ 20 Myr; Miret-Roig et al. 2020).

HR 4796A: This is the one of the most well-studied debris disks in the context of dust characterization. HR 4796A harbors a large and narrow ring with a semi-major axis of $\sim 1'' \approx 77$ au that is inclined by $\sim 76^\circ$ degrees from pole-on (Fig. 12).

Dust properties for this source have been inferred from SED (Augereau et al. 1999; Li and Lunine 2003; Rodigas et al. 2015), reflectance spectra (Debes et al. 2008; Köhler et al. 2008; Rodigas et al. 2015; Milli et al. 2017; Ren et al. 2023b), SPF (Schneider et al. 2009; Perrin et al. 2015; Milli et al. 2015, 2017, 2019; Olofsson et al. 2020; Ren et al. 2020; Chen et al. 2020; Arriaga et al. 2020; Schmid 2021). Rodigas et al. (2015) performed simultaneous modeling of reflectance colors and SED using the Mie theory with the EMA (Bruggeman). They found that the best fit porosity to SED and reflectance spectra are different: the former favors a higher porosity ($\sim 70\%$) and the latter does a lower porosity ($\sim 30\%$). When the two constraints (reflectance spectra+SED) were combined, the model only provides a mediocre fit with a slight preference for a lower porosity ($\sim 10\%$). The SPF for this source has a unique trend: a strong forward scattering peak with a gradual enhancement of intensity toward larger scattering angles (Fig. 12). Such behavior can be either due to either iron-rich grain composition (Chen et al. 2020) or grain morphology, i.e., large particles with rough surface (Milli et al. 2019). In the presence of surface roughness, the incident light onto the dust surface will be diffusely reflected, rather than specularly reflected (e.g., Fresnel reflection), and diffuse reflection can make back scattering rather bright, as with the case of lunar phase (Hapke 1981; Mukai et al. 1982; Min et al. 2010). Min et al. (2016) demonstrated using DDA calculations that light scattering by compact dust aggregates (a fractal dimension $\gamma \sim 3$) shows the enhanced back scattering (see also Grynko et al. 2020; Penttilä et al. 2021) similar to what is seen in the HR 4796 disk, whereas such a trend is absent for fluffy dust aggregates ($\gamma \sim 2$) with monomers smaller than the wavelength (Volten et al. 2007; Tazaki et al. 2016). From laboratory measurements, Muñoz et al. (2017) studied SPF of mm-sized non-spherical compact grains at optical wavelength and found a similar backscattering enhancement. These studies suggest that, if the enhanced backward scattering is due to grain morphology, less porous grains are favorable for explaining SPFs, although quantitative porosity value remains unknown.

Overall, dust properties inferred from various observations of HR 4796A seem to be in favor of the presence of less porous grains, based on SED analysis (Rodigas et al. 2015) and the observed enhanced backscattering behavior (Milli et al. 2017, 2019). However, the narrowing down more detailed properties are still to be done.

AU Mic:

AU Mic is one of a few debris disks around M-type stars. The strongest constraint on dust porosity in AU Mic seems to be coming from polarization measurements with

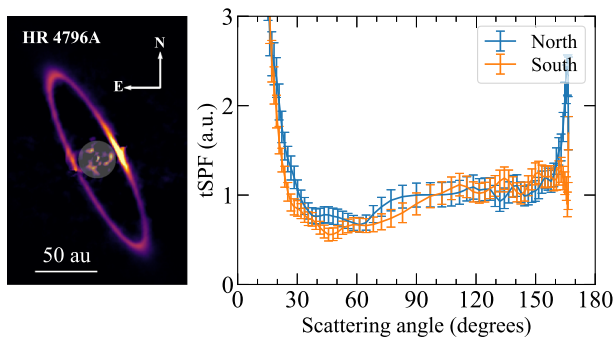


Fig. 12 Total intensity image of HR 4796A (left) and the tSPFs extracted for the northern and southern sides (right) reduced by Milli et al. (2017). The image was reduced with the masked classical angular differential imaging (mcADI; Milli et al. 2012). The tSPFs were corrected for the mcADI flux losses and the convolution effect by the instrumental PSF, but not for the limb brightening, which results in a small hump at $\sim 90^\circ$ (see Olofsson et al. 2020). The peak beyond 160° seen in the northern SPF is likely an artifact

HST/ACS at $0.6\ \mu\text{m}$ (Graham et al. 2007). They found a DoLP rising steeply from 5% to 35% between 20 and 50 au and reaching a maximum of $\sim 40\%$ within 80 au. Based on the radial dependence of observed surface brightness and DoLP, Graham et al. (2007) found grains that show a strong forward scattering and a high degree of polarization are compatible with the data. By using the Mie theory with the real part of refractive index being treated as a free parameter, they obtained $n = 1.03 \pm 0.03$. This values correspond to a porosity of 91–94% depending on if the matrix is either ice or rock assuming the Maxwell–Garnett mixing rule. Qualitatively similar conclusions have been obtained in more recent studies by Fitzgerald et al. (2007), Shen et al. (2009) and Arnold et al. (2022). In Fitzgerald et al. (2007), they constructed grain models based on multiwavelength surface brightness data and SED assuming the refractive index of Mathis and Whiffen (1989) (a porous mixture of silicate, carbon, and ice) or astronomical silicate. They found a compatible fit quality to surface brightness and SED regardless of porosity, but the compact model is ruled out to explain the observed DoLP reported in Graham et al. (2007). Shen et al. (2009) performed light scattering simulations of Ballistic Aggregates using DDA and compared the results of Graham et al. (2007) and found aggregates with a porosity of $\sim 60\%$ (so-called BAM2 model, see Fig. 5 for exemplary morphology of BAM2). Arnold et al. (2022) carried out MCMC fitting to estimate grain properties based on spatially resolved scattered light spectra obtained with HST/STIS (Lomax et al. 2018). Porous spheres or agglomerated debris particles (ADP) (Zubko et al. 2015), where both of them have a porosity of $\sim 76\%$, fit equally well to the wavelength and radial dependence of surface brightness, whereas non-porous spherical models only show a poor fit. They also confirm that their porous models are compatible with the DoLP reported in Graham et al. (2007). Using a Herschel $70\ \mu\text{m}$ image, Matthews et al. (2015) pointed out that a halo component is spanning from 40 to 140 au, which is beyond the outer edge of the planetesimal belt (~ 40 au). Due to low luminosity of AU Mic, radiation pressure is insufficient to blow out small grains, and hence the stellar winds

might blow them out (Augereau and Beust 2006; Matthews et al. 2015; Arnold et al. 2019). Matthews et al. (2015) pointed out that high porosity grains are favorable for an efficient transport to the halo region via the stellar winds due to their larger cross sections. Note that their argument is for a halo region, and hence, dust porosity around the planetesimal belt at ~ 40 au might not necessarily have the same porosity as the halo region. To summarize, all modeling efforts for the AU Mic disk (particularly for outer disk regions) so far point to the presence of porous grains with a porosity of ~ 60 – 94% based on the Mie theory with the EMA, ADP models, or BAM2 models.

β Pic: Earlier modeling of β Pic's dust properties revealed an apparent conflict: Li and Greenberg (1998), based on SED modeling, favored highly porous aggregates, whereas Golimowski et al. (2006), using scattered light images and color, favored less porous grains. Ballering et al. (2016) found that this tension can be resolved when a wider parameter space in grain composition is explored. They modeled SED and scattered light with the Mie theory with EMA, and their best-fit dust model is made of predominantly astronomical silicate and refractory organics with little amount of vacuum and ice. Although they do not discuss if the model shows a compatible level of DoP ($\sim 10\%$ at K band) (Tamura et al. 2006), it seems not challenging as non-porous grains readily show a low DoP (see, e.g., Fig. 5).

Recently, Rebollido et al. (2024) observed the disk with JWST/NIRCam and MIRI and found that the secondary disk has a bluish color in the mid-IR, whereas it is reddish in the main disk. Moreover, they found a unique structure called 'cat's tail', and such a structure could be explained by the presence of dust particles characterized with a high radiation pressure efficiency, i.e., fluffy aggregates made of organics. Based on these results, they proposed that the main disk and the secondary disk (including the cat's tail) are composed of different types of dust grains: the former consists of more non-porous grains and the latter consists of more fluffy aggregates.

To summarize this subsection, debris disk observations have so far suggested various porosities: less porous grains in the ring region in the HR 4796A disk, porous grains at least in the halo region of the AU Mic disk, and possibly a mixture of high and low porosity grains for the main disk and secondary disk in β -Pic, respectively. Dust in a single system is likely not characterized by a single porosity value, but instead exhibits a range of porosities within the disk. This idea is supported by observations of comet 67P, where both compact and fractal dust families have been identified (Sect. 3.1). In the three debris disks discussed above, the inferred porosity values differ, which may reflect variations in dust properties depending on the region observed, specifically, how close the observations probe to the planetesimal belt.

4 Laboratory and modeling studies

In the first two subsections, we describe results of laboratory experiments and dust growth models relevant to the ISM and protoplanetary disks. Regarding the experiments, we consider two cases: (i) formation of grains in envelopes of evolved stars (mainly of asymptotic giant branch (AGB) stars) and their subsequent growth in the ISM and planet-forming disks and (ii) recondensation of grains in the diffuse ISM.

The latter is related to the idea of a practically complete destruction of “stardust” in the ISM by supernova shocks (Draine 2003; Jones and Nuth 2011; Zhukovska and Henning 2013). Then we briefly discuss cosmic dust materials. The last subsections are devoted to atomistic modeling of cosmic and astrochemical modeling.

4.1 Dust growth in the interstellar medium

In the experiments simulating the formation of cosmic dust in envelopes of evolved stars and their subsequent growth in the ISM, gas-phase condensation techniques, such as laser ablation and condensation as first demonstrated by Smalley et al. in their foundational work on fullerenes (Kroto et al. 1985), laser- and plasma-enhanced pyrolysis as commonly used in chemical vapor deposition (see Yi et al. 2021 for a review), and electron/ion beam sputtering as widely used in the deposition of coatings and thin films (see El-Awadi 2023 for a review), combined with deposition of condensed particles on substrates are used. The typical low pressure (a few mbar) regime of quenching atmospheres applied for condensation zones is comparable to the pressure conditions for dust condensation in AGB stars (Lodders and Fegley 1999). Deposition of grains simulates the dust growth in the ISM and leads to the formation of porous fractal grain aggregates.

For example, researchers of the Laboratory Astrophysics Group of the Max Planck Institute for Astronomy have for many years performed laser ablation of graphite targets for carbon dust and silicon-based targets (e.g., MgSi, FeSi, MgFeSi) for silicate dust in their work. Evaporated species condense in a quenching atmosphere of a few mbar He/H₂ (for carbon grains) or He/O₂ (for silicate grains) forming nm-sized particles. Condensed particles are extracted adiabatically from the ablation chamber decoupling the particles from the carrier gas and generating a particle beam, which is directed onto a substrate. To characterize the condensed materials and to determine their composition, structure and morphology, sophisticated ex situ analytical methods such as high-resolution transmission electron microscopy (TEM), scanning electron microscopy (SEM), atomic force microscopy (AFM), and energy dispersive X-ray (EDX) spectroscopy have been used by the group. TEM and EDX spectroscopy deliver a direct view inside the grains and the information on the composition, structure, sizes, and shapes of individual grains. SEM and AFM provide information on the morphology of the condensed grain layers.

The analysis of dust grain samples shows that the dust layers consist of individual spherical particles of a few nm in size and porous random-shaped aggregates of up to several tens of nm in size. Thus, the morphology of dust particles on a substrate can be understood as a layer of dust aggregates having a fractal structure (fractal distribution of grain monomers) and a very high (up to 90%) porosity. Such grain aggregates present analogous of dust grains in the ISM, and in protostellar envelopes and planet-forming disks, for which they represent building blocks of larger aggregates having a similar structure and morphology (considering the fractal nature of the grain growth).

Microscopy images of dust grains produced by laser ablation and subsequent deposition on a substrate are presented in Fig. 13. These are typical images, and the reader can find many similar examples in the literature (e.g., Jäger et al. 1998, 2008, 2009;

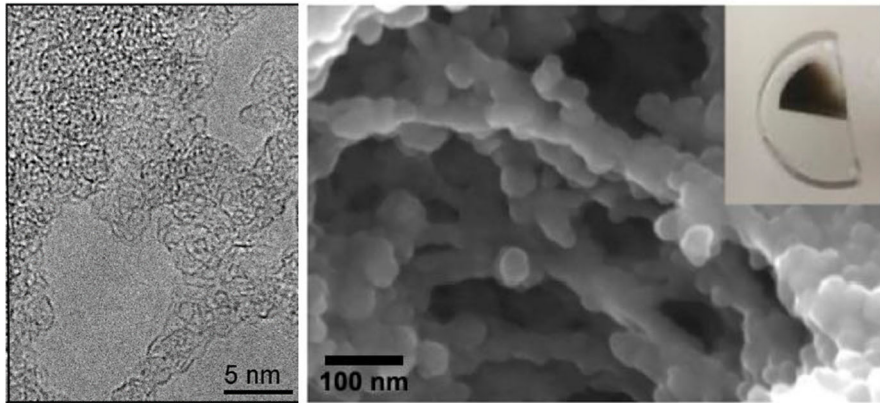


Fig. 13 TEM (left) and SEM (right) images of amorphous carbon (left) and amorphous silicate (right) grains produced by gas-phase condensation of nm-sized grains and their subsequent deposition onto a substrate. Inset: a laboratory sample—a layer of carbon grains on a KBr substrate. Images reproduced with permission from [left] Potapov et al. (2020), copyright by the author(s); and [right] from Potapov et al. (2019), copyright by APS

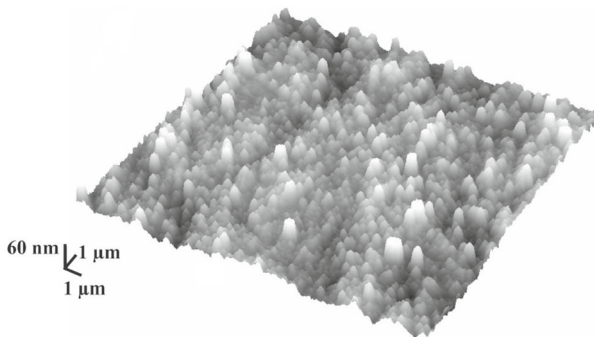


Fig. 14 AFM image of a 200 nm thick amorphous silica thin film physical vapor deposited on a polished metal substrate. Image reproduced with permission from Thrower et al. (2009a), copyright by the author(s)

Sabri et al. 2014; Gavilan et al. 2016; Potapov et al. 2019, 2024). What is clearly seen in the images is a very high porosity of dust grain aggregates on the level of nanoparticles as well as large aggregates.

A much less sophisticated experimental approach can be taken using standard thin film deposition technologies. For example, McCoustra and co-workers have for over 15 years employed amorphous silica deposited on polished copper or stainless steel substrates in their work (see, e.g., Thrower et al. 2009b; Collings et al. 2015). Simple electron-beam evaporation is used to promote physical vapor deposition on room temperature substrates. The resulting thin films, illustrated by the AFM image in Fig. 14, are sufficiently thick that there is no access to the underlying substrate from the gas phase and there is no likelihood of metal substrate-mediated hot electron chemistry. High porosity of the dust layer is clearly seen.

An alternative to electron beam evaporation is ion sputtering in which ions mechanically remove material from a target for deposition on the substrate is being explored in some laboratories (Sobrado et al. 2023). The presence of reactive gases can ensure deposition of oxides, nitrides, and other materials. Specific designs of sputter source, (e.g., Pratontep et al. 2005; Ellis et al. 2016; Palmer et al. 2016; Sanzone et al. 2021) permit growth of films and powders with size-selected particles. Either approach can be extended to produce thin films of virtually any of the materials in Table 1 below (see Sect. 3.3).

In the experiments simulating the re-formation of cosmic dust in the ISM (Krasnokutski et al. 2014; Rouillé et al. 2014; Fulvio et al. 2017), laser vaporization of SiO, silicate, or graphite targets was carried out followed by matrix isolation of laser-vaporized atomic and molecular species, e.g., Si, Mg, SiO, and carbon chains in neon or argon. After annealing and complete evaporation of the Ne/Ar matrix, the formation of silicate and carbon grains was detected. The condensed grains had the structures and porosity like the grains produced by laser evaporation and subsequent deposition (exemplified by Fig. 13).

The aforementioned experimental results are in agreement with the results of modeling of grain growth in the ISM (Ossenkopf 1993; Ossenkopf and Henning 1994; Ormel et al. 2009; Hirashita and Il'in 2022) showing porosity of dust aggregates in the range of ~30–80%. Two main approaches were used in these models to simulate growth of spherical grains of a constant internal density: (i) particle-cluster aggregation (PCA), where an aggregate is created by adding each constituent particle from a random direction and (ii) cluster-cluster aggregation (CCA), where an aggregate is created by sticking with the same-sized cluster from a random direction (Meakin 1991; Mukai et al. 1992). The CCA approach leads to more fluffy and porous grain aggregates. Figure 15 shows an example of the results of CCA simulations of dust growth in the dense ISM from (Ossenkopf 1993) where the porosity of dust aggregates of ~80% was demonstrated. We note here that if we compare Fig. 13 (grain aggregates from experiments), Fig. 15 (grain aggregates from simulations), and Fig. 6 (a real extraterrestrial particle), we will find a great similarity.

Space weathering may efficiently change the composition and structural, morphological (porosity), optical and chemical properties of the dust. Interactions of heavy ions and X-rays, analogs of cosmic rays, with analogs of cosmic dust grains have been studied (Jäger et al. 2016; Gavilan et al. 2016; Dartois et al. 2017; Pino et al. 2019). Structural and compositional changes of dust grains have been demonstrated, however, no attention has been paid to the porosity and surface reactivity of dust grains, as has been done, for example, for thermal annealing. Thermal annealing of silicate grains causes the coalescence of grains leading to an increase of the sizes of individual grains and to a consistent decrease of the porosity of grain aggregates. Moreover, the grain surface becomes chemically less active. It was shown that the average size of silicate grains increases from about 6 to 30 nm and their porosity decreases from about 90% to 40% with annealing from room temperature to 900 °C (Potapov et al. 2024). Also, not much attention has been paid to changes in optical properties of analogs of cosmic dust grains due to space weathering. There is only a handful of studies of the influence of UV and ion irradiation (Mennella et al. 2001;

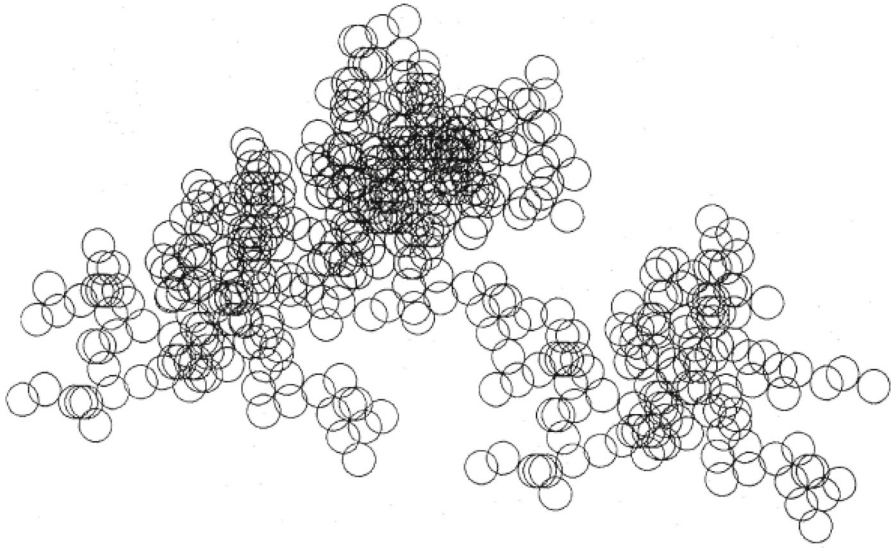


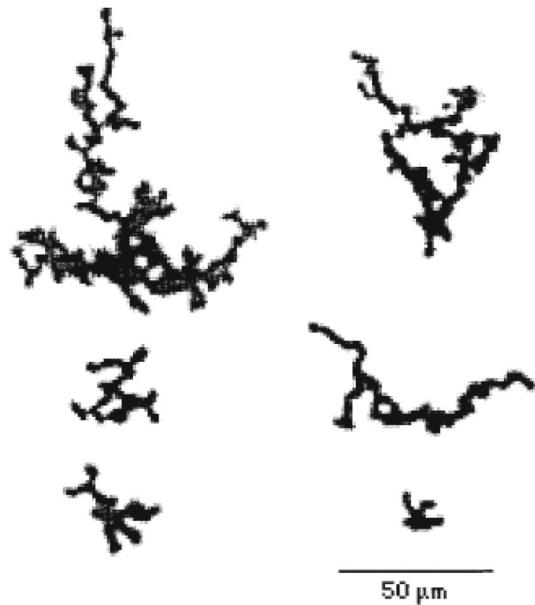
Fig. 15 A result of numerical simulations of dust growth. Clusters consisting of 512 single grains of identical size grew by ballistic cluster–cluster agglomeration. Image reproduced with permission from Ossenkopf (1993), copyright by ESO

Gadallah et al. 2012; Jäger et al. 2016; Dartois et al. 2017). The influence of temperature has been investigated a bit more intensely, see (Potapov and Bouwman 2022) for a review.

Absence of interest to changes in porosity and surface reactivity of dust grains due to space weathering was, probably, due to the popularity of the compact dust model described in Sect. 1, considering that dust has no or very limited influence on the physico-chemical processes on its surface. However, in the alternative model (fractal dust) these changes may influence and, in some cases, define the efficiency of such processes as well as optical properties of dust grains. The latter may dramatically influence interpretation of astronomical spectra. Thus, new results on the influence of space weathering on the optical, morphological and chemical properties of analogs of cosmic dust grains would provide an important piece of puzzle of the evolution of cosmic dust grains in astrophysical environments.

The results on thermal annealing of dust grains are relevant to warm/hot environments, such as inner parts of protostellar envelopes and planet-forming disks and the atmospheres of exoplanets. As for exoplanet atmospheres, simulations have shown that the porosity of particles in atmospheric clouds may affect the structure and composition of clouds and has to be taken into account (Samra et al. 2020). Influence of high temperatures on the growth of grains and on the porosity, chemical activity and optical properties of grain aggregates are open questions representing doorways to future research.

Fig. 16 Examples of aggregates observed in the dust jet extracted from the turbomolecular pump. The monomers are monodisperse SiO_2 spheres with a diameter of $1.9\ \mu\text{m}$. Image reproduced with permission from Wurm and Blum (1998), copyright by Elsevier



4.2 Dust growth in protoplanetary disks

In protostellar envelopes and planet-forming disks, grains continue to grow. The first stages of dust coagulation in disks lead to the formation of fractal aggregates of up to at least several μm in size. Laboratory collisional studies (Wurm and Blum 1998; Blum and Wurm 2000; Krause and Blum 2004; Blum and Wurm 2008; Güttler et al. 2010) and Blum (2018) for a review corresponding to the initial stage of dust aggregation showed that aggregation of micrometer-sized grain monomers leads to the formation of fluffy particles with a fractal dimension of 1–2 and the porosity of up to more than 90%. An example of porous grain aggregates formed through collisions is shown in Fig. 16. In those collisional experiments (Wurm and Blum 1998), SiO_2 grains sedimented with constant velocity in a tube-shaped vacuum chamber forming a confined jet of high number density of grains. A similar result, highly porous aggregates (volume filling factor 0.11 ± 0.01) was obtained in collisional experiments on μm -sized water ice particles (Gundlach et al. 2011). In those experiments, the particles and their aggregates were produced by spraying dispersed water droplets into a dry, cold gas (nitrogen) environment with subsequent sedimentation of the particles. The results of experimental collisional studies are mainly in agreement with the results of modeling of grain growth in protoplanetary disks also showing high porosity of dust aggregates at the first stage of dust coagulation (Wada et al. 2008, 2009; Suyama et al. 2008; Okuzumi et al. 2012; Wada et al. 2013; Kempf et al. 1999; Okuzumi et al. 2009; Wada et al. 2007; Ormel et al. 2007).

Although the initial growth leads to the formation of fluffy, open-structured aggregates, their later porosity evolution is rather controversial if such a structure is maintained as they grow to (sub)millimeter sizes. This is mainly because collisional

strength of aggregates, which depends on the monomer size and composition as well as porosity of aggregates, and the impact velocity are still highly uncertain in a disk environment (Blum 2018). One of the crucial factors for the porosity of grain aggregates created by collisions can be the impact speed. Depending on the impact speed, collisions result in sticking without deformation (hit-and-stick) for low velocities, sticking with deformation/compaction or bouncing of grain aggregates for moderate velocities, and catastrophic disruption (fragmentation) for higher velocities (Güttler et al. 2010). Usually, the collision speed increases with the aggregate size, and the hit-and-stick tend to happen in the first stage, whereas the latter two happen in later stages of dust aggregation. Figure 17 taken from Kataoka et al. (2013) shows evolution of the internal density of dust aggregates during their growth, assuming perfect sticking (no bouncing and no fragmentation). The results confirm that dust particles can evolve into highly porous aggregates at the first hit-and-stick stage (porosity reaching up to $\sim 99.99\%$) and stay fractal even in the collisional compression stage, as suggested from MD simulations (Suyama et al. 2008; Wada et al. 2009). In this scenario, dust aggregation can directly lead to the formation of planetesimals without invoking any hydrodynamic clumping of solid particles (Okuzumi et al. 2012; Kataoka et al. 2013; Arakawa and Nakamoto 2016; Homma and Nakamoto 2018; Kobayashi and Tanaka 2021), although gravitational instability could be triggered during the fluffy growth (Michikoshi and Kokubo 2017). There are mechanisms that are thought to inhibit fluffy growth, such as bouncing/efficient compaction/fragmentation/erosion upon collision (e.g., Zsom et al. 2010; Krijt et al. 2015, 2016; Tanaka et al. 2023; Lorek et al. 2018; Estrada et al. 2022; Estrada and Umurhan 2023; Michoulier et al. 2024). When bouncing collision occurs, the porosity is reduced to $\sim 60\%$ after sequential bouncing collisions (Weidling et al. 2009; Zsom et al. 2010). Note that there is a debate if fluffy aggregates are subject to bouncing collisions between numerical and laboratory studies (Wada et al. 2011; Seizinger and Kley 2013; Kothe et al. 2013; Brisset et al. 2017), although more recently, Arakawa et al. (2023) pointed out that not only porosity but also aggregate size affects the probability of bouncing, which might explain why numerical and experimental studies show apparently different conclusions about bouncing. Another effect that could potentially be important is collisional fragmentation (Dominik and Tielens 1997; Paszun and Dominik 2009; Wada et al. 2009, 2013; Hasegawa et al. 2021). If collisional fragmentation happens, we would not be able to complete the proposed journey to icy planetesimals.

In summary, although it is widely accepted that growing aggregates have some porosity, but it remains rather inconclusive how much porosity they will have due to uncertainties in a number of conditions such as adhesion energy (surface composition) of the monomers, size of the monomers, and the impact velocity. With that said, disk observations now start to tell us about porosity, as we discussed in Sect. 3.3.1. Those observational studies suggest that aggregates may have a fluffy structure at least when they are micron sizes (see Fig. 10), but (sub)millimeter-sized aggregates seem to have a porosity less than $\sim 99\%$. The occurrence of collisional fragmentation has been favored from disk observations as well (Okuzumi and Tazaki 2019; Jiang et al. 2024). However, it is worth pointing out that those (sub)millimeter-sized aggregates might be the secondary origin, that is, they are not primordial aggregates of interstellar grains,

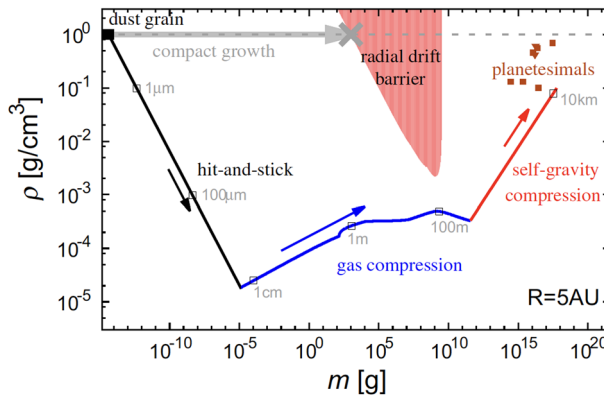


Fig. 17 Pathways in the planetesimal formation in the minimum mass solar nebula model. The gray line shows the constant density evolutionary track, which corresponds to the compact growth. The black, green, blue, and red lines are the evolutionary track through dust coagulation via fluffy aggregates. Each line represents different mechanisms of dust coagulation, which are hit-and-stick, gas compression, and self-gravity compression. The red shaded region represents where the radial drift timescale is less than the growth timescale, which is equivalent to radial-drift region. The brown squares indicate the properties of comets, and the triangles represent their upper limit. The radii of dust aggregates for 1 μm , 1 cm, 1 m, 100 m, and 10 km are also written. Image reproduced with permission from Kataoka et al. (2013), copyright by ESO

but those produced by collisions of massive bodies like planetesimals, as proposed in Tatsuuma et al. (2024).

4.3 Cosmic dust materials

The choice of materials for laboratory experiments is guided by knowledge from estimates of the elemental inventory in space derived from a combination of Big Bang and stellar nucleosynthesis and tempered by observations of materials in a range of spectroscopic windows. Dorschner (2010) in Henning (2010) nicely describes the historical development of our understanding of dust mineralogy in linking spectroscopic observations (e.g., the 217 nm bump in the interstellar extinction curve commonly attributed to presence of graphitic grains, and the observations of silicate vibrations in the infrared consistent with both amorphous and crystalline materials) with the composition of meteorites as they represent an end point for processing of carbonaceous and siliceous materials through the many phases of star formation and ending in cometary environments (Rubin and Ma 2017). Ott (2010), in the same volume, highlights the discovery of fossil grains in primitive meteorites as representative of the parent dust cloud from which the Solar System formed.

From this discussion, we can establish an inventory of likely materials on which to base further laboratory exploration. This is presented in Table 1. It is interesting to note that none of these materials is known naturally to be micro- or mesoporous. Porosity in these materials is most likely to be associated with amorphization of the material and surface heterogeneity. However, physico-chemical alteration in space environments can produce materials that exhibit such porosity, e.g., carbon nanotubes and related

Table 1 Materials inventory of the major minerals for dust models in laboratory astrophysics experiments based on Table 1 from Ott (2010). This list ignores the metallic elements also likely to be present

Carbonaceous materials

Amorphous carbon

Graphite

Diamond

PAHs

Fullerenes

Silicon derivatives

Silicon carbide (SiC; carborundum)

Silicon nitride (Si₃N₄)

Oxides

Silicon dioxide (SiO₂, silica)

Aluminum oxide (Al₂O₃; sapphire)

Magnesium aluminum oxide (MgAl₂O₄, spinel)

Silicates

(Fe,Mg)₂SiO₄, Olivine

(Fe,Mg)₂Si₂O₆, Pyroxene

materials, or aluminosilicates (zeolites). The latter are well-known terrestrially as size- and shape-selective industrial catalysts.

4.4 Atomistic modeling of nanoporous materials

Attempts to model the effects of dust grain porosity typically assume that a general physical understanding of such systems can be obtained without consideration of the atomistic level structure and properties. Following this assumption, porous dust models are typically created using aggregates of monomers with sizes ranging between a few nanometers and a few microns as discussed in Sect. 4.1. Such studies have provided estimates of how porosity could affect dust extinction (Sect. 2) and have simulated the evolution of porosity in dust aggregates in various astrophysical environments (Sect. 3). Here, we focus on models of porous systems in which atoms are the fundamental building blocks. Such atomistic level modeling is typically applied to systems possessing pore sizes smaller than 10 nm, where it can provide a uniquely detailed perspective.

Although there are currently very few atomistic modeling studies that have been directly applied to astronomical dust, such methods have been used for decades to understand technologically important porous materials. As astronomically relevant examples, we refer to studies on nanoporous silica-based materials to illustrate how atomistic modeling can provide otherwise unobtainable physico-chemical insights. Atomistic modeling initially involves the bottom-up atom-by-atom construction of realistic porous structures. Subsequently, these modeling methods can be used to theoretically characterize the physico-chemical properties of such systems, such as: atomic-scale structural features (e.g., detailed morphology of pores and surfaces), spectroscopic characteristics (e.g., IR and UV spectra), and phenomena occurring within pores (e.g., adsorption and diffusion of chemical species).

As previously mentioned in this review, the porosity of cosmic dust remains largely unexplored, and its atomistic level characterization is even less understood. Therefore, we provide a brief background to atomistic modeling methods applied to porous silica-based materials, which could potentially be applied to the structural modeling of porous cosmic dust. We note that, although the typical pore sizes in cosmic dust are still unknown, most reported atomistic modeling studies of porous silicas have focused on materials with pore diameters < 10 nm due to their industrial importance.

4.4.1 Atomistic modeling methods

Firstly, we briefly introduce the most commonly employed methods to model materials at an atomistic level. The most computationally efficient methods are based on classical molecular mechanics (MM), for which current state-of-the-art simulations can treat systems possessing up to a few million atoms. MM methods use interatomic potentials (IPs), also known as force fields, to calculate the energy, structure, and properties of the system, neglecting the electrons of the system. Typically, IPs consist of a set of analytical functions that have been empirically parameterized to represent different atomic-level interactions (e.g., chemical bonds, electrostatics, van der Waals). Some IPs also incorporate extended parameter sets to describe the energetics of chemical reactions [e.g., ReaxFF (Duin et al. 2003; Pitman and van Duin 2012)]. Well-parameterized IPs are available for describing the interatomic interactions in some astronomically relevant dust materials such as silicates (Pedone et al. 2022) and water ice (González and Abascal 2011; Karssemeijer et al. 2014a,b). However, for more chemically complex systems (e.g., numerous different molecular species interacting within a porous material) accurate parameterization is more difficult and suitable IPs are often lacking. As such, the applicability of MM modeling is limited to systems for which IP parameters have been developed. We note that, as an alternative to using empirically determined parameters, machine learning is now being widely used to develop more accurate and general IPs which are starting to be used for modeling astronomical dust (Tang et al. 2023). Even with such advances, the fundamental limitation of MM modeling is that it does not explicitly describe electronic degrees of freedom. As such, MM modeling cannot be reliably applied in scenarios where a detailed understanding of electronic effects is important (e.g., astrochemical reactions, UV adsorption spectra).

To overcome the electronic limitations of MM methods, one can use quantum mechanical (QM) methods. QM methods are often referred to as first principles methods, as they account for the electronic structure of the system from solving the electronic Schrödinger equation. Among the various available QM modeling methodologies, density functional theory (DFT) is the most popular and widely used due to its relatively high computational efficiency. This efficiency derives from computing the properties of the system via a function of the electronic density (i.e., a density functional) rather than explicitly from the wavefunction. As an accurate general description of this functional for arbitrary systems of atoms is still unknown, hundreds of DFT functionals have been developed. In practice, only a few DFT functionals are commonly used [e.g., B3LYP (Becke 1993; Lee et al. 1988), PBE (Perdew et al. 1996)], which generally provide a reasonably accurate description of the electronic structure

and related properties for a wide range of molecular and solid-state systems. Generally, DFT methods provide a more accurate and fuller description of a system than IP-based MM methods.

Despite the computational effectiveness of DFT methods, such simulations are limited by the size of the systems they can handle. Currently, with the aid of high-performance computing and massively parallel calculations, such calculations are still limited to models containing up to a few thousand atoms. This constraint places much stronger size limits on the applicability of DFT modeling to treat porous dust systems compared to MM methods. As a compromise between DFT and MM methods, semiempirical methods offer a relatively computationally inexpensive QM-based approach to overcome the size limitations of DFT. Semiempirical methods are derived from pure QM methods but incorporate various approximations (e.g., omission of bi-electronic integrals) and empirical parameters to avoid costly computations. Due to these simplifications and parameterizations, semiempirical methods are faster than their QM counterparts, enabling the treatment of large chemical systems that are otherwise untenable with pure QM methods. However, similar to MM methodologies, the accuracy of semiempirical methods heavily depends on the suitability of the parameterization for the specific case under study. There are various semiempirical methods, but the most frequently used are those based on tight-binding approaches, which derive from DFT such as SCC-DFTB (Elstner et al. 1998). Recently, for example, Grimme and coworkers developed the GFN-xTB family (Bannwarth et al. 2021), a set of tight binding-based methods that model covalent H-bond, and dispersion interactions with improved accuracy, and are parameterized for almost the entire periodic table of elements (up to $Z = 86$).

Apart from the choice of calculation method, there are two main system-based approaches to atomistically modeling materials: (i) the periodic system approach and (ii) the cluster approach (Rimola et al. 2021). Periodic systems involve a repeating unit cell defined by lattice parameters (i.e., the cell lengths along the three spatial directions and the angles between them) to create a periodic system that extends infinitely by applying periodic boundary conditions (PBC). For bulk materials, this repetition is three dimensional (3D), while for surfaces, it is two dimensional (2D). In contrast, the cluster approach models the material as a discrete finite system without considering PBC. Figure 18 shows examples of these two approaches as applied to an extended silicate crystal and an amorphous silicate nanoparticle (Zamirri et al. 2019).

The simplest way to approximately model a porous material at the atomic scale is by using an extended (“open”) surface model. Here, for suitably large pores, we can assume that the local properties of a porous wall are similar to those of an isolated extended surface in vacuum. For example, both extended silica surfaces and the interior surfaces of porous silica have exposed silanol (Si-OH) groups, which largely determine their adsorptive properties (Rimola et al. 2013). Therefore, an extended silica surface model with an appropriate silanol density can also serve as a model for the Si-OH covered interior pore surface of a mesoporous silica material (Ugliengo et al. 2008; Delle Piane et al. 2014b). Within this framework, open surfaces can be modeled using either a cluster or a periodic approach. Clearly, however, open surfaces and real surfaces inside a porous material are not the same, and this approximation ignores several potentially important factors. For example, modeling a porous material with

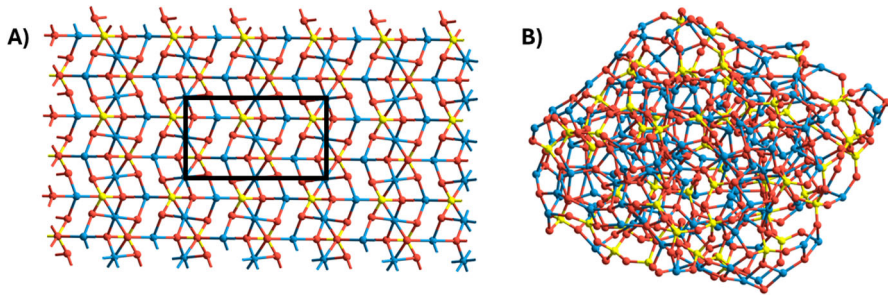


Fig. 18 Atomistically detailed structural models for forsterite (Mg_2SiO_4). **A** A periodic approach, modeling crystalline forsterite (repeat unit cell outlined in black), and **B** a cluster approach, modeling a finite amorphous system. Atom color key: Si – yellow, Mg – blue, O – red

an extended surface neglects the long-range influence of the surrounding pores and the local effects of an enclosed pore surface. Such issues are particularly important in phenomena like adsorption and diffusion of chemical species, which become increasingly confined as the pore size becomes smaller. To address the approximations of an open surface approach, more accurate atomistic models explicitly account for the pore structure. Below we divide our discussion of such nanoporous models into two parts, following the conventional classification of porous silica-based materials based on pore diameter (d): (i) mesoporous materials with $d = 2 - 50$ nm, and (ii) microporous materials with $d < 2$ nm. In both cases, we briefly discuss possible physico-chemical properties of these systems that could be astronomically relevant.

4.4.2 Mesoporous models

Mesopores (with $d \geq 2$ nm) are large compared to the dimensions of most small molecules likely to be encountered in astrophysical environments (e.g., H_2 , CO, H_2O , CH_3OH). Such species can thus diffuse through such materials relatively unimpeded, at least as far as pore size is concerned. During diffusion, molecules will repeatedly collide with the interior pore walls, likely leading to eventual adsorption at interior pore wall sites where they interact the most strongly. On Earth, water molecules tend to strongly interact with the surfaces of amorphous silica where they dissociate and form surface bound hydroxyl groups (i.e., silanol groups: Si-OH). As such, the interior pore walls of laboratory-synthesized mesoporous silicas are covered with silanol groups. For mesoporous silicate dust particles, we may also expect interior silanols, but from arising from reactions with hydrogen and atomic oxygen (Jones and Williams 1984), rather than from water molecules. The presence of such strongly bound Si-OH groups on extraterrestrial silicates has been confirmed in cometary material (Mennella et al. 2020) and in lunar silicates (Zeller et al. 1966). Chemisorbed hydroxyl groups are susceptible to desorption via interaction with strong UV radiation (Imai et al. 1996). The coverage of silanol groups on the exterior surface of silicate dust grains in the diffuse ISM is thus likely to be low. However, silanol groups within a mesoporous silicate material would be more protected from external radiation and would be more likely to persist at higher coverages.

Experimentally synthesized stable mesoporous silica materials usually possess relatively dense amorphous pore walls. Models of such amorphous porous materials can be derived from an initially non-porous model (typically a dense crystalline phase) which is amorphized using molecular dynamics (MD) simulations through a melt/quench scheme (Ugliengo et al. 2008; Williams et al. 2016; Delle Piane et al. 2018). MD solves Newton's equations of motion for atoms, thus providing a time-dependent description of the system's atomistic dynamic evolution. Performing MD simulations at high temperatures on an initially crystalline system induces the atoms to disorder (i.e. induces melting). Subsequent rapid decrease of the simulation temperature quenches the system while maintaining the disordered atomic positions.

To generate atomistic models of mesoporous materials one can then remove atoms from the non-porous dense analogue to create pore spaces with a desired size and shape. Here, it is crucial to proceed cautiously during atom removal to ensure structurally stable and chemically sound structures. For example, for ionic materials (e.g., silicates) stoichiometry and electroneutrality must be maintained (Martínez-González et al. 2018), while for molecular materials (e.g., water), the chemical bonds of the molecular moieties should not be broken (Zamirri et al. 2018; Ferrero et al. 2023). For example, in the case of mesoporous silica this atom removal process often results in under-coordinated oxygen atoms that can be saturated with hydrogen atoms to form Si-OH groups. Note, that one can also choose to add extra silanol groups to the interior pore surfaces to create mesoporous models with desired Si-OH surface coverages. Finally, the as-generated porous system is structurally relaxed by minimizing the forces on all atoms and the stress on the unit cell. Figure 19 illustrates the computational procedure to generate a realistic atomistic model for a mesoporous amorphous silica from periodic cell extracted from crystalline α -quartz following: (i) amorphization of the initial non-porous crystalline structure through melt/quench MD simulations, (ii) removal of atoms to create pore spaces, and (iii) optimization of the system to achieve a structurally relaxed (stable) structure. The advantage of using a periodic approach when applying this procedure is that application of PBC to a suitable of the final cell with a single pore intrinsically generates a perfectly regular array of pores. Figure 20 shows the result of applying PBC to a porous unit cell (outlined in blue) to generate an array of pores to represent an extended mesoporous silica material (Ugliengo et al. 2008).

Use of such models (see Fig. 20) can help in providing detailed atomic scale insights into the characteristic IR response of Si-OH groups within mesoporous silicates (Ugliengo et al. 2008) and how small molecules (e.g., H_2O) diffuse through such a Si-OH covered pore systems (Coasne and Ugliengo 2012). Much experimental work has focused on the behavior of water in mesoporous silicas, where the combined roles of nanoporosity and surface Si-OH groups can be significant (Saliba et al. 2016). In such systems, nanoscale confinement leads to a decrease in the melting/freezing point temperature, density, and surface tension of water (Knight et al. 2019) which could have implications for astrochemical ice formation/stability in mesoporous grains. These physico-chemical changes are fundamentally linked to the underlying changes in hydrogen bonding in these systems (Musat et al. 2008; Le Caër et al. 2011). Atomistic modelling of water-filled mesoporous silicas with selected pore sizes and Si-OH coverages and can provide highly detailed insights into the IR spectroscopic shifts

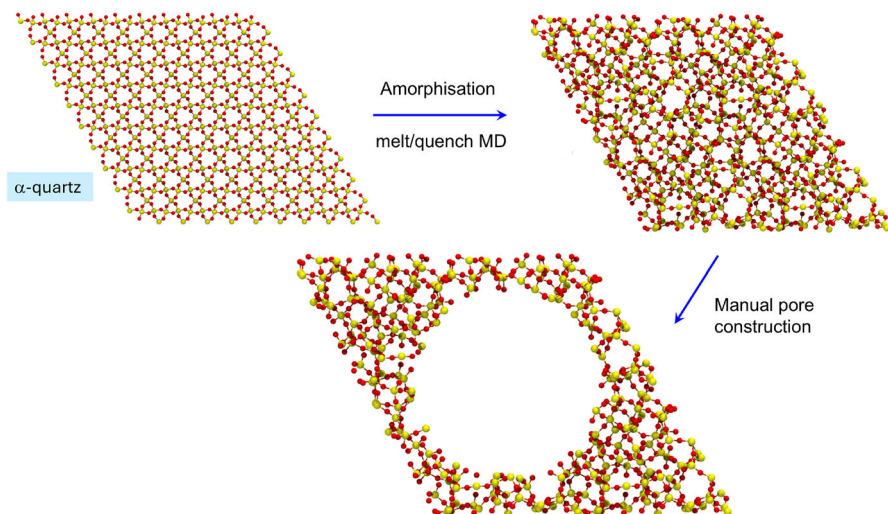


Fig. 19 Atomistic modeling of a porous system, using the transformation from a periodic cell of crystalline α -quartz to a cell of an amorphous porous silica containing one mesopore. The first step consists in the amorphization of the initially crystalline structure by molecular dynamics (MD) simulations following a high temperature melt and low temperature quench process. In the second step atoms are removed to construct a pore. Finally, the system is structurally relaxed. Atom color key: Si – yellow, O – red

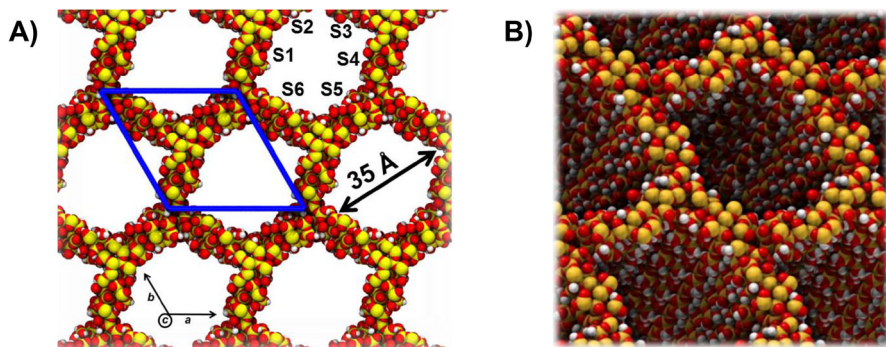


Fig. 20 **A** Atomistic model of a mesoporous silica after addition of Si-OH groups and application of PBC. The unit cell is outlined in blue. The pore diameter is also highlighted (35 Å), along with potential binding sites (S1–S6). **B** Three-dimensional view of the atomistic mesoporous model. Atom color key: Si – yellow, O – red, H – white

associated with such changes (Senanayake et al. 2021; Burris et al. 2016), which may be observationally detectable.

4.4.3 Microporous models

Microporosity refers to smallest pore sizes ($d < 2$ nm), which can be of the order of the sizes of small molecules. In principle, one can generate microporous models by following the strategy outlined for mesoporous models, by removing atoms from

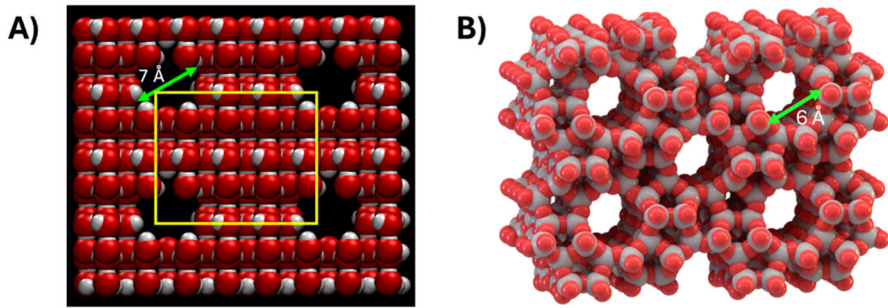


Fig. 21 **A** Microporous water ice (oxygen – red, hydrogen – white) with pores generated by removing water molecules from the crystalline P-ice phase. The pore diameter is also highlighted (7 Å) and the unit cell is shown in yellow. **B** A crystalline microporous silica zeolite (oxygen – red, silicon – gray) with pore diameter indicated

a dense precursor material. Figure 21A illustrates this process for microporous water ice, in which small pores are generated by removing water molecules from a compact crystalline ice phase. For silicates, many microporous solids are known which have complex crystalline structures that are distinct from any dense phase. These materials, known as zeolites (see Fig. 21B), have been widely studied by atomistic modeling methods due to their technological applications involving adsorption, diffusion and separation of small molecules (Smit 2008; Keil et al. 2000). Different zeolites have distinct degrees of porosity made up from micropores and channels with characteristic sizes and topologies. These, often subtle, differences can have a relatively large influence on the ease with which different small molecules diffuse through these materials.

The smallest micropore sizes ($d < 0.5$ nm) can be similar in size to numerous astronomically abundant small molecules such as H_2 , CO and H_2O . Here, we are in the highly confined regime where even a single molecules can significantly interact with the pore walls in multiple directions. Simple atomistic scale models of such highly confined molecules can rationalize how the size of the micropores with respect to the confined molecules can contribute to differences in diffusion and adsorption. Such models, for example, predict that the physisorption of small molecules inside small micropores can be up to eight times larger than that on the corresponding flat surface (Derouane et al. 1988). For such situations, detailed atomistic modeling of confined H_2 molecules has also shown that the flexibility of the silicate structure is essential for facilitating inter pore diffusion (van den Berg et al. 2004b). As such, the structural response of the microporous system needs to be taken into account for understanding diffusion rates of highly confined molecular species (van den Berg et al. 2004b).

Although studies of zeolites can provide some insights of astronomical relevance, these crystalline silica-based materials with well-ordered micropore systems are unlike the disordered multiscale porosity likely exhibited by porous silicate dust (e.g. as in IDPs). An alternative method for constructing atomistic models of porous materials is through aggregation. In principle, aggregation can bring together particles of many different sizes to form porous fractal aggregates in which a hierarchy of pore sizes can exist. Here, we consider the formation of a microporous silicate from the aggregation of ultrasmall nanosilicate grains (Bromley 2024). Nanosilicates with diameter less

than 3 nm are likely to be produced in high numbers in the ISM due to processing of larger grains by SNe shockwaves (Jones et al. 1996). Although it has been estimated that nanosilicates account for a relatively small mass fraction of available silicon (approximately 5–10% (Hensley and Draine 2017; Li and Draine 2001)) these dust species are so small that they would be numerically much more abundant than larger dust species.

Nanosilicates could eventually potentially aggregate in more protected translucent or molecular cloud environments (Krasnokutski et al. 2014). Fractal nanosilicate aggregates may also be formed during circumstellar dust nucleation and growth (Kimura et al. 2022). We also note that laboratory-made fractal aggregates of nano-sized silicate particles can reproduce observed IR spectra of silicate dust (Ishizuka et al. 2015). We expect that the astrochemical and astrophysical impact of microporosity in nanosilicate aggregates to have some similarities with those observed for microporous silicate zeolites.

The process of aggregation can be approximately modeled by placing an isolated nanosilicate in a repeat simulation cell using PBC, and then gradually reducing the unit cell parameters. As the unit cell size is reduced, nanosilicate structures in adjacent cells start to interact with each other and form bonds. Continuation of this process, with structural optimization at each cell size reduction step, eventually creates a three-dimensional microporous structure. The upper part of Fig. 22 illustrates this procedure in which an olivinic (Mg_2SiO_4)₃ nanosilicate is used to produce a periodic microporous silicate model (Rimola and Bromley 2021). In the lower part of Fig. 22 the calculated IR spectra are shown for each respective step of the aggregation process. Observed IR spectra of silicate grain populations are typically dominated by two broad features centred at around 9.8 μm (i.e., 1020 cm^{-1}) and 18 μm (i.e., 556 cm^{-1}) corresponding to Si-O stretching and O-Si-O bending vibrational modes, respectively. Due to their ultrasmall size and non-bulk-like atomistic structures, nanosilicate grains are predicted to have characteristically different IR spectra. Typically, the IR spectra of nanosilicates exhibit more peaks with frequencies that are shifted with respect to the IR spectra of larger amorphous grains (Escatllar et al. 2019; Zeegers et al. 2023). Such a spectrum can be seen in the lower right of Fig. 22. Upon aggregation into a microporous silicate the IR spectra evolve towards a more typical silicate spectrum. However, even when fully aggregated, the IR spectrum still retains some fine structure which may indicate that nanoporous silicates could be observationally distinguished from denser silicate grains. Clearly, further atomistic modeling and laboratory experiments are required to consolidate these preliminary findings.

4.5 Astrochemical modeling

Much of the interest in porosity in astrochemical models has been driven by laboratory studies of ice composition and structure, but there are shared features between the ice and grain porosity scenarios, as well as between the models used to simulate them. Awad et al. (2005) developed a model for chemistry on an ice structure with crack-like porous features; the model was devised to replicate laboratory experiments, such that CO molecules in a CO–H₂O ice mixture would be partially protected from reactive

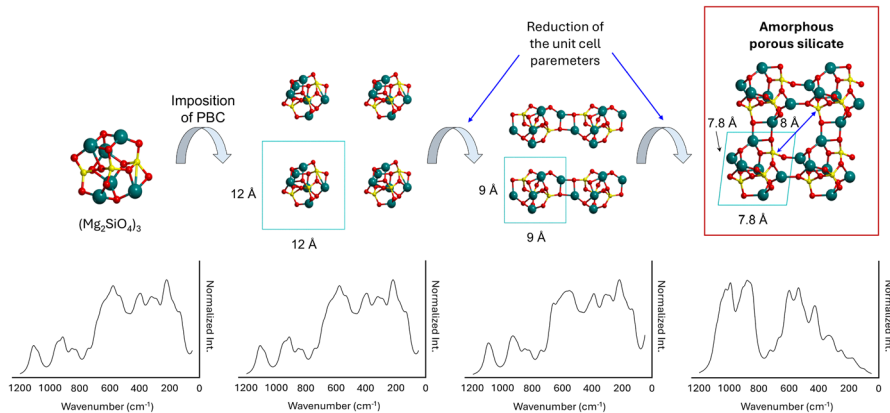


Fig. 22 Top: Atomistic modeling of an aggregation-induced microporous silicate. From left to right: A $(\text{Mg}_2\text{SiO}_4)_3$ nanosilicate is selected. PBC are imposed by introducing the isolated nanosilicate into a $12 \times 12 \times 12 \text{ \AA}$ cubic unit cell. Reducing the unit cell parameters to $9 \times 9 \times 9 \text{ \AA}$ and optimizing the structure induces an initial interaction between clusters of adjacent unit cells. The process of cell size reduction and structural optimization is stopped once a minimum energy is reached. In this case a microporous silicate structure with $8 \text{ \AA}$ diameter micropores is obtained. The unit cell at each step is shown in blue. Atom color key: Si – yellow, Mg – blue, O – red. Bottom: Simulated IR spectrum corresponding to each structure throughout the aggregation process. For further details see Rimola and Bromley (2021)

H atoms adsorbing onto the surface. The competition between efficient production of H_2 on the outer ice surface via H recombination, and the more limited penetration of H into the cracks, allowed some of the CO to avoid conversion to H_2CO or CH_3OH .

Perets and Biham (2006) constructed the first rate equation-based chemical model to simulate grain porosity explicitly, working under the hypothesis that porosity could provide the higher rate of grain-surface H_2 production deemed necessary to explain H_2 abundances in photon-dominated regions (PDRs). The model considered only the grain-surface chemistry, and was limited to the $\text{H} + \text{H} \rightarrow \text{H}_2$ system under steady-state conditions. Diffusive hydrogen was allowed to exist in two locations; the external grain surface that was coupled to the gas phase via adsorption and desorption; and an internal system of pores accessible via diffusion through “edge” sites (making up 5% of external binding sites) that linked the internal and external surfaces. While both H and H_2 could pass through the edge sites, desorption within the pores was not allowed, on the assumption that such species would be re-adsorbed on an inner wall. Thus, H atoms in particular could be retained within the pores at greater abundance than would be otherwise expected, increasing their conversion to H_2 . Different levels of porosity, expressed as the ratio of internal to external binding sites were tested, ranging from 10–1000. The effect of the inclusion of porosity in the model was to extend the temperatures at which efficient H_2 production could be produced (although not to high enough temperatures to explain efficient H_2 production in PDRs).

The GRAINOBLE model by Taquet et al. (2012) is the only rate equation-based treatment of a full gas-grain interstellar chemical network to consider porous structures. Technically, this model apparently considered porosity in the grains as well as in the ice mantles, but was more focused on the latter. Their treatment of grain-surface

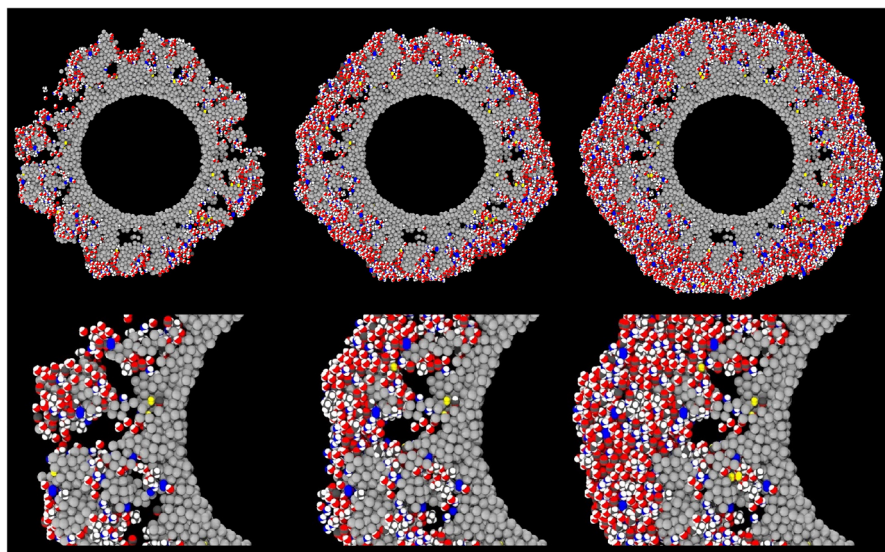


Fig. 23 Cross-sectional images produced from chemical simulations on a $100 \text{ \AA}$ radius porous grain, using the off-lattice Monte Carlo kinetics model MIMICK. Results at three moments in the early stages of ice build-up are shown; lower panels represent a zoomed-in view of a section of each upper panel. Gray spheres represent the carbon atoms composing the dust grain. The solid inner region of the grain was removed to simplify the calculations; this inner void plays no part in the model. Grain-surface atoms are represented by white (H), red (O), black (C) and blue (N) spheres. Molecules are similarly represented as collections of such atoms in appropriate structures. H_2 molecules are highlighted in yellow. Image reproduced from Christianson and Garrod (2021), copyright by the author(s)

chemistry employed a so-called multilayer model, of a type similar to the one first proposed by Hasegawa and Herbst (1993), allowing active chemistry only in the upper layer of the ice (or initially on the bare grain surface), with material beneath being stored as layers of bulk ice. As with Perets and Biham (2006), the porous structures could be entered from the surface via edge sites; however, whereas Perets and Biham (2006) considered an expansive porous structure much larger than the outer surface, Taquet et al. (2012) envisioned a system of pores whose available reactive surface was defined to be less than that of the outer surface layer. While the model prohibited pore-bound species from desorbing, the generically small size of each individual pore surface (9 binding sites) would make the trapping effect much weaker, in comparison with that seen in Perets & Biham's model. Furthermore, the Taquet model rendered trapped pore material chemically inert once it was incorporated into the bulk ice. This model therefore likely says little about the effects of *grain* porosity in particular. The recent Monte Carlo kinetics model by Song et al. (2024) also concentrates exclusively on the effects of ice porosity.

The models by Christianson and Garrod (2021) currently represent the only attempt to simulate explicitly the grain-surface chemistry that would occur on a porous interstellar grain. Their MIMICK model simulates surface chemical activity using an off-lattice microscopic Monte Carlo kinetics technique in which the positions of atoms and molecules are calculated at run time, based on the local surface potentials, which

also govern the mobilities of those species on the surface. The model can simulate chemistry on any pre-defined 3-D surface structure. Christianson and Garrod (2021) created a selection of porous and non-porous grains by first producing a spherical, carbonaceous grain (with amorphous surface structure), and then randomly depositing further grain atoms using a hit-and-stick method. The result was a broadly spherical grain with an open porous structure. Gas-phase CO molecules and H, C, O and N atoms (with fixed total budget) were then deposited onto the surface over periods on the order of 10^4 – 10^5 yr. These species and their chemical products were allowed to diffuse, react and thermally desorb. The desorption treatment included the explicit calculation of the trajectory of the ejected species, allowing it to re-adsorb onto any surface obstructing its path, and thus allowing the more volatile species in the model to be retained more easily within the pores than on the outer surface.

Cross-sections through one of the porous grains at three periods during the build-up of ice are illustrated in Fig. 23. In some areas, the grain-pore structures are seen not to become completely filled with molecules, but are nevertheless closed over by the growing ice mantle, leaving voids within the deeper regions. With the formation of a thick ice mantle, the porous structure was lost and the grain took on a regular and roughly spherical morphology.

The overall chemical composition of the ice was found not to vary substantially between the porous and non-porous grain cases; nor indeed was the production of the volatile H₂ molecule much altered. The main effect of the porous structure was found instead to be the trapping of H₂. This was caused by a combination of (i) porous structures that could be enclosed by the growing ice, and (ii) the enhanced binding energies experienced by H₂ molecules when encountering larger species (such as water) or highly irregular microscopic surface structures in the pores. The trapped H₂ did not need to be formed inside the pores; the porous structures acted rather as a trap for otherwise mobile, volatile species formed elsewhere. The authors posited that such an effect would be larger if gas-phase H₂ adsorption were considered (which is found to be a substantial computational hurdle in models of this kind). It was also speculated that other volatile, and largely non-reactive, species such as atomic He could become trapped deep within the ices in a similar fashion.

5 Impact and potential implications of porosity

5.1 Atomistic and astrochemical modeling

5.1.1 Calculating properties of nanoporous systems

Once an atomistic structural model has been generated, its physicochemical properties can be theoretically characterized. Regarding observational astronomy, spectroscopic properties are probably most relevant. Here, atomistic modeling can simulate a range of spectroscopies (e.g., IR, UV, microwave) with varying degrees of accuracy which can be compared with observations. The significance of using atomistic modeling in this way is that it directly links the spectral properties to an atomic-level (and/or quantum-level) description of the system in question. For example, using the atomistic

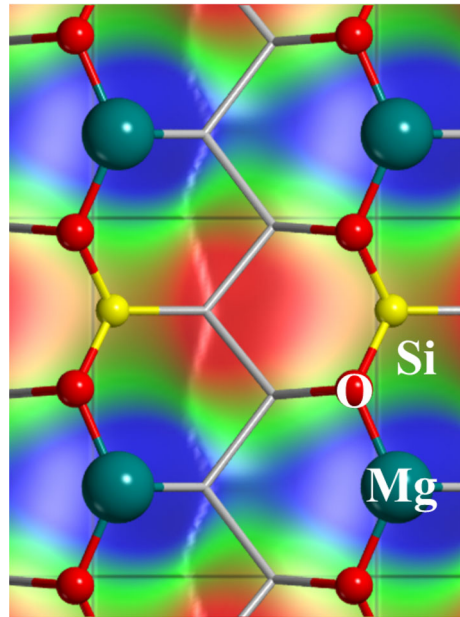
structure of a silicate dust grain we can calculate the atomic displacements associated with all vibrational normal modes and their associated dipolar variations, and thereby simulate IR spectra. An example of this type of calculation is shown in Fig. 22. By analyzing the detailed structures associated with the simulated spectra and comparing these spectra with the observed IR spectra, we can infer possible characteristics of the astronomical dust under study (Zamirri et al. 2019; Zeegers et al. 2023). We note that other non-observational spectroscopic properties, such as Raman and solid-state NMR spectra, can also be simulated using atomistic modeling (Delle Piane et al. 2014a; Gignone et al. 2015). Here, simulated data can be compared with data from laboratory-based experimental characterization (e.g., of porous dust analogs, Dib et al. 2021).

Besides spectroscopy, atomistic modeling is also able to simulate the adsorption and diffusion of chemical species inside porous materials. One fundamental property of great interest in astrochemistry is how strongly molecules interact with dust grain surfaces (i.e., molecular binding energies – BEs, Minissale et al. 2022). The first step in calculating the BE of an adsorbed molecule is to consider the adsorption of a single molecule. The high surface area of interior pore walls possesses several potential binding sites with varying energetic stabilities and, consequently, different BEs. Therefore, detailed sampling of the pore walls to cover all possible binding sites is of paramount importance to obtain good statistical averages. Identification of likely strong adsorption sites on pore walls can make use of electrostatic potential maps (EPMs). EPMs highlight regions of positive and negative electrostatic potentials, indicating where interactions with negative and positive charges would be strongest, respectively. Figure 24 shows the EPM of a crystalline forsterite (010) surface (Navarro-Ruiz et al. 2014), in which the Mg^{2+} cations are associated with regions of positive electrostatic potential, while O^{2-} anions are associated with a negative electrostatic potential. These maps are useful for identifying binding sites that follow the electrostatic complementarity principle, such as ion/dipole interactions (e.g., between a Mg^{2+} cation of the silicate surface and a negatively polarised O atom of a molecular adsorbate).

For small pore sizes, sampling of binding sites can be done manually since the number is expected to be limited. However, for large pore sizes, manual sampling can be overwhelming, and automated procedures can facilitate the task. Such automated procedures are currently implemented in programs for sampling binding sites of external surfaces of interstellar interest, such as the ACO-FROST program (Germain et al. 2022) for sampling large H_2O ice cluster models and the Polycleaver program (Mates-Torres and Rimola 2024) for sampling extended periodic ionic surfaces (see Fig. 25A and B, respectively). Applying these algorithms to porous materials can be beneficial for accurately sampling the space of possible binding sites for a single molecule.

Once a set of binding sites has been identified, the adsorbed molecule together with the porous system can be optimized using a suitable modeling method to find the most energetically stable adsorption configuration. Comparing the energy of such a configuration with those of the separate porous system and the isolated relaxed molecule allows one to calculate BEs for each adsorbed configuration. From a sampling of many such configurations a statistically reliable distribution of the BEs can be obtained. Additionally, calculating the IR spectra of the adsorption complexes can

Fig. 24 Electrostatic potential map corresponding to a repeat fragment of the crystalline forsterite Mg_2SiO_4 (010) surface. Blue regions represent positive electrostatic potentials, mainly centered on the Mg^{2+} cations. Red regions represent negative electrostatic potentials, mainly centered on the O^{2-} anions



help identify any adsorption-induced vibrational shifts, which can be compared with observational and experimental data.

Exhaustive sampling of binding sites can also be useful for increasing the loading of adsorbed species, eventually forming monolayer structures of adsorbates covering the pore walls (Gierada et al. 2016). This building-up process allows for the derivation of BE variations as adsorbate loading increases. For high loading scenarios, it is recommended that these “static” optimization evaluations of BEs (effectively at 0 K) be complemented with finite temperature MD simulations. The use of MD can capture dynamic effects, which can be significant at the temperatures found in warmer astrophysical environments. For instance, for adsorption based on H-bond interactions, MD simulations can capture the dynamics of H-bonds, showing how they continuously break and reform. For adsorption based on weak dispersive forces, MD simulations allow visualization of the dynamic behavior of adsorbates on the pore wall, providing a more comprehensive atomic-scale picture beyond the static snapshot given by geometry optimizations (Piane et al. 2016; Delle Piane et al. 2013).

Within the context of porous dust, using atomistic modeling to sample the BEs of water molecules inside a porous silicate model would be interesting due to the likely deposition of water ice inside the pores of cosmic dust Potapov et al. (2020). Such modeling could be performed for a range of water loadings and the corresponding simulated IR spectra compared with of experimental data on H_2O ice interacting with porous silicates.

Computational codes that simulate dust grain-surface chemistry (often in tandem with gas-phase processes) are a commonly used tool that allows the chemical evolution to be studied as a function of time and physical conditions. However, there exist exceedingly few astrochemical codes that take porosity into account, either in the icy

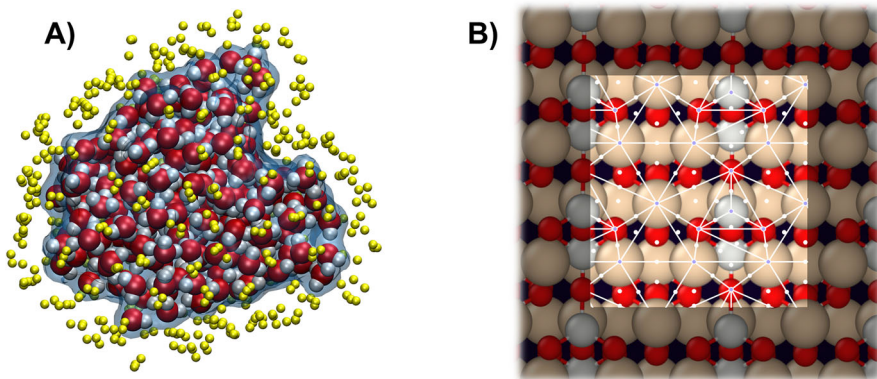


Fig. 25 Automated procedures for an exhaustive sampling of binding sites: A) through the ACO-FROST program (Germain et al. 2022) for large H₂O ice clusters, where the yellow grid points represent potential binding sites, B) through the Polycleaver program (Mates-Torres and Rimola 2024) for periodic ionic surfaces (in this case the crystalline forsterite (010) surface), where the network point represent potential surface binding sites

dust-grain mantles (e.g. Awad et al. 2005; Taquet et al. 2012; Garrod 2013; Song et al. 2024) or in the grains themselves (Perets and Biham 2006; Christianson and Garrod 2021).

The usual computational approach taken to interstellar grain-surface chemistry is to assume a spherical grain with a single, representative radius, commonly 0.1 μm . Thus, these grains are typically intended to represent the smaller subunits of interstellar dust, rather than larger aggregates. Upon this surface, atoms and/or molecules adsorbed from the gas phase are allowed to react, usually driven by the diffusion of relatively mobile physisorbed species such as atomic H. Under dense conditions, in which the grains are very cold, this leads to the build-up of ice mantles that are chemically stable, and which are mostly composed of small molecules that include water, CO and CO₂. In such simulations, the surface of the grain is often implicitly assumed to be smooth, as manifested in the single-valued binding energies and diffusion barriers that are assigned individually to each chemical species on the surface. While such methods may be considered microscopically to be rather crude, they have been successful in capturing the broad behavior of grain-surface chemistry and ice-mantle compositions in a range of astrophysical environments.

In fact, multiple different approaches exist to simulate the chemistry on a technical level. These range from the kind of rate equation-based models (such as the classic work by Hasegawa et al. 1992, and its successors) that use single-valued input parameters to provide the abundances of chemical species on the average grain, to much more complex Monte Carlo kinetics treatments (e.g., Chang et al. 2005; Cuppen and Herbst 2005; Garrod 2013) that allow microscopic surfaces to be dictated explicitly and individual atoms and molecules to be tracked on the surface. Needless to say, the latter method is far more computationally expensive than the former, and is usually limited to a very rigid set of physical conditions. Nevertheless, it is possible to take porosity into account, on some level, using either technique.

Porosity has the potential to influence the behavior of grain-surface chemical models in several important ways. Firstly, the presence of porosity increases the available surface area in comparison to the typically considered solid, spherical grain. This may slow down diffusive surface reactions, but could also result in slower (and thinner) ice-mantle build-up, leading to longer exposure of less mobile surface species (e.g., CO) to chemical attack by mobile reactants like atomic H. The underlying grain material would also remain exposed for longer, leading to more rapid surface diffusion rates for some species.

Depending on the nature of the porosity, i.e., whether a more open, fractal structure, or a closed system of pocket-like enclosures, atoms and molecules residing within the pores may be restricted from desorbing effectively, and may even become entirely trapped within. This could have several effects, such as enhancing reactivity among volatile species, retaining volatile products beyond their desorption temperatures, and potentially shielding trapped product molecules from chemical or photolytic attack over long timescales (see also Sect. 5.2).

5.1.2 Information needed to refine chemical models

Interstellar chemical models of grain-surface chemistry on porous grains have a long way to go. While microscopically exact treatments (e.g. MIMICK, above) are well suited to tackling the structural aspects of the problem, the widespread applicability of these models is severely limited by their extreme computational demands. Such models also do not, as yet, include photolysis of molecules, which could provide a clearer distinction between the molecular content of ice stored inside potentially protective grain-pore structures versus outside them. Some degree of code optimization might allow the idea of the trapping of volatiles to be tested more comprehensively.

Unfortunately, it is not clear that current treatments of porosity using simpler modeling methods are capable of accurately reproducing the formation of ices within the pores, due to their lack of microscopic detail. This would manifest in the treatment of the possible filling and enclosure of grain pores as the ices grow. Neither the porosity in the grains nor in their ice mantles is simple to simulate accurately in rate-based models. However, due to the relatively rigid, unchanging structures of dust-grain pores, as opposed to those that might be present within the ice mantles, such models might be better suited to the former than to the latter. If porosity in interstellar grains in fact manifests as a very open, fractal structure, the influence of porosity would be relatively straight forward to model, by simply adjusting the surface area available for reactions. In this scenario, trapping and shielding would likely be no more of a concern than it is with existing smooth, spherical grain models.

A clearer picture of the true degree and nature of interstellar dust-grain porosity would be a substantial motivator for the development of more detailed treatments of such features in gas-grain chemical models. Uncertain quantities include the precise degree and nature of the porosity, as discussed in this review, which is related also to the degree of connectivity within the pore structures. This connectivity, both within the pores and between the pores and the nominal outer grain surface, may be a key factor in determining the nature of the surface kinetics occurring in the pores. The models would be greatly assisted by the availability of more explicit laboratory experiments of

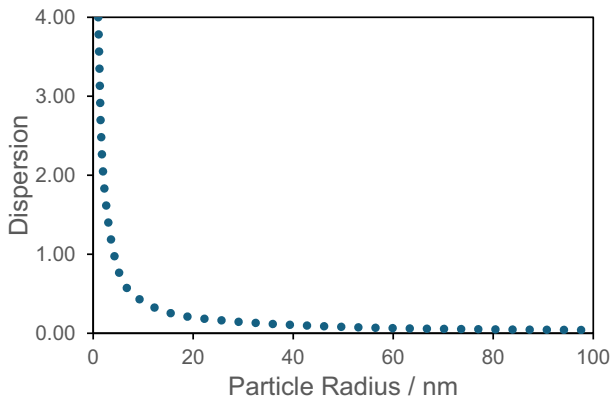


Fig. 26 The effect of decreasing particle size on dispersion as given by equation 3 for a spherical particle of radius in the range given comprising of an agglomerate of 1 nm particles

surface chemistry on well-defined porous grain-surface analogs, which would allow simulations of both the laboratory and interstellar environments to be constructed.

5.2 Surfaces, pores, and their impact on gas-grain chemistry

5.2.1 Surface area

In considering the implications of a fractal dust structure as discussed in the preceding sections, it is crucial that we understand the impact of reducing the scale of the dust particles. Figure 26 illustrates the issue through the concept of dispersion commonly employed in the catalysis literature (Bowker 2011). In that literature, dispersion D , is defined as the ratio of the number of surface atoms (N_S) to the total number of atoms (N_T) in a particle. It is commonly used in relation to the metal particles deposited on a catalytic support:

$$D = \frac{N_S}{N_T}. \quad (14)$$

However, we can adapt this concept to where larger particles may be agglomerates of smaller particles by considering the numbers of smaller particles comprising the larger. If we define the radius of the larger particle, r_L , in terms of the smaller, r_S , then

$$N = \frac{r_L}{r_S} \quad (15)$$

and for spherical particles we have

$$D = \frac{4}{N}. \quad (16)$$

In effect the dispersion gives us insight into the effective surface area of the agglomerated materials compared to a single large particle. As an illustration, for a 100 nm

particle composed of 1 nm grains, we might expect the maximum total surface area of the agglomerate to be some 25 times that of a single particle, i.e., $1/D$. Laboratory experiments comparing the surface areas of a compact particle and a porous fractal aggregate consisting of nm-sized monomers showed that the surface area of the aggregate is several hundred times that of a compact particle (Potapov et al. 2020).

There are mathematical methods allowing for estimation of a fractal dimension and a surface area of an aggregate from its geometrical parameters and interaction with light (e.g., Carr et al. 1992; Besselink et al. 2016). More directly, O₂ adsorption can be used to characterize the surface area and porosity/morphology of grain aggregates. The technique is analogous to isothermal adsorption measurements, which are typically performed at higher temperatures (Gregg and Sing 1982; Rouquerol et al. 1999). However, these methods have never been applied to analogs of cosmic dust particles.

While the spherical assumption might be valid to some extent for larger particles, as grain dimensions approach the nanometer scale then particles are likely to be far from spherical as illustrated in Fig. 27 for small SiO clusters.

This has two effects. Firstly, the sum of the small particle surface areas may be substantially larger than in the spherical limit. Additionally, and more importantly, atoms at surfaces commonly experience lower coordination than those in bulk materials and as such are naturally much more reactive. A simple comparison of the interaction of cyclohexane and benzene with an agglomerated silica cluster surface (M.R.S. McCoustra, unpublished data) using temperature programmed desorption methods demonstrates that the former interacts weakly with the silica surface as might be expected. While the latter is known from the literature to form a strongly bound monolayer on such surfaces (Thrower et al. 2009a, b). The efficacy with which partial electron transfer occurs from π orbitals of the benzene molecule to the low coordination number Si centres on the silica cluster mediates this process.

In the simplest sense, increased surface area on which deposition and reaction might occur means that reactivity at the gas-grain interface might increase. This might be particularly true for surface-assisted recombination reactions (e.g., $H + H \rightarrow H_2$) and reactions involving activated atoms within the grain surface (e.g., energetically-triggered formation of CO and CO₂ from H₂O on various carbon surfaces, see (Potapov and McCoustra 2021) for a review, where the rate of reaction scales effectively with grain surface area. However, within the Langmuir–Hinshelwood framework (considering diffusion of at least one of the reactants as a prerequisite for the reaction) that dominates surface chemistry in space, diffusion could be slowed in an agglomerate compared to a large particle as diffusion now needs to occur between particles. As with crystallite boundaries on polycrystalline surfaces such boundaries may represent a significant barrier to diffusion and consequently slow reaction rates (Rabkin et al. 1999; Wang et al. 2017; Zhou et al. 2019). On the other hand, recent results demonstrated efficient diffusion of CO₂ and NH₃ molecules through the pores of dust aggregates in contrast to diffusion into bulk ices of each other (Potapov et al. 2025).

When considering the additional surface area that porosity may impart to dust grains, it is necessary to consider both intrinsic porosity (associated with the material itself) and extrinsic porosity (associated with the morphology of the dust grain agglomerate). Intrinsic porosity within the materials will add to the surface area available for reactions if the pores are connected to the surface. Porosity as closed off void

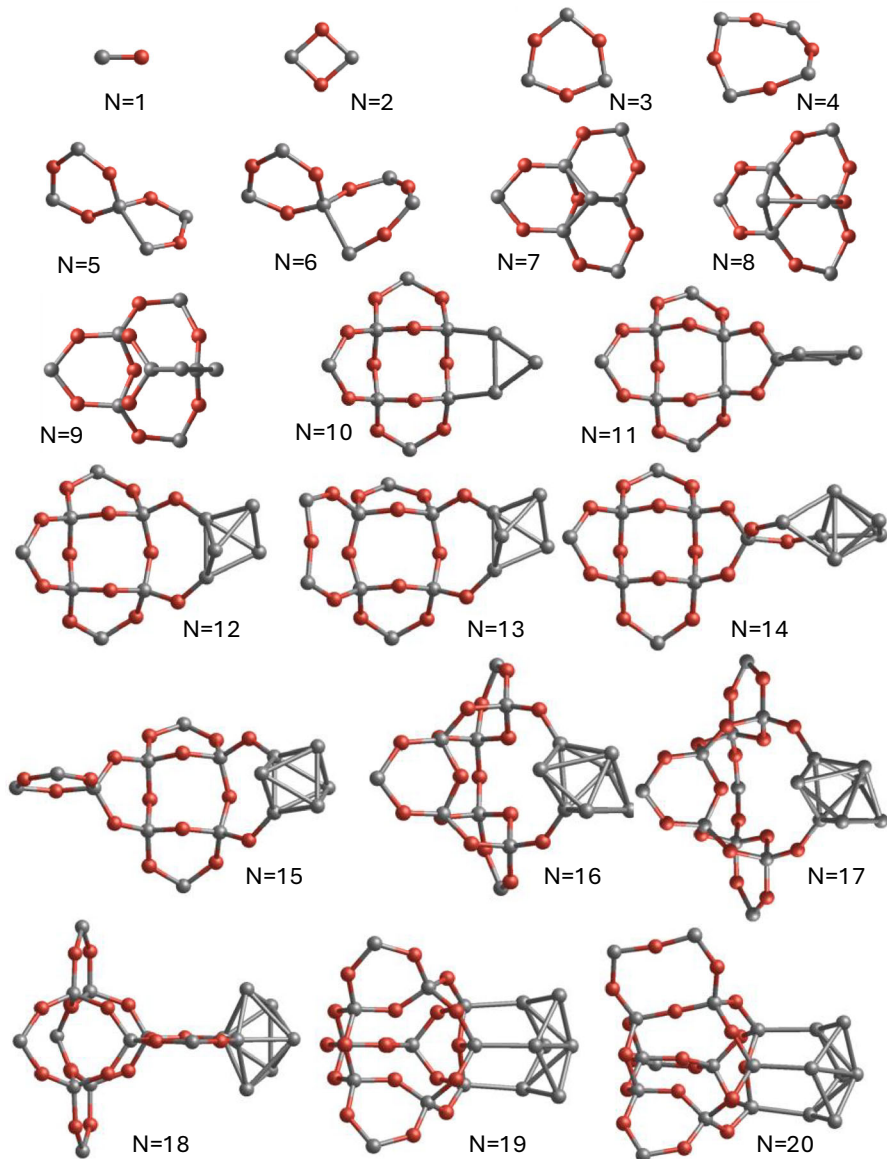


Fig. 27 Small $(\text{SiO})_N$ clusters for $N = 2 - 20$. Atom color key: Si – red, O – gray. Image reproduced with permission from Bromley et al. (2016), copyright by RSC

space will not add to the available surface area. Extrinsic porosity is related to the morphology of the agglomerate. Extended agglomerates where small particles are held together in simple chains may possess some extrinsic porosity in crevices around the contact points between the agglomerated grains, but these are unlikely to add significantly to the surface area of the agglomerate. In more compact structures, the impact

of pores and voids on the surface area of the agglomerate may be significant. It is worth noting that both types of porosity may act, under the correct circumstances, to store gaseous reagents beyond their normal desorption temperatures enabling reactions on pore surfaces at higher temperatures and local pressures (Goh et al. 2024).

In relation to intrinsic porosity in the materials from which grains compose, we are considering silicates from the two main families, $(\text{FeO})_x(\text{MgO})_y(\text{SiO}_2)_z$ and $(\text{FeO})_x(\text{Al}_2\text{O}_3)_y(\text{SiO}_2)_z$, and carbonaceous materials of various forms. These materials form in the outflows of large AGB stars under near thermal equilibrium conditions. The silicates may form as either crystalline or glassy solids which likely have negligible intrinsic porosity. Amorphization by cosmic radiation may introduce defects to the lattice but generally the intrinsic porosity will remain low. In contrast, water alteration of these materials in specific environments where this is possible can produce materials that exhibit lamellar (clay) and cage (zeolite) structures that will introduce nanoscale porosity to material (e.g., Eberl 1984; Chipera and Apps 2001). Of course, these altered materials are equally subject to radiation alteration that will seek to remove the nanoscale porosity and return the material to a glassy state (Wang et al. 2000; Consolaro et al. 2024).

In terms of carbon materials, intrinsic porosity is well-known specific systems, e.g., within fullerenes and nanotubes and the lamellar structure of graphite. Materials like diamond and hydrogenated amorphous carbon are, however, less likely to show such intrinsic porosity. The extrinsic porosity of agglomerated carbon grains will likely parallel that in silicate grains.

5.2.2 Catalysis

High dust grain porosity and a correspondingly large surface area as discussed above have an important consequence—the availability of active dust grain surfaces for physico-chemical processes in various astrophysical environments. There is no question that dust surfaces are available in low-density (diffuse interstellar clouds) and warm/hot (atmospheres of exoplanets, protostellar envelopes and protoplanetary disks inside the snowline) environments due to the absence of molecular ices, which might cover dust grains and thus make the dust surface material unavailable for surface processes. However, the scientific community is still far from reaching a consensus regarding cold and dense environments, such as dense interstellar clouds, protostellar envelopes and protoplanetary disks beyond the snowline. The widely accepted view of grains in such environments presents grains as a compact refractory dust core covered by a thick (tens or hundreds of monolayers) ice layer. In such a case, processes occurring on and in the ice are independent of the properties of the dust material. However, the aforementioned study (Potapov et al. 2020) demonstrated that porous grains in cold environments can be covered by only a sub-monolayer or a few monolayers of ice, especially if that ice can agglomerate (Rosu-Finsen et al. 2016). Thus, bare dust grain surfaces are potentially available for chemical reactions in a wide range of environments. In such a case, the dust can actively participate in surface processes and, depending on the properties of the dust material, may play a role of a classical catalysis. This new view was also presented and discussed in (Potapov and McCoustra 2021).

While there remains much to explore in terms of grain surface photochemistry, our knowledge of that field is substantive in comparison to our knowledge of catalytic processes (i.e., processes in which the grain reduces the reaction and/or diffusion activation barrier accelerating the reaction) on grain surfaces. The previous research of the catalytic formation of simple molecules, such as H_2 and H_2O , and more complex species, such as $\text{NH}_4^+\text{NH}_2\text{COO}^-$, on dust grain analogs was recently reviewed (Potapov and McCoustra 2021). Here, we highlight ideas in that area that have recently opened new doors on astrocatalysis.

(1) Silicate grains contain iron and other catalytically active transition metals (e.g., Ni, Co, Mn). It is well established that space weathering nucleates the growth of iron (and other metal) nanoparticles in the surface regions of grains (e.g., Hapke 2001; Pieters and Noble 2016; Burgess and Stroud 2021). Iron and its neighbors are well known to catalyze key industrial processes from the Haber–Bosch synthesis of ammonia, through Fischer–Tropsch chemistry for alkane and alcohol formation from H_2 and CO to chemistries tied to the bottom-up synthesis of carbon nanomaterials (PAHs and nanotubes specifically) from simple unsaturated hydrocarbons like acetylene and ethylene (Twigg 1989).

(2) Carbonaceous and silicate materials can both behave as substrates for the deposition of gas transition metal atoms introduced in the gas phase by sputtering in shocked regions. Recent computational work by Rimola and co-workers nicely illustrates the potential for such single atoms to engage in catalytic chemistry (Pareras et al. 2023, 2024).

(3) Nanostructured carbons and transition metal clusters are metallic in nature. This opens a wealth of potential chemistry linked to the generation of electron–hole pairs (which dominate photochemistry on metals), and cavity-enhancement thereof, which is known to be highly efficient (Chakarov et al. 2001; Bergeld et al. 2008).

These factors represent opportunities for exploration by the solid state and surfaces laboratory astrophysics community and link it very strongly to the catalysis community.

5.2.3 Relaxation

It is well known that surfaces effectively behave as a third body in atom and radical recombination reactions on grains by providing pathways enabling electronic and vibrational relaxation of the nascent reaction product. The formation of H_2 from physisorbed H atoms on a variety of surfaces nicely illustrates this effect (Wakelam et al. 2017). H_2 formation on graphite surfaces also nicely illustrates that unless the internal (ro-vibrational) degrees of freedom are strongly coupled into the surface then relaxation at the surface may not be as efficient as expected (Islam et al. 2007; Latimer et al. 2008).

Grain surfaces also provide a pathway to relaxing vibrationally and electronically excited species that either impact on surfaces from the gas phase or are already adsorbed on surfaces and excited. Of course, the more surface is available, the more effective are these processes. In both instances, however, relaxation is fundamentally governed by Fermi’s Golden Rule and the energy–time Uncertainty Principle. Underpinned by the nature of the electronic states and the conical intersections that link

them, these ideas lead us to the Jablonski Diagram, determine spectroscopic line profiles, and yield symmetric Lorentzian profiles for transitions in isolated molecules (Atkins and Friedman 2005). Efficient nonradiative mechanisms reduce electronic and vibrational excited state lifetimes and hence homogeneously, and symmetrically, broaden linewidths often resulting in Gaussian or Voigt line profiles. In the gas phase, photon-driven processes, temperature (average molecular speed – Doppler Broadening) and pressure (collision frequency – Pressure Broadening) are the principle broadening mechanisms resulting in homogeneous broadening of gas phase line profiles (Demtröder 1996). On solid surfaces, molecular translation and rotation are frustrated and weakly interacting adsorbates on simple insulating solids can therefore exhibit relatively narrow linewidths. The classic example of this is found in the work of Ewing and co-workers (Chang et al. 1990, 1995). These authors estimate the natural linewidth for the vibration of carbon monoxide (CO) on the NaCl (100) surface at 5 K to be of the order of 10^{-8} cm^{-1} , and suggest that the observed linewidth, 0.07 cm^{-1} , results from the residual heterogeneity of the NaCl surface. In contrast, on conductor surfaces, transition dipoles couple with the free electrons in the conductor band structure providing an efficient mechanism for relaxing excited adsorbates via electron – hole pair creation (Ueba 1997; Arnolds 2011). The resulting line profiles are broad, for example varying from around 5 to 15 cm^{-1} for CO on conductor single crystal surfaces, and asymmetric, reflecting Fano coupling between the adsorbate vibration and the non-adiabatic electron–hole pair continuum of the substrate (Gadzuk and Luntz 1984; Langreth 1985). Additionally, these systems, as with halide surfaces, are often subject to further broadening due to environmental heterogeneity (Ryberg 1985). Environmental heterogeneity reaches its extreme with the profiles of vibrational lines of adsorbates interacting with supported metal and metal oxide catalysts (Ryberg 1985) as which silicate minerals might be considered.

An interesting and relevant example from McCoustra and co-workers illustrates the potential for exploring the impact of surface heterogeneity and adsorbate photostability on surfaces in the IR through studies of line shapes for CO on amorphous silica and amorphous solid water (Taj et al. 2017, 2021). Herein, evidence is presented from the similarity of CO line profiles in these two systems, the origins of these line profiles are indeed different, with the former likely associated with an efficient IR photon-induced desorption channel and the latter with efficient vibrational energy relaxation into the amorphous solid water phonon bath.

5.2.4 Shielding

While the efficacy or otherwise of surface relaxation maybe crucial to defining the stability of species adsorbed on surfaces, we should recognize the simpler shielding role of the corresponding bulk beneath the surface. Both silicate and carbonaceous materials directly absorb radiation at a variety of wavelengths and especially in the short wavelength ultraviolet. As such adsorbate species are only exposed to destructive radiations from the 2π steradians above the surface on which the adsorbate sits. Access to adsorbates by from the remaining 2π steradians below the surface on which the adsorbate sits is attenuated by the scattering and adsorption of the substrate itself. Moreover, grain surface molecules, potentially including complex organic molecules,

formed at early stages of the evolution of cosmic environments, i.e., in diffuse interstellar clouds (e.g., Potapov et al. 2017; Dulieu et al. 2019; Ioppolo et al. 2021; Garrod et al. 2022), can be shielded from external radiation fields due to the growth (aggregation) of the grains and, thus, survive during the travel of the grains from the ISM through protostellar envelopes and protoplanetary disks to planetary system and atmospheres of planets.

5.3 Planet formation, binding sites, and origin of water

The efficiency of the formation of planets in protoplanetary disks depends on the amount of solid-state material available at locations of future planets (Min et al. 2011; Thommes and Duncan 2006). Outside of the water snowline, the density of material is enhanced due to the presence of water (the main constituent of ices in cold environments) and other molecular ices (Hayashi 1981). Moreover, coagulation models (Wada et al. 2009, 2013; Kimura et al. 2020) and laboratory experiments (Gundlach et al. 2011; Gundlach and Blum 2015) confirm that sticking efficiency of water-ice-coated dust grains is much higher as compared to rocky (iceless) grains. In addition, simulations demonstrated that high porosity of icy aggregates triggers significant acceleration in collisional growth (Okuzumi et al. 2012; Kataoka et al. 2013; Kobayashi and Tanaka 2021), although these models are being challenged as ALMA observations favor grains with a modest amount of porosity (see Sect. 3.3.1). Both factors are argued to have facilitated the formation of giant planets in the Solar System (Stevenson and Lunine 1988; Lissauer and Stevenson 2007), with the snowline located within the asteroid belt at about 3 AU from the Sun (Morbidelli et al. 2000).

The amount of solid mass available for planet formation beyond the snowline as well as the efficiency of dust coagulation as linked to the stickiness of ices are still being debated. Regarding the amount of solid mass, we refer the interested reader to Morbidelli et al. (2015) and references therein. Regarding the efficiency of dust coagulation, for water ice the efficiency strongly depends on the amount of water (water ice thickness) on dust grains (Kimura et al. 2020). The situation is worse if the CO₂ ice forms an outer ice layer on dust grains. It was demonstrated by laboratory experiments (Musiolik et al. 2016a,b) and models (Arakawa and Krijt 2021) that the stickiness of CO₂ ice is much lower as compared to H₂O ice. This result was favored in observational modeling of protoplanetary disks (Okuzumi and Tazaki 2019; Jiang et al. 2024). We note that the case of an outer CO₂ ice layer is relevant to colder parts of protoplanetary disks, beyond the snowline of CO₂ located at about 10 AU from the Sun.

The above discussion focuses on a general statement regarding planet formation and here porosity may also play an important role, in particular with regards to the water content of the Earth which formed inside the nebular snow line. In the laboratory experiments studying thermal desorption of ices, water ice desorbs completely at 160–180 K (Bolina et al. 2005; Collings et al. 2004; Smith et al. 2011). This temperature defines the location of the snowline. It is typically assumed that dust grains inside the snowline are dry, which motivates the need for water supply to the Earth from beyond the snowline perhaps via dynamically reshuffling of solids in the nebula

due to the presence of, e.g., Jupiter (Raymond et al. 2004; Rubie et al. 2015; Krijt et al. 2023). However, more realistic laboratory experiments modeling dust grains in cold environments as dust/ice mixtures have demonstrated that a considerable part of water molecules mixed with silicate grains is trapped (strongly bound) on grains at temperatures exceeding the desorption temperature of water ice (Potapov et al. 2018a, b, 2021, 2024). The amount of trapped water is directly defined by the number of binding sites, which in turn is defined by the surface area of grains which is enhanced with porous grains with variable sub-structure. The results of (Potapov et al. 2024) demonstrated that the trapped water is physisorbed as water molecules rather than dissociatively chemisorbed (i.e., as chemically bonded $-OH$ groups). These water molecules can persist up to about 470 K, which is well above the desorption temperature of water ice. This implies the existence of sites in porous silicates where water molecules can be very strongly bound. As mentioned in Sect. 4.4.3, models of small molecules physisorbed inside micropores show that the molecular binding in such cases can be up to eight times larger than on the corresponding flat surface (Derouane et al. 1988). Temperature-dependent IR experiments on microporous silicate zeolites also show that water molecules can be trapped inside micropores up to at least 423 K (Singh and White 2018). These results strongly imply that micropores in porous silicate grains could trap water molecules and retain them during planetary accretion processes at relatively high temperatures.

Water molecules trapped in refractory dust grains may be present in the solid state in astrophysical environments, where we do not expect them, e.g., in the diffuse ISM, in protoplanetary disks inside the water snowline, and in the warm/hot atmospheres of exoplanets. Comparison of laboratory and observational spectra provided evidence of the presence of solid-state water in the diffuse ISM (Potapov et al. 2021). Comparison of laboratory spectra and spectra of cometary particles and meteorites provided evidence for the presence of trapped water in extraterrestrial particles (Potapov et al. 2022). Analysis of recent JWST observations provided evidence of water in the solid state inside the water snowline in a protoplanetary disk (Potapov et al., submitted). The estimated concentration of H_2O is similar to that of the present-day bulk Earth and consistent with recent measurements of enstatite chondrite meteorites. This result, if generalized, would imply that most habitable zone planets are born with water budgets comparable to Earth's.

The microphysics of how porous grains interact with radiation may also influence the volatile composition of planet forming materials. For instance (Najita et al. 2001) noted the prevalence of energetic stellar X-ray emission that irritates dust and gas in protoplanetary disks (Glassgold et al. 1997; Feigelson and Montmerle 1999). They showed that when an X-ray is absorbed by an aggregate comprised of smaller particles, the energy transfer from a sub-unit to the whole grain is impeded leading to a higher local temperature for a longer period of time. This potentially can foster local non-thermal desorption of volatile ices via “spot heating”, which is centrally dependent on the structure of the silicate or carbonaceous refractory dust. A similar process may be present when cosmic rays, which may also be present (Cleeves et al. 2013; Padovani et al. 2018), impact volatile ice coated dust grains (Sipilä et al. 2021).

Thus, the consideration of porous, fractal grains may change our understanding of the mechanisms and efficiencies of grain growth and volatile incorporation into

planetesimals/pebbles and rocky planets inside disk snow lines, whether for water and organics or more volatile components such as CO or CO₂. This can ultimately influence the volatile content of forming bodies. This ranges from the water content of the Earth, a central component of its habitability, but also the materials present in other planets, asteroids, and comets.

6 Conclusions

Dust porosity is a crucial factor in understanding physicochemical and structural properties of dust itself as well as the evolution of dust in astrophysical environments. However, while results of laboratory experiments and dust evolution models clearly speak for high porosity of cosmic dust, results of the analysis of astronomical observations are more ambiguous. One of the problems is that models that describe observations have many degenerate parameters, e.g., porosity can be “compensated” for by a “grain size distribution”. While astronomical observations of the ISM in general do not contradict results of grain growth models and laboratory experiments, astronomical observations of planet-forming disks are more diverse.

However, if we integrate results of the analysis of observations of different environments from the ISM through protoplanetary disks to debris disks and the Solar System, we see a logical trend, which, together with the experimental and modeling results, draw a clear picture of increasing porosity in increasingly evolved environments. The sequential growth of dust grains traveling from the diffuse ISM to the dense ISM and then to protoplanetary disks and planetary systems is accompanied by an increase of the sizes of compact grain units (monomers) and by an evolution of their porosity, which is relatively low at the beginning of the journey and very high at its end before the processes leading to the formation of planetesimals.

There are questions immediately raised by this picture. What are the reasons for the observed diversity of astronomical observations? Is it linked to different conditions in the astrophysical environments or imperfect dust models and/or laboratory data? What is the origin of low porosity in the diffuse ISM, considering fractal growth starting from nm-sized particles? Is the degree of porosity dependent on whether grain growth in a particular environment occurs through aggregation of pre-formed subunits, or at the atomic/molecular scale (particularly as the grain core nucleates)? What are mechanisms leading to growth of compact grain units (monomers) with grain growth? Is this conclusion not biased by the Solar System measurements?

There are many more open questions and considerable gaps in our knowledge. Moreover, to understand the evolution of dust and planet formation process, it is crucial to establish links between the dust particles observed in the ISM, in planet-forming disks, and in the Solar System. It is clear that observations, models, and laboratory experiments should be combined and work together to understand the complete picture of the dust evolution in space. In the following, we try to formulate a few promising research directions in observations, experiments, and modelling covering a desired science program on cosmic dust porosity.

Observations: To push forward our understanding of dust porosity in disks, careful studies of light scattering properties and its application to the actual disk observations are mandatory. Multiwavelength polarimetric observations of protoplanetary disks are required across a broad range of targets. Infrared observations will also be valuable for constraining grain composition, which in turn can help to solve for dust parameter degeneracy. More statistics is required for the Solar System cometary particles. For this, new sample-return missions to comets are crucial.

Experiments: Laboratory optical data for porous dust grains and their mixtures with molecular ices, at various temperatures from 10 s (ISM) to 100 s (disks, exoplanets) of K are required for reliable analysis of observations. Study of the influence of space weathering on the optical, morphological and chemical properties of analogs of cosmic dust grains would provide an important piece of puzzle of the evolution of cosmic dust grains in astrophysical environments and links between the dust particles in the ISM, planet-forming disks, the Solar System. Influence of high temperatures relevant to the exoplanet atmospheres on the dust grain growth and the porosity, chemical activity and optical properties of grains represent another important but practically uncharted territory. Considering a high porosity and a correspondingly large surface area of cosmic dust grains, the studies of physical-chemical surface processes relevant to astrophysical environments should be continued with an impact on laboratory experiments involving dust surfaces.

Modeling: New advanced models of porous dust grains using new laboratory data mentioned above are required for the analysis of modern multiwavelength observations of various astrophysical environments and for understanding the origin of the diversity in porosity. Radiative transfer modeling using 3D radiative transfer models coupled with a sophisticated light scattering model for porous grains/aggregates should be applied for a broad range of protoplanetary disks. Structural modeling of porous cosmic dust grain with a range of astrophysically relevant chemical compositions beginning from atomistic level is required for characterization of cosmic dust and its laboratory analogs. Considering a high porosity and a correspondingly large surface area of cosmic dust grains, such studies should aim to model physical-chemical surface processes relevant to astrophysical environments and work in parallel with astrochemical modeling involving dust surfaces.

But even having possibility to realize all the ideas above, there are two big elephants in the room: (i) how to describe porosity in a model and (ii) how to combine optical constants appropriately. Optical scattering theory is solid but perhaps we need to use more Monte Carlo—based methods as we do with electrons rather than ray tracing methods to integrate transmission, absorption and scattering into a single picture. Moreover, now, in the era of quickly developing artificial intelligence, we should look for potential for a unified approach that uses machine learning to address these problems.

With this review, we cover the likely prevalence and consequences of dust porosity and how it can be investigated by laboratory, modeling and observational methods. We thereby hope to provide a solid platform for a broad discussion on cosmic dust porosity aiming at better understanding of the properties and evolution of astrophysical environments.

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Declarations

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