Grain surface chemistry in astrophysical objects
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Molecular hydrogen formation on dust grains in the high redshift universe.

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We study the formation of molecular hydrogen on dust grain surfaces and apply our results to the high redshift universe. We find that a range of physical parameters, in particular dust temperature and gas temperature, but not so much dust surface composition, influence the formation rate of H$_2$. The H$_2$ formation rate is found to be suppressed above gas kinetic temperatures of a few hundred K and for dust temperatures above 200-300 K and below 10 K. We highlight the differences between our treatment of the H$_2$ formation process and other descriptions in the literature.

We also study the relative importance of H$_2$ formation on dust grains with respect to molecular hydrogen formation in the gas phase, through the H$^-$ route. The ratio of formation rates of these two routes depends to a large part on the dust abundance, on the electron abundance, and also on the relative strength of the FUV (extra-)galactic radiation field. We find that for a cosmological evolution of the star formation rate and dust density consistent with the Madau plot, a positive feedback effect on the abundance of H$_2$ due to the presence of dust grains can occur as early as a redshift of $z \sim 3 - 5$. This effect begins for a dust-to-gas mass ratio as small as $10^{-4} - 10^{-3}$ of the galactic value.
4.1 Introduction

H$_2$ formation in the universe is a process which has been studied extensively in the past decades, but which is still not well understood. In the interstellar medium, H$_2$ formation occurs on grain surfaces, permitting three-body reactions that are much more efficient than gas phase reactions (Gould & Salpeter 1963). Many studies have been performed over the years and focussed on explaining the mechanisms involved in the H$_2$ formation process on grain surfaces. It is clear that this process is governed by the mobility of the H atoms on the grain, as well as the energies binding the H atoms to the surface. The mobility of an adatom (the atom that is bound to the surface) is the combination of two processes: thermal diffusion and quantum tunneling. Therefore, an adatom can move on the surface of the grain, from site to site, through these two processes according to the temperature of the grain and the characteristics of the surface (Barlow & Silk 1976; Leitch-Devlin & Williams 1984; Tielens & Alamandola 1987). On astrophysically relevant surfaces (olivine and amorphous carbon), an adatom can bind in two energetically different sites: physisorbed sites and chemisorbed sites. Physisorbed atoms are weakly bound to the surface and are mobile for low grain temperatures (around 10 K), whereas chemisorbed atoms are bound stronger to the surface and become mobile for a grain temperature of a few hundred K (Barlow & Silk 1976; Aronowitch & Chang 1980; Klose 1992; Fromherz et al. 1993; Cazaux & Tielens 2002). Therefore, H$_2$ formation strongly depends on the metallicity of the system (i.e., the dust abundance), the considered grains (olivine or amorphous carbon), the temperature of the grains and the atomic hydrogen abundance.

Studies of H$_2$ formation in low metallicity systems – e.g., the high redshift universe – have already been performed (c.f. Tegmark et al. 1997). H$_2$ at high redshift is of prime importance since it is considered to be the only coolant below 10$^4$ K. Therefore, as discussed by many authors, H$_2$ plays a crucial role in the formation of the first stars (Haiman, Rees, & Loeb 1996; Haiman, Thoul, & Loeb 1996; Tegmark et al. 1997), and thus determines the end of the dark ages (Haiman, Abel, & Rees 2000). Other authors discussed the possibility of HD as a more efficient coolant because this molecule possesses a nonzero dipole moment, even though its abundance is much lower (Galli & Palla 1998; Nakamura & Umemura 2002). Norman & Spaans (1997), estimate a redshift of about unity, where H$_2$ formation in the gas phase and H$_2$ formation on grain surfaces are equally important. At high redshift, H$_2$ formation proceeds through the H$^-$ route, until a high enough metallicity is reached to form H$_2$ through three-body reactions. Below a redshift of unity, grain surface reactions become more important relative to the (inefficient) H$^-$ route.

These issues are of more than academic interest since the presence of H$_2$, either through the H$^-$ or dust grain routes, is instrumental in the ability of primordial gas to cool and contract to form stars. Because no dust grains are available prior to the formation of popIII objects, the H$^-$ route is crucial in starting up the star formation process, but the subsequent expulsion of metals in supernova explosions and ambient dust formation can strongly enhance the formation of molecular hydrogen (Hirashta, Hunt, & Ferrara 2002). The construction of comprehensive models for the effects of dust grains on early galaxy evolution and their observational consequences is underway (c.f. Hirashta, Hunt, & Ferrara 2002; Spaans & Norman 1997; Kauffmann & Charlot 1998; Somerville, Primack & Faber 2001), motivated by upcoming observatories like ALMA and JWST. In general, such studies adopt the H$_2$ formation rate of Hollenbach & McKee (1979). Although a good order of mag-
4.2 H\textsubscript{2} formation

4.2.1 Dust grain route

In this section we study the formation of H\textsubscript{2} on interstellar grain surfaces. First, we discuss the typical range of the H flux in diffuse interstellar clouds. Second, we study the intrinsic properties of the grain (olivine or carbonaceous), the impact of the parameters characterizing the surface of the grain, and the role of the grain size distribution.

**H flux**

A grain in the ISM is irradiated by H atoms from the gas phase. The H flux in a diffuse interstellar cloud is given by

$$F_H = \frac{n(H)v_H}{N_S},$$

(4.1)

where $N_S$ is the number of sites per cm$^2$ on the surface of the grain, $n(H)$ the density of H atoms in the gas phase, and $v_H$ the mean velocity of these atoms. We assume $N_S = 2 \times 10^{15}$ sites cm$^{-2}$ for a 0.1 $\mu$m grain, the density of H atoms to be between 1 and 100 particles per cm$^3$, and the velocity of these atoms to be between 1 and 10 km s$^{-1}$. Therefore, we consider a range for the flux of $5 \times 10^{-11} \leq F_H \leq 5 \times 10^{-8}$ where $F_H$ is the flux of H atoms in monolayer per second (mLy s$^{-1}$).
**Characteristics and nature of the grains**

A. **Surface characteristics**

In this section we present the characteristics of the grain surface which are relevant to the model we are using in this paper. This model has been discussed by Cazaux & Tielens (2002a), and describes how \( \text{H}_2 \) forms on grain surfaces.

When an atom hits a grain, it can either be bound to the surface, if it arrives in an empty site, or it can go back into the gas phase, if the site is occupied. This process follows Langmuir kinetics. An adatom can bind to the surface in two energetically different sites: a chemisorbed site or a physisorbed site. According to the interaction between the atom and the surface, the mobility of the adatom is set. Coming from the gas phase the atoms are first physisorbed. Then they can either cross the barrier to go to a chemisorbed site (depicted in Fig. 4.1) by moving perpendicular to the surface, or go to another physisorbed site, by moving along the surface. Considering an adatom H, the relevant parameters for our study are the desorption energies of chemisorbed hydrogen, \( E_{\text{H}} \), of physisorbed hydrogen \( E_{\text{H}_2} \), and of molecular hydrogen \( E_{\text{H}_2} \), as well as the energy of the saddle point between a physisorbed and a chemisorbed site \( E_s \) and the factor \( \mu \) which is the fraction of the newly formed molecules which stays on the surface. Fig. 4.1 illustrates these parameters, in the case of a barrier between a physisorbed and a chemisorbed site. Under steady state conditions, the \( \text{H}_2 \) recombination efficiency (i.e., the fraction of incoming atoms leaving the grain as \( \text{H}_2 \) molecules) varies with these parameters. When we know the different physical processes involved in \( \text{H}_2 \) formation on grain surfaces, we can understand the impact of each parameter on the \( \text{H}_2 \) formation, and at which range of gas and dust temperatures it occurs.

![Figure 4.1](image.png)

**Figure 4.1**. Barrier between a physisorbed site and a chemisorbed site for an atom, \( k \), bound to the surface. When an atom crosses this barrier, it moves perpendicularly to the surface. Here, we consider hydrogen or deuterium atoms. Their energies are different because D atoms are more tightly bound to the chemisorbed and physisorbed sites than H atoms due to zero point energy difference. \( E_a \) is the energy of the saddle point. In this work only H atoms are considered.
At low and high dust temperatures, variations in the flux affect the H$_2$ recombination efficiency. At low dust temperatures, this can be explained by the Langmuir kinetics. If the flux is low, the atoms, after a stay in the physisorbed sites, move into the chemisorbed sites without encountering other incoming atoms from the gas phase. If the flux is large, the physisorbed atoms, before moving to the chemisorbed sites, encounter some incoming atoms from the gas phase and are both released into the gas phase again. This explains the less efficient H$_2$ formation at high fluxes. On the contrary, at high dust temperatures, only a small fraction of the atoms coming onto the grain go to chemisorbed sites. When the flux increases, the number of chemisorbed H atoms just increases too, and the H$_2$ formation is more efficient since the grain surface is occupied by more H atoms. This impact of the flux on the H$_2$ recombination efficiency is presented Fig. 4.2.

![Figure 4.2](image_url)

**Figure 4.2**. H$_2$ recombination efficiency at low and high dust temperatures for 4 different fluxes: solid line $5 \times 10^{-11}$, dashed line $5 \times 10^{-10}$, dot-dashed $5 \times 10^{-9}$, dots $5 \times 10^{-8}$. The parameters are $E_{\text{H}_2} = 340$ K, $E_{\text{H}_2} = 600$ K, $E_S = 200$ K, $E_{\text{H}_2} = 10,000$ K and $\mu = 0.02$.

Another parameter which affects the H$_2$ formation at low dust temperatures is the H$_2$ desorption energy. H$_2$ can form and stay on the surface of the grain until a temperature is reached that allows evaporation of these molecules. This desorption process is driven by the desorption energy of H$_2$, $E_{\text{H}_2}$, and consequently this parameter has a big impact on the H$_2$ recombination efficiency, as presented in Fig 4.3, left panel.

At higher dust temperatures, the desorption energy of physisorbed atoms, as well as the energy of the saddle point, affect the H$_2$ formation process. Indeed, the only obstacle to form H$_2$ at higher dust temperatures, is the evaporation of the physisorbed H atoms before recombination. At these dust temperatures the physical process to form H$_2$ is the encounter of a physisorbed H and a chemisorbed H atom. This means that the incoming H atom, which is physisorbed, has to cross the barrier presented in Fig. 4.1, and hence the energies $E_{\text{H}_2}$ and $E_S$ have a big impact on the H$_2$ recombination efficiency, as shown in Fig. 4.3, right panel and Fig. 4.4, left panel.
Finally, when the dust temperature is too high to enable the physisorbed atoms to recombine before they evaporate, the H$_2$ formation process reduces to the recombination of two chemisorbed H atoms. Of course, this process depends on the desorption energy of the chemisorbed atoms, as illustrated in Fig. 4.4, right panel. When the dust temperature is high enough to enable chemisorbed H evaporation, these atoms leave the grain before recombining, and H$_2$ formation is quenched.

B. Olivine versus carbon

The composition of dust in the diffuse interstellar medium is still uncertain. According to observations, this composition includes silicates, amorphous carbon, polycyclic aromatic hydrocarbons (PAHs), graphite organic refractories, and many more (Mathis, Rumpl, & Nordsieck 1977). Most models combine all these elements to obtain the interstellar extinction curve and to compare it with observations. Weingartner & Draine (2001) and Li & Draine (2001, 2002) have developed a carbonaceous-silicate grain model which successfully reproduces observed interstellar extinction, scattering and infrared emission. This model consists of a mixture of carbonaceous and silicate grains with a grain size distribution chosen to reproduce the extinction curves obtained by observing the Milky Way, the Large Magellanic Cloud (LMC) and the Small Magellanic Cloud. This model requires the presence of very small carbonaceous grains, and appears to be a viable explanation for the observations. Therefore, we calculate H$_2$ formation only on carbon and silicate grains. The surface characteristics of these two grains have been discussed in Cazaux & Tielens (2002). The experiments done by Pirronello et al. (1997a, 1997b and 1999) and Katz et al. (1999) have benchmarked the model that we are using here (Cazaux & Tielens 2002), and the derived parameters are reported in table 2.1.
4.2. H$_2$ formation

Figure 4.4. (a) H$_2$ recombination efficiency for 4 different desorption energies of physisorbed H, $E_{H,\text{p}}$: solid line 400 K, dashed line 600 K, dot-dashed 800 K, dots 1000 K. Fixed parameters are $F_H = 10^{-10}$, $E_{H,\text{p}} = 510$ K, $E_S = 200$ K, $E_{H,\text{c}} = 10,000$ K and $\mu = 0.02$. (b) H$_2$ recombination efficiency for 4 different energies of chemisorbed H desorption, $E_{H,\text{c}}$: Solid line 15,000 K, dashed line 10,000K, dot-dashed 8000 K, dots 5000 K. Fixed parameters are $F_H = 10^{-10}$, $E_{H,\text{p}} = 340$ K, $E_{H,\text{p}} = 600$ K, $E_S = 200$ K and $\mu = 0.02$.

Table 4.1. Model parameters for silicate and carbonaceous surfaces

<table>
<thead>
<tr>
<th>Surface</th>
<th>$E_{H,\text{p}}$</th>
<th>$\mu$</th>
<th>$E_S$</th>
<th>$E_{H,\text{p}}$</th>
<th>$E_{H,\text{c}}$</th>
<th>$\nu_{H,\text{p}}$</th>
<th>$\nu_{H,\text{c}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Olivine</td>
<td>340</td>
<td>0.3</td>
<td>200</td>
<td>650</td>
<td>$\sim$30000</td>
<td>$2 \times 10^{12}$</td>
<td>$1 \times 10^{13}$</td>
</tr>
<tr>
<td>Carbon</td>
<td>540</td>
<td>0.4</td>
<td>250</td>
<td>800</td>
<td>$\sim$30000</td>
<td>$3 \times 10^{12}$</td>
<td>$2 \times 10^{13}$</td>
</tr>
</tbody>
</table>

$E_{H,\text{p}}$, $E_{H,\text{p}}$, and $E_{H,\text{c}}$ are the desorption energies of H$_2$, physisorbed H (H$_{\text{p}}$) and chemisorbed H (H$_{\text{c}}$), and $E_S$ is the energy of the saddle point between two physisorbed sites. $\mu$ is the fraction of the newly formed H$_2$ which stays on the surface and $\nu_{H,\text{p}}$ and $\nu_{H,\text{c}}$ are the vibrational frequencies of H$_2$ and H in their surface sites. The frequency factor for each population $i$ is written as $\nu_i = \sqrt{\frac{2 N_S E_i}{m_i}}$, where $N_S$ is the surface number density of sites on the grain, $m$ the mass of the species, and $E_i$ the energy of the site where the species is bound (physisorbed or chemisorbed). (a). For more details about the determination and calculation of these parameters, see Cazaux & Tielens (2003).

The H$_2$ recombination efficiency on olivine and carbonaceous grains as functions of the flux and the temperature is presented in Fig. ??.
Figure 4.5. H\textsubscript{2} recombination efficiency as a function of the dust temperature and the flux for olivine grains (left) and for amorphous carbon grains (right).

C. The H\textsubscript{2} formation rate

In astrophysical environments, the recombination rate can be written as

\[ R_d = \frac{1}{2} n(H) v_{TH} n_d \sigma_d \epsilon_{H2} S_{H1}, \]  

(4.2)

where \( n(H) \) and \( v_{TH} \) are the number density and the thermal velocity of H atoms in the gas phase, \( n_d \sigma_d \) is the total cross section of interstellar grains, \( \epsilon_{H2} \) is the recombination efficiency that is discussed in detail in (Cazaux & Tielens 2002) and \( S_{H1} \) is the sticking coefficient of the H atoms which depends both on the dust and the gas temperature. \( S_{H1} \) is given by (Hollenbach and McKee 1979)

\[ S_{H1}(T) = \left( 1 + 0.4 \times \left( \frac{T_d + T_g}{100} \right)^{0.5} + 0.2 \times \frac{T_g}{100} + 0.08 \times \left( \frac{T_g}{100} \right)^2 \right)^{-1}, \]  

(4.3)

where \( v_{TH} \) is of the order of \( 1.45 \times 10^5 \frac{T_g}{100} \text{ cm s}^{-1} \). We consider typical grains with a radius of 0.1 \( \mu \text{m} \) and a material density of 3 g cm\(^{-3}\) (Hollenbach and McKee 1979). Therefore, the typical mass of a dust grain is about \( 1.256 \times 10^{-14} \text{ g} \). We can write \( n_d = 1.329 \times 10^{-10} \xi_d n_{H1} \), where \( \xi_d \) is the dust to gas mass ratio, which is equal to 0.01 under Galactic conditions, and \( n_{H1} \) is the density of hydrogen in all forms. The recombination rate can be written as

\[ R_d = 3.025 \times 10^{-17} \epsilon_{H2} \frac{\xi_d}{0.01} n_{H1} n(H) S_{H1} \frac{T_g}{100}, \]  

(4.4)

as previously calculated by Tielens & Hollenbach (1985). Due to the functional dependence of \( S_{H1} \) on the gas and dust temperature, the choice of olivine or amorphous carbon as the
substrate is of little consequence for the temperature behavior of $R_d$ and we take olivine as the substrate in the remainder of the paper. This choice is illustrated in Fig. 4.6, where $R_d$ is plotted as a function of $T_g$ and $T_d$ for a hydrogen density $1 \text{ cm}^{-3}$ and $\xi_d = 0.01$. For the gas and dust temperatures of interest in this work, the substrates give similar behaviors of $R_d$ within a factor of two.

Figure 4.6. H$_2$ recombination rate as a function of the dust and the gas temperature for olivine grains (left) and for amorphous carbon grains (right).

4.2.2 The H$^-$ route

In the absence of dust particles, H$_2$ can be formed through gas phase reactions. This gas phase route is driven by the recombination of H atoms with H$^-$ ions,

$$\text{H} + \text{H}^- \rightarrow \text{H}_2 + e^-,$$

and has a rate coefficient $k_2$ that is approximately constant in the temperature range between 100 K and 32,000 K, with $k_2 = 1.3 \times 10^{-9} \text{ cm}^3 \text{ s}^{-1}$ (De Jong 1972; Haiman, Thoul & Loeb 1996; Schmeltekopf, Fehsenfeld & Ferguson 1967). The equilibrium H$^-$ density is determined by the relation (Donahue & Shull 1991; De Jong 1972)

$$n_{H^-} = \frac{k_3 n_{H} n_{e}}{k_2 n_{H} + k_3 J_{21} + k_4 n_{H^+}},$$

where $n(H) \approx n_{H_2}$ and $k_1$ is the formation rate of H$^-$ via electron attachement, $\text{H} + e^- \rightarrow \text{H}^- + h\nu$, with $k_1 = 1.83 \times 10^{-18} T_g^{0.8770}$. We consider three main processes responsible for the disappearance of H$^-$. First, associative detachment, $\text{H}^- + \text{H} \rightarrow \text{H}_2 + e^-$, that we consider to be the most important gas phase route to form H$_2$, with a rate coefficient $k_2$ (as discussed
above). Second, photodetachment, $\text{H}^- + h\nu \rightarrow \text{H} + e^-$ with a rate coefficient $k_3 \times J_{21}$, where $J_{21}$ is the radiation field in units of $10^{-21}$ erg s$^{-1}$ cm$^{-2}$ Hz$^{-1}$, and $k_3 = 3.1 \times 10^{-11}$. Third, mutual neutralization, $\text{H}^- + \text{H}^+ \rightarrow 2\text{H}$ with a rate coefficient $k_4 = 7 \times 10^{-7} T^{-0.5}$ cm$^3$ s$^{-1}$. We assume that the disappearance of $\text{H}^-$ is mainly due to the formation of $\text{H}_2$ and we neglect the neutralization of $\text{H}^-$ by ionizing radiation or by the encounter with $\text{H}^+$ (Donahue & Shull 1991). These assumptions are valid for the radiation field that we adopt below. Therefore, we can write the equilibrium $\text{H}^-$ density as

$$n_{\text{H}^-} = \frac{k_1 n_e}{k_2}, \quad (4.7)$$

and we write the $\text{H}_2$ formation rate through the $\text{H}^-$ route as

$$R_g = k_1 n_{\text{H}^-}^2 \xi_e, \quad (4.8)$$

with $\xi_e$, the electron abundance given by $\xi_e = \frac{n_e}{n_{\text{H}^-}}$.

### 4.3 $\text{H}_2$ formation at high redshift

#### 4.3.1 A comparison between the $\text{H}^-$ and dust grain routes to $\text{H}_2$ formation

We first compare the microphysics of $\text{H}_2$ formation on dust grains and in the gas phase by treating the most influential variables as completely free. Our motivation is the substantial uncertainty that still exists regarding the dust and gas temperature of primordial gas as well as the free electron abundance and FUV radiation field at high redshift. The general results of this section can be incorporated by the reader into any cosmological model. We compute the ratio of $\text{H}_2$ formation through the dust and gas routes as

$$\frac{R_d}{R_g} = 1.65 \times 10^3 \frac{\xi_e}{\xi_{\text{e}}} \frac{S_{\text{H}}}{T_g^{0.8779}} \epsilon_{\text{H}_2} \sqrt{\frac{T_g}{100}} \quad (4.9)$$

Figs. 4.7 and 4.8 show the ratio $R_d/R_g$ as functions of $T_d$, $T_g$, and $\xi_e$. We find that the dust to electron ratio $\xi_e$ is the dominant parameter for the behavior of the ratio $R_d/R_g$.

In Fig. 4.9 we present the surface $\frac{R_d}{R_g}=1$ as a function of the 3 free parameters. These two figures show for which conditions the gas phase route and the dust grain route to $\text{H}_2$ formation are equal. At low dust grain temperatures, as shown by Fig. 4.9, the required ratio $\xi_e$ varies considerably. This is easily explained by the fact that at these temperatures, $\text{H}_2$ once formed, mostly stays on dust grains (the temperature of the grain is then too low to enable evaporation). Therefore, for these considered temperatures, $\text{H}_2$ formation through the dust route is extremely small, and the physical conditions to obtain the equality through the two different routes give a extremely high ratio $\xi_e$. This range of temperatures is quite small (between 0 and 10K). Because we know that the grain temperature is typically larger than 10K, we consider a range of temperatures between 10 and 100K for the dust grains. For this considered range, as shown in Fig. 4.9, the ratio $\frac{\xi_e}{\xi_{\text{e}}}$ required for $\frac{R_d}{R_g}=1$, varies slightly with the dust and the gas temperature. In conclusion, $\text{H}_2$ formation through the $\text{H}^-$ route is equal to $\text{H}_2$ formation through the dust route if the ratio $\frac{\xi_e}{\xi_{\text{e}}}$ lies between 0.1 and 0.8.
4.3. H₂ formation at high redshift

Figure 4.7–. Dust to H⁻ route ratio for the H₂ formation rate as a function of \( \xi_e / \xi_d \) and the temperature of the dust \( T_d \). The gas temperature is set at 100 K (left) and at 500K (right).

4.3.2 Cosmological evolution of physical quantities

Model

In order to make a cosmological assessment of the relative importance of the dust grain and H⁻ route contributions to the total H₂ formation rate, we adopt a cosmological model for the density, dust abundance, electron abundance and radiation field strength as a function of redshift. Our microscopic model shows that the equivalence of the dust grain and H⁻ route to form H₂ occurs for a dust to electron ratio \( \xi_d / \xi_e \) between 0.1 and 0.8. Therefore, in this section, we construct a cosmological model to estimate at which redshift this equivalence occurs, if at all. Like in Norman & Spaans (1997) and Hirashita, Hunt, & Ferrara (2002), we consider a disk galaxy with a radius \( R_{disk} \) and a scale height \( H \). \( R_{disk} \) depends on the redshift as \( R = 10(\Omega_{b,g} / \Omega_c) \frac{1}{(1 + z)^{1/3}} \) kpc, where \( \Omega_{b,g} \) is the baryonic mass fraction in the protogalactic disk, following the treatment of Kauffmann (1996) for a biasing parameter of \( b \approx 1.5 \). The height to disk size ratio, \( \eta = H/R \), as discussed by Norman & Spaans (1997), is of the order of 0.01-0.03, although this value is uncertain and can be as high as 0.1 (Hirashita, Hunt, & Ferrara 2002). We wish to emphasize that the model galaxy constructed here is intended to represent a dwarf or sub-\( L^* \) disk galaxy, typical of the bulk of all disk galaxies, that starts to form stars at a redshift of a few and continues to do so at a relatively vigorous pace (much like the Milky Way and the LMC).
Figure 4.8. Dust to \( \text{H}^\text{-} \) route ratio for the \( \text{H}_2 \) formation rate as a function of the temperature of the dust \( T_\text{dust} \) and of the gas \( T_\text{gas} \). The dust to electron ratio \( \xi_\text{dust}/\xi_\text{e} \) is set at 0.01 (left) and at 1 (right).

**Electron density**

The adopted electron fraction, \( \xi_\text{e} \), as described by Norman & Spaans (1997), following Donahue & Shull (1991), is written as

\[
\xi_\text{e} = 0.02 T_\text{gas}^{0.42} \sqrt{\frac{J_{21}}{n_\text{H}}} \quad (4.10)
\]

We consider the radiation field to be a combination of a background UV radiation field and an internally generated UV radiation field.

\[
J_{21} = J_{21}^{\text{background}} + J_{21}^{\text{internal}}. \quad (4.11)
\]

In our model, we consider the gas to be optically thick around 1000 \( \text{Å} \), and the spectral index of the radiation field to be \( \alpha = 5 \), which is typical for a radiation field produced by massive stars. Note that a spectral index of \( \alpha = 1 \) would be appropriate for a radiation field produced by quasars. In our model we consider only the contribution made by massive stars. Therefore, the background radiation field, as discussed in Kitayama & Ikeuchi (2000), can be written as

\[
J_{21}^{\text{background}} = 8.18 \times 10^{-13} I_{21} \tau_\perp^2 (\nu_{\text{H}1}) s^{-1}, \quad (4.12)
\]

where \( \tau_\perp \) is the optical depth perpendicular to the disk, given by \( \tau_\perp = 6.3 \times 10^{-18} N_\perp \) with \( N_\perp \) the hydrogen column density perpendicular to the disk. \( I_{21} \) is the UV background intensity, in units of \( 10^{-21} \text{ ergs s}^{-1} \text{ cm}^{-2} \text{ str}^{-1} \text{ Hz}^{-1} \), which depends on the redshift, and can be written (Kitayama & Ikeuchi 2000) as

\[
I_{21} = \left( \frac{1+z}{7} \right)^{-6} \quad 6 \leq z \leq 20 \quad (4.13)
\]
4.3. H₂ formation at high redshift

Figure 4.9–. These surfaces represent the different conditions under which the dust route contribution to the H₂ formation rate is equal to that of the H⁺ route for low dust temperatures. The dust to electron ratio \( \frac{\Phi_d}{\epsilon} \) is plotted as a function of \( T_d \) and \( T_e \) for low dust temperatures from 4 to 10 K (left), and for higher dust temperatures from 10 to 100 K (right). Note that on the left panel, \( \log(\frac{\Phi_d}{\epsilon}) \) is plotted because this quantity varies enormously for the considered range in dust temperatures.

\[
I_{21} = 1 \quad 3 \leq z \leq 6 \tag{4.14}
\]

\[
I_{21} = \left( \frac{1 + z}{4} \right)^4 \quad 0 \leq z \leq 3. \tag{4.15}
\]

The internal UV radiation field, as discussed by Norman & Spaans (1997), results from stellar emission and thus depends on the star formation rate. Therefore, we can use equation 4.12 to obtain

\[
J_{21}^{\text{internal}} = 8.18 \times 10^{-13} \left( \frac{\Phi_d}{\epsilon} \right)^{\frac{8}{7}} (\nu H I) s^{-1} \tag{4.16}
\]

where \( J_{21}^{\text{internal}} \) has the same units as \( I_{21} \) and is directly proportionnal to the star formation rate (SFR), and \( \tau || = 6.3 \times 10^{-18} N || \) with \( N || \) the hydrogen column density along the radius of the disk. We compute the SFR in our model using Hirashita & Ferrara (2002) at high redshift \( z \geq 5 \), and we match it onto the Madau plot for \( z \leq 5 \). At low redshift, we assume the SFR to be constant with a value comparable to the Galactic value of \( 3 M_\odot \text{yr}^{-1} \). For redshifts between 3 and 9, we parameterize the SFR as \( a (1 + z)^b \), with \( a \) and \( b \) determined by the limit conditions at \( z = 3 \) and \( z = 9 \). At high redshift, from 9 to 20, we assume the SFR to be constant with a value of 0.003 \( M_\odot \text{yr}^{-1} \). Hence,

\[
SFR = 0.003 \quad 9 \leq z \leq 20 \tag{4.17}
\]

\[
SFR = 10^5 (1 + z)^{-7.5} \quad 3 \leq z \leq 9 \tag{4.18}
\]

\[
SFR = 3 \quad 0 \leq z \leq 3 \tag{4.19}
\]
The above is a purely pragmatic approach whose only purpose is to define a reasonable star formation history for a model disk galaxy. This parameterization is not intended as an attempt to explain the Madau plot.

For the hydrogen column densities parallel and perpendicular to the disk, we consider in our calculations a disk with a radius $R_{\text{disk}}$ and an height $H$ as given above. Therefore, the hydrogen column densities are written as

$$N_{\parallel} = n_H \frac{R_{\text{disk}}}{2}, \tag{4.20}$$

where we adopt a mean distance between the stellar sources and the bulk of hydrogen gas equal to $\frac{R_{\text{disk}}}{2}$, typical for a system where most of the baryonic mass and light are concentrated within $R_{\text{disk}}$.

$$N_{\perp} = n_H \eta R_{\text{disk}}, \tag{4.21}$$

where $n_H$ evolves with redshift as $n_H = 5(\frac{\Omega_M}{0.01})(1 + z)^3$ (Norman & Spaans 1997).

**Dust abundance**

We can compute the dust-to-gas mass ratio, following Norman & Spaans (1997) from:

$$\xi_d = \frac{2}{3} \frac{M_d}{M_g} \frac{y \times \beta}{H_0 \times M(z_d)} \int_{z_d}^{1} SFR \frac{dz}{(1 + z)^2}, \tag{4.22}$$

where $\xi_d \approx \frac{1}{3}$ is the fraction of metals locked into grains, $y \approx 0.02$ is the yield of metals like C and O (Woosley & Weaver 1995), $\beta = 0.12$ is the fraction of stars formed that will become supernovae (Yepes et al. 1997), $H_0 = 75$ km/s/Mpc is the Hubble constant and $M \sim 7 \times 10^9 \ M_\odot$ is the gas mass of the galaxy at redshift 0, typical of a galaxy that has converted a substantial fraction of its original gas mass into stars, but still contains a large reservoir of gas as well (like the Milky Way and the LMC). For these numbers, our model galaxy contains about an order of magnitude more mass in the form of stars as it does in the form of atomic hydrogen at $z = 0$ (Zwaan et al. 1997). Finally, the integral in the equation above is the contribution to the metallicity of the gas by stars that have ended their evolution at a redshift larger than $z_d$.

**Results**

The cosmological model that we adopt for the dust abundance and the electron fraction exhibits a strong redshift dependence. In Fig. 4.10, the electron fraction is presented as a function of the gas temperature and the redshift. We note the strong dependence of the electron fraction on redshift and the weak dependence it has on the gas temperature $T \sim \tau^{0.42}$. The decreasing electron fraction with increasing redshift is easily explained by the fact that $T \sim n_H R_{\text{disk}} \sim (1 + z)^2$ and $J_2 \sim \tau^{-8/3}$. The resulting value of $\xi_d$ at $z \sim 0$ is consistent with the electron abundance of the Milky Way and the LMC in the diffuse/ionized ISM.

In Fig. 4.11 the dust abundance is presented. The slope of this curve follows our adopted star formation law. At a redshift of zero the dust abundance is comparable to that of the LMC. We feel that such a limiting value for $\xi_d$ is a sensible one to use for the bulk of the baryonic matter residing in dwarf and sub-L* galaxies.
4.3. $H_2$ formation at high redshift

![Figure 4.10](image)

**Figure 4.10**. The electron density plotted as a function of the temperature of the gas $T_g$ and the redshift. Note the weak dependence of $\zeta_e$ on the gas temperature in comparison to the redshift dependence.

![Figure 4.11](image)

**Figure 4.11**. The dust-to-gas mass ratio as a function of the redshift for our model disk galaxy, see the text for parameter values.

The ratio of the dust abundance over the electron fraction is calculated with our cosmological model and is presented in Figs. 4.12. In these two figures we overplotted our microscopic model in order to determine at which conditions the dust or the $H^-$ route dominates. The flat surface (which is independent of redshift) represents the dust to electron ratio for which the dust route contribution to the $H_2$ formation rate is equal to that of the $H^-$ route.
according to our microscopic model. The other surface represents the cosmological model. The section of the cosmological surface above the plane surface determines the cosmological parameters for which the dust route dominates. Conversely, the section of the cosmological surface below the plane surface shows the cosmological parameters for which the H$^-$ route dominates. For low dust temperatures (around 10 K) the gas phase route is the dominant process until a redshift of 3, for a gas temperature of 500 K, and until a redshift of 5, for a gas temperature of 100 K. After this phase, the dust route dominates until \( z \sim 0 \). For larger dust temperatures (around 100 K), the gas phase route dominates until a redshift of 4, for a gas temperature of 100 K. For higher gas temperatures, the gas phase route dominates until lower redshift. Finally, for gas temperature higher than 350 K, the gas phase route is the dominant \( \text{H}_2 \) formation process for all redshifts.

**Figure 4.12-.** The dust to electron ratio \( \frac{\text{Dust}}{\text{Electron}} \) is plotted as a function of the temperature of the gas and the redshift, for a fixed dust temperature of 10 K (left) and 100 K (right). The plane surface represents the dust to electron ratio for which the dust route contribution to the H\(_2\) formation rate is equal to that of the H$^-$ route according to our microscopic model. The other surface represents the cosmological model. The section of the cosmological surface above the plane surface determines the cosmological parameters for which the dust route dominates. Conversely, the section of the cosmological surface below the plane surface shows the cosmological parameters for which the H$^-$ route dominates. Left: The figure shows that the dust route dominates, for a dust temperature of 10 K, below a redshift of 3-5, depending on the ambient gas temperature. Right: This figure shows that the dust route dominates, for a dust temperature of 100 K, below a redshift of 4 if the gas temperature is of the order of 100 K. However, for high gas temperatures, the H$^-$ route can dominate at any redshifts.

### 4.4 Conclusions and discussion

We have studied the formation of H\(_2\) on dust grain surfaces at high redshift and we have related our results to the contribution made by gas phase reactions, i.e., through the H$^-$
route. We have found that the substrate (olivine or amorphous carbon) has a modest impact on the resulting H\textsubscript{2} formation rate. The recombination efficiency depends strongly on the dust temperature below 10 K and above 200-300 K. The role of the gas temperature is more limited, but suppresses the H\textsubscript{2} formation rate above several hundred K due to a reduced sticking coefficient. We wish to stress that the microphysical results on the recombination efficiency and the H\textsubscript{2} formation rate are robust and independent of any galactic context.

We adopted a cosmological model to determine at which cosmological parameters the dust and gas phase contributions to the H\textsubscript{2} formation rate are equal, and thus when, in the universe’s history, the dust grain route becomes the dominant H\textsubscript{2} formation process. That is, when the presence of dust, a result of star formation, leads to an enhancement of the H\textsubscript{2} formation rate, which in turn can boost the H\textsubscript{2} abundance (depending on the internal FUV radiation field that can dissociate H\textsubscript{2}) and hence the ambient cooling rate. Such a cycle constitutes a positive feedback loop (Hirashita, Hunt, & Ferrara 2002) and can enhance the star formation rate inside a galaxy.

Our results show that, within the uncertainties of our cosmological model for the evolution of disk galaxies, the conditions for this positive feedback first occur at a redshift between 3 and 5 and for a dust-to-gas mass ratio $10^{-4}$-$10^{-3}$ times lower than Galactic. This redshift range is large and depends strongly on the dust grain and gas temperatures (microphysics) that we adopted as well as on the star formation rate (macrophysics) that we used. Indeed, for high dust/gas grain temperatures, the atoms desorb/bounce from/off the grain surface which decreases the H\textsubscript{2} formation rate. On the other hand, a high gas temperature favors gas phase formation of H\textsubscript{2}. This clearly shows the importance of both dust and gas temperature to determine which of these two routes dominates. At very high redshift, $z > 15-20$, the temperature of the dust is coupled to the temperature of the CMB, which increases like $1+z$. The dust grains are then too warm to allow an important dust route contribution. So even if dust would be present at these redshifts, it would not boost the H\textsubscript{2} formation rate until the universe had cooled down considerably through cosmological expansion.

In fact, once the presence of dust boosts the H\textsubscript{2} formation rate, and hence the star formation rate through the enhanced cooling rate, around $z \sim 3-5$, the production of stellar photons will raise the mean dust (and gas) temperature. This constitutes a minor effect when the shielding dust columns are large and the McKee criterium is satisfied (McKee 1989), but might be quite important in the first, metal-poor stages of star formation. In any case, the magnitude of the positive feedback that the presence of dust has on the H\textsubscript{2} formation rate requires a careful treatment of the impact that (enhanced) star formation activity has on the dust (and gas) thermal equilibrium. We postpone these matters to a future paper.

Finally, recent observations of distant quasars (Bertoldi et al. 2003) at redshifts around $z\sim6$ showed that these objects possess a metallicity close to solar. These quasars represent large over-densities in the Universe and our study concentrates on the evolution of a typical sub-L* galaxy, that we assume to be more representative of the average galaxy population. In any case, these distant quasars, rich in metals, possess both a high dust grain abundance and the physical conditions to allow efficient H\textsubscript{2} formation on dust surfaces.