Formation and evolution of molecular hydrogen in disc galaxies with different masses and Hubble types

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ABSTRACT

We investigate the physical properties of molecular hydrogen ($H_2$) in isolated and interacting disc galaxies with different masses and Hubble types by using chemodynamical simulations with $H_2$ formation on dust grains and dust growth and destruction in interstellar medium. We particularly focus on the dependences of $H_2$ gas mass fractions ($f_{H_2}$), spatial distributions of $H_1$ and $H_2$, and local $H_2$-scaling relations on initial halo masses ($M_h$), baryonic fractions ($f_{\text{bary}}$), gas mass fractions ($f_g$), and Hubble types. The principal results are as follows. The final $f_{H_2}$ can be larger in disc galaxies with higher $M_h$, $f_{\text{bary}}$, and $f_g$. Some low-mass disc models with $M_h$ smaller than $10^{10} M_{\odot}$ show extremely low $f_{H_2}$ and thus no/little star formation, even if initial $f_g$ is quite large ($>0.9$). Big galactic bulges can severely suppress the formation of $H_2$ from dust grains whereas strong stellar bars cannot only enhance $f_{H_2}$ but also be responsible for the formation of $H_2$-dominated central rings. The projected radial distributions of $H_2$ are significantly more compact than those of $H_1$ and the simulated radial profiles of $H_2$-to-$H_1$-ratios ($R_{\text{mol}}$) follow roughly $R^{-1.5}$ in Milky Way-type disc models. Galaxy interaction can significantly increase $f_{H_2}$ and total $H_2$ mass in disc galaxies. The local surface mass densities of $H_2$ can be correlated with those of dust in a galaxy. The observed correlation between $R_{\text{mol}}$ and gas pressure ($R_{\text{mol}} \propto P_g^{0.92}$) can be well reproduced in the simulated disc galaxies.

Key words: stars: formation – ISM: molecules – galaxies: evolution – galaxies: ISM – infrared: galaxies.

1 INTRODUCTION

Formation and evolution processes of molecular hydrogen ($H_2$) and interstellar dust in galaxies can be strongly coupled, because the surface of dust grains can be the major formation sites of $H_2$ (e.g. Gould & Salpeter 1963; Hollenbach & Salpeter 1971). Dust has long been considered to play decisive roles in several aspects of star and galaxy formation, such as radiative cooling processes in star-forming clouds (e.g. Herbst 2001) and the formation of metal-poor low-mass stars in the early universe (e.g. Schneider & Omukai 2010). Likewise, $H_2$ is an essential element in giant molecular clouds (GMCs) where star formation (SF) is ongoing (e.g. Blitz et al. 2007; Fukui & Kawamura 2010) and its physical properties (e.g. mass densities) are key parameters for the observed star formation laws in galaxies (e.g. Bigiel et al. 2008; Leroy et al. 2011). Thus, the better understanding of the formation and evolution processes of both dust and $H_2$ in interstellar medium (ISM) can lead to the deeper understanding of galaxy formation and evolution in general.

Physical properties of $H_2$ have long been investigated for galaxies with different Hubble types (e.g. Young & Scoville 1991, hereafter YS91; Boselli et al. 2014), in different environments (e.g. Leon, Combes & Menon 1998; Wilson et al. 2009), and at different redshifts (e.g. Daddi et al. 2010; Tacconi et al. 2010; Bauermeister et al. 2013), and their origins have not been clarified yet. Recent extensive observational studies on $H_1$ and $H_2$ properties of galaxies and their correlations of galaxy parameters for a large number of galaxy samples have provided valuable information on scaling relations of gas and stars and thus new constraints on galaxy formation and evolution. (e.g. Catinella et al. 2010; Saintonge et al. 2011). Resolved structures and kinematics of GMCs in nearby galaxies such as M31, M33, and the Large Magellanic Cloud (LMC) have enabled astronomers to reveal the physical factors for the conversion from $H_1$ to $H_2$ and the possible typical lifetime of GMCs in galaxies (e.g. Blitz et al. 2007; Fukui & Kawamura 2010).

In spite of these observational progresses, a number of key long-standing problems on $H_2$ properties of galaxy have not been resolved yet. Among them is the origin of the diverse $H_2$ properties along the Hubble sequence (e.g. YS91). It is well known that the mass ratio of $H_2$ to $H_1$ (referred to as $R_{\text{mol}}$) is quite diverse (more than two orders of magnitudes) for a given Hubble type and it is systematically higher in early-type disc galaxies (YS91). This diverse
H$_2$ properties along the Hubble sequence has been confirmed in the latest observations with a larger number of galaxy samples (e.g. Boselli et al. 2014). It is theoretically unclear what global galaxy parameters (e.g. bulge-to-disc ratios) can determine the observed H$_2$-to-H I ratios ($R_{H_2}$) in galaxies.

Furthermore, one of other unresolved problems is related to the observed radial distributions of H$_2$ in galaxies and their correlations with stellar parameters of galaxies (e.g. Blitz et al. 2007). Wong & Blitz (2002) showed that the ratio of H$_2$ to H I surface density in a galaxy depends on the projected distance ($R$) from the galactic centre such that it can be best fit to $R^{-1.5}$ (or $R^{-1}$, see their fig. 14). Some early-type spirals (e.g. M31) are observed to have intriguing ring-like structures (e.g. YS91). Recent observations have revealed that the mass ratio of H$_2$ to stars ($M_{H_2}/M_*$) is quite different between galaxies with different Hubble types and even within a same type (e.g. Boselli et al. 2014). These observations have not been explained clearly by previous theoretical studies of galaxy formation and evolution, though they would have some profound implications on galaxy formation.

Recent significant progresses in observational studies of H$_2$ properties of galaxies with different types at different $z$ appear to have triggered extensive theoretical and numerical studies of H$_2$ formation in galaxies. For example, recent numerical simulations of galaxy formation and evolution have incorporated the conversion of H$_2$ formation from H I on dust grains (e.g. Pelupessy, Papadopoulos & van 2006; Robertson & Kravtsov 2008; Gnedin, Tassis & Kravtsov 2009; Christensen et al. 2012; Kuhlen et al. 2012; Thompson et al. 2014). Recent semi-analytic models of galaxy formation (e.g. Fu et al. 2010; Lagos, Lacey & Baugh 2012) adopted the H$_2$ formation model-dependent gaseous metallicities and densities proposed by Krumholz, McKee & Tumlinson (2009) and thereby investigated the time evolution of H$_2$ contents in galaxies.

However, these previous numerical studies of galaxy formation and evolution with H$_2$ formation have not incorporated the evolution of dust (e.g. abundances and masses) explicitly in their models, and accordingly could not discuss the importance of the joint evolution of dust and H$_2$. It is ideal for any theoretical studies of H$_2$ formation in galaxies to include the formation and evolution processes of both dust and H$_2$ in a self-consistent manner, because their evolution can be strongly coupled through SF. Given that recent observational studies have revealed a number of important correlations between dust and H$_2$ properties in galaxies (e.g. Corbelli 2012), it would be essential for theoretical studies of H$_2$ formation in galaxies to incorporate a model for the formation and evolution of dust in ISM.

Our previous studies constructed a new chemodynamical model that includes both the H$_2$ formation on dust grains and the formation and destruction of dust in ISM in a self-consistent manner (Bekki 2013a, 2014; hereafter B13a and B14, respectively; Yozin & Bekki 2014b). They therefore could discuss the time evolution of dust and H$_2$ properties in galaxies at their formation epochs. However, they did not discuss how the physical properties of H$_2$ in galaxies can possibly depend on their global parameters such as their total masses and Hubble types. Therefore, the following three questions are unresolved: (i) what can drive the observed diversity in H$_2$ properties between different galaxies, (ii) whether and how dust can play a role in controlling H$_2$ properties of galaxies, and (iii) what is responsible for the observed H$_2$–dust correlations in galaxies.

The purpose of this paper is twofold as follows. First, we investigate whether the adopted model of H$_2$ formation self-consistently including dust evolution can explain the observed fundamental properties of H$_2$ in galaxies. In this first investigation, we focus particularly on the observed correlations between mass ratios of H$_2$ to H I and other galaxy parameters (e.g. Wong & Blitz 2002; Blitz & Rosolowsky 2006; Blitz et al. 2007). Second, we investigate how the physical properties of H$_2$ in galaxies depend on the total halo masses ($M_h$), baryonic mass fractions ($f_{\text{baryon}}$), gas mass fractions ($f_g$), Hubble types (e.g. bulge-to-disc ratios, $f_b$), and the formation redshifts of galaxies by using mainly isolated models of disc and dwarf galaxies. We also try to understand how galaxy interaction can influence the time evolution of global H$_2$ properties of galaxies in this second investigation.

The plan of the paper is as follows. We describe some details of the chemodynamical model with the formation and evolution of dust and H$_2$ adopted by the present study in Section 2. We present the numerical results on the physical correlations between H$_2$ properties and galaxy parameters (e.g. masses) in disc galaxies in Section 3. In this section, we also discuss the dependences of the results on the adopted model parameters. In Section 4, we discuss the latest observational results on H$_2$ properties of galaxies and provides some implications of some key results derived in this paper. We summarize our conclusions in Section 5.

In the present paper, we do not discuss the latest results from Atacama Large Millimeter/submillimeter Array (ALMA), such as the molecular outflow driven by active galactic nuclei (AGN; e.g. Combes et al. 2014) and total ISM masses probed by dust emission in 107 galaxies from $z = 0.2$ to 2.5 (Scoville et al. 2014). These new observational results will be addressed by our future works with a more sophisticated chemodynamical model with H$_2$ formation.

2 THE MODEL

2.1 A new simulation code

We adopt our new simulation code recently developed in our previous works (B13a, B14) in order to investigate spatial and temporal variations of H$_2$ in disc galaxies with different masses and Hubble types. The adopted code can be run on GPU-based machines (clusters), where gravitational calculations can be done on GPUs whereas other calculations (e.g. SF and hydrodynamics) can be done on CPUs. The code adopts the smoothed particle hydrodynamics (SPH) method for following the time evolution of gas dynamics in galaxies.

The present simulations include the formation of dust grains in the stellar winds of supernovae (SNe) and asymptotic giant branch (AGB) stars, the time evolution of interstellar radiation field (ISRF), the growth and destruction processes of dust in the ISM, the H$_2$ formation on dust grains, and the H$_2$ photodissociation due to far-ultraviolet (FUV) light in a self-consistent manner. Although we can investigate the formation of polycyclic aromatic hydrocarbon (PAH) dust in carbon-rich AGB stars and the time evolution of dust by using the simulation code, we do not extensively investigate the dust properties in the present study. Instead, we briefly discuss the possible physical correlations between dust and H$_2$ properties in disc galaxies.

The new simulation code does not include the effects of feedback of AGN on ISM and the growth of supermassive black holes (SMBHs) in galaxies so that we cannot investigate how the feedback can change the spatial distributions and mass budgets of dust and H$_2$ in galaxies. Although it is an important issue whether and how the AGN feedback effects can influence the dust properties of ISM and thus the H$_2$ contents, we will discuss this in our future papers.

The new code allows us to choose whether some physical effects (e.g. dust formation etc.) are included or excluded (i.e. ‘switched
on or off') so that we can investigate how the physical effects are important in the evolution of gas and stars in galaxies. Accordingly, we summarize the physical effects that are included in the present study in Table 1 for clarity.

Since the major formation site of H₂ in ISM is the surface of dust grains, it is crucial for any theoretical study on H₂ evolution of galaxies to properly investigate the time evolution of dust abundances in disc galaxies. Given that both observational and theoretical studies have shown that dust-to-metal ratios can be diverse (e.g. Hirashita 1999; Galametz et al. 2011), we need to refrain from deriving dust abundances from metallicities by assuming constant dust-to-metal ratios. The present code indeed enables us to investigate the time evolution of different dust components in galaxies so that we can more properly predict the time evolution of H₂ in galaxies. We mainly focus on isolated disc galaxies composed of dark matter halo, stellar disc, stellar bulge, and gaseous disc: some new results on H₂ properties in forming galaxies at high redshifts (z) are discussed in B14. Since the details of the physical models for the formation and evolution of dust and H₂ are given in B13a and B14, we briefly describe the models in the present paper.

### 2.2 A disc galaxy

#### 2.2.1 Structure and kinematics

The total masses of dark matter halo, stellar disc, gas disc, and bulge of a disc galaxy are denoted as \( M_h \), \( M_g \), \( M_{\text{gas}} \), and \( M_b \), respectively. The total disc mass (gas+stars) and gas mass fraction are denoted as \( M_a \) and \( f_g \), respectively, for convenience. The mass ratio of the disc \( (M_s + M_g) / M_h \) to the dark matter halo \( (M_h) \) in a disc galaxy is a ‘baryonic mass fraction’ and denoted as \( f_{\text{bary}} \). The bulge-to-disc ratio is defined as \( M_b / M_h \), and represented by a parameter \( f_b \). The four key parameters in the present study are \( M_h, f_g, f_{\text{bary}}, \) and \( f_b \).

In order to describe the initial density profile of dark matter halo in a disc galaxy, we adopt the density distribution of the Navarro–Frenk–White (NFW) halo (Navarro, Frenk & White 1996) suggested from cold dark matter (CDM) simulations:

\[
\rho(r) = \frac{\rho_0 (r/r_s)(1 + r/r_s)^2}{(1 + r/r_s)^2},
\]

where \( r \), \( \rho_0 \), and \( r_s \) are the spherical radius, the characteristic density of a dark halo, and the scale length of the halo, respectively. The \( \rho \) parameter \( (\rho = r_{\text{vir}}/\rho_\text{s}) \), where \( r_{\text{vir}} \) is the virial radius of a dark matter halo) and \( r_{\text{vir}} \) are chosen appropriately for a given dark halo mass \( (M_{\text{halo}}) \) by using the \( c-M_{\text{halo}} \) relation for \( z = 0 \) and 2 predicted by recent cosmological simulations (e.g. Neto 2007; Muñoz-Cuartas et al. 2011).

The bulge of a disc galaxy has a size of \( R_b \) and a scale length of \( R_{0,b} \) and is represented by the Hernquist density profile. The bulge is assumed to have isotropic velocity dispersion and the radial velocity dispersion is given according to the Jeans equation for a spherical system. The bulge-to-disc ratio \( (f_b = M_b/M_h) \) of a disc galaxy is a free parameter ranging from 0 (pure disc galaxy) to 4 (bulge dominated). The ‘Milky Way (MW)-type’ models are those with \( f_b = 0.17 \) and \( R_0 = 0.2R_s \), where \( R_s \) is the stellar disc size of a galaxy. We adopt the mass–size scaling relation of \( R_0 = C_b M_h^{0.5} \) for bulges so that we can determine \( R_b \) for a given \( M_h \). The value of \( C_b \) is determined so that \( R_b \) can be 3.5 kpc for \( M_h = 10^{10} M_\odot \) (corresponding to the mass and size of the MW’s bulge).

The radial \((R)\) and vertical \((Z)\) density profiles of the stellar disc are assumed to be proportional to \( \exp(−R/R_0) \) with scale length \( R_0 = 0.2R_s \) and to \( \sech^2(Z/Z_0) \) with scale length \( Z_0 = 0.04R_s \), respectively. The gas disc with a size \( R_g = 2R_s \) has the radial and vertical scale lengths of \( 0.2R_s \) and \( 0.02R_s \), respectively, for models other than the fiducial MW-type models. The radial and vertical scale lengths of the gas disc in the fiducial MW-type models are set to be \( 0.1R_s \) and \( 0.02R_s \), respectively. In the present model for the MW type, the exponential disc has \( R_s = 17.5 \) kpc and \( R_g = 35 \) kpc.

In addition to the rotational velocity caused by the gravitational field of disc, bulge, and dark halo components, the initial radial and azimuthal velocity dispersions are assigned to the disc component according to the epicyclic theory with Toomre’s parameter \( Q = 1.5 \). The vertical velocity dispersion at a given radius is set to be 0.5 times as large as the radial velocity dispersion at that point.

The total numbers of particles used for dark matter halo \( (N_{\text{dm}}) \), stellar disc \( (N_s) \), and gaseous disc \( (N_g) \) in a simulation are 700,000, 200,000, and 100,000 respectively. The total number of particle for bulge is \( f_b N_s \), which means that \( N_b = 33 \) 400 for the MW-type disc galaxy model with \( f_b = 0.167 \) and 400 000 for the big bulge model with \( f_b = 2 \). Therefore, the total number of particles is \( N = 1033 \) 400.
for the fiducial MW-type model and $N = 1400000$ for the big bulge model. The gravitational softening length for each component is determined by the number of particle used for each component and by the size of the distribution (e.g. $R$, and $r_{\text{vir}}$) and the value is described later.

### 2.2.2 Gas-phase metallicity and its radial gradient

Observations have shown that (i) there is a mass–metallicity relation in disc galaxies (e.g. Tremonti et al. 2004) and (ii) most of disc galaxies show negative metallicity gradients (i.e. higher metallicity in inner regions) with the slopes being different in different galaxies (e.g. Zaritsky et al. 1994). We therefore determine the initial mean metallicity of the gas disc in a galaxy according to the observed mass–metallicity relation for the adopted total halo mass ($M_h$) and gas mass fraction for the galaxy. For example, a MW-type disc galaxy with $M_h = 10^{12} M_\odot$ ($M_\star = 6 \times 10^{10} M_\odot$) and $f_g = 0.09$ (corresponding to the fiducial model later described) can have [Fe/H] = 0.

The gas-phase metallicity of each (gaseous and stellar) particle is given according to its initial position: at $r = R$, where $r (R)$ is the projected distance (in units of kpc) from the centre of the disc, the metallicity of the star is given as

$$[\text{Fe/H}]_{r=R} = [\text{Fe/H}]_{R=0} + \alpha R. \quad (2)$$

where $\alpha$ is the slope of the metallicity gradient in units of dex kpc$^{-1}$. Since the present results on global properties of $H_2$ do not depend on $\alpha$, we mainly show the results of the models with $\alpha = 0$. We however discuss briefly how the present results can change if we adopt a steeper metallicity gradient of $\alpha = -0.04$, which is the observed value of our MW (e.g. Andreewsky et al. 2004).

#### 2.2.3 Low-z versus high-z discs

Since we mainly investigate $H_2$ properties of disc galaxies at $z = 0$, we construct the disc model by using the $c-M_h$ relation for dark matter haloes at $z = 0$ (e.g. Neto 2007; Muñoz-Cuartas et al. 2011). We however investigate a number of disc models that can represent disc galaxies at high $z$ by using the $c-M_h$ relation dependent on $z$ (Muñoz-Cuartas et al. 2011). In constructing the disc models at high $z$, we consider the following two theoretical and observational results. First, the mean density of a dark matter halo ($\rho_{\text{dm}}$) with $M_h$ at $z$ is $(1 + z)^3$ times higher than that of a dark matter halo with the same $M_h$ at $z = 0$ ($\rho_{\text{dm},0}$). Second, the stellar disc size of a galaxy at $z$ ($R_\star$) is $(1 + z)^{-0.4}$ times larger than that at $z = 0$ ($R_{\star,0}$). Therefore, the mean density of a dark matter halo in a disc galaxy at $z = 0$ is as follows:

$$\rho_{\text{dm}}(z) = \rho_{\text{dm},0}(1 + z)^3, \quad (3)$$

where $r_{\text{vir}}(z) \propto \rho_{\text{dm},0}^{-1/3}$ for a given $M_h$. The stellar disc size is given as follows:

$$R_\star(z) = R_{\star,0}(1 + z)^{-0.4}, \quad (4)$$

which means that the size ratio of $r_{\text{vir}}$ to $R_\star$ is proportional to $(1 + z)^{-0.6}$. For example, $c$ and $r_{\text{vir}}$ for a disc galaxy with $M_h = 10^{12} M_\odot$ at $z = 0$ are 10 and 245 kpc, respectively, whereas they are 4.5 and 82 kpc at $z = 2$. The simulated dark matter haloes are assumed to have a scaling relation of $r_{\text{vir}} \propto M_h^{0.5}$ at $z = 0$ and 2.

#### 2.3 Star formation

Since SF can proceed in molecular clouds, we adopt the following ‘$H_2$-dependent’ SF recipe (B13a) using molecular gas fraction ($f_{H_2}$) defined for each gas particle in the present study. A gas particle can be converted into a new star if (i) the local dynamical time-scale is shorter than the sound crossing time-scale (mimicking the Jeans instability), (ii) the local velocity field is identified as being consistent with gravitationally collapsing (i.e. $\nabla v < 0$), and (iii) the local density exceeds a threshold density for SF ($\rho_{\text{th}}$). We mainly investigate the models with $\rho_{\text{th}} = 1$ cm$^{-3}$ in the present study.

A gas particle can be regarded as a ‘SF candidate’ gas particle if the above three SF conditions (i)–(iii) are satisfied. It could be possible to convert some fraction ($\alpha f_{H_2}$) of a SF candidate gas particle into a new star at each time step until the mass of the gas particle becomes very small. However, this SF conversion method can increase dramatically the total number of stellar particles, which becomes numerically very costly. We therefore adopt the following SF conversion method. A SF candidate $i$th gas particle is regarded as having a SF probability ($P_{\text{sf}}$):

$$P_{\text{sf}} = 1 - \exp\left(-C_{\text{sf}} f_{H_2} \Delta t \rho_{\text{th}}^{-2}\right), \quad (5)$$

where $C_{\text{sf}}$ corresponds to a star formation efficiency (SFE) in molecular cores and is set to be 1, $\Delta t$ is the time step width for the gas particle, $\rho$ is the gas density of the particle, and $\alpha f_{H_2}$ is the power-law slope of the Kennicutt–Schmidt law (star formation rate (SFR) $\propto \rho^{\alpha f_{H_2}}$; Kennicutt 1998). A reasonable value of $\alpha = 1.5$ is adopted in the present study. This SF probability has been already introduced in our early chemodynamical simulations of galaxies (e.g. Bekki & Shioya 1998).

At each time step random numbers ($R_i; 0 \leq R_i \leq 1$) are generated and compared with $P_{\text{sf}}$. If $R_{sf} < P_{\text{sf}}$, then the gas particle can be converted into a new stellar one. In this SF recipe, a gas particle with a higher gas density and thus a shorter SF time-scale ($\alpha f_{H_2} \rho \propto \rho^{1-\alpha f_{H_2}}$) can be more rapidly converted into a new star owing to the larger $P_{\text{sf}}$. Equally, a gas particle with a higher $f_{H_2}$ can be more rapidly converted into a new star. We thus consider that the present SF model is a good approximation for SF in molecular gas of disc galaxies.

Each SN is assumed to eject the feedback energy ($E_{\text{SN}}$) of $10^{51}$ erg and 90 and 10 percent of $E_{\text{SN}}$ are used for the increase of thermal energy (‘thermal feedback’) and random motion (‘kinematic feedback’), respectively. The thermal energy is used for the ‘adiabatic expansion phase’, where each SN can remain adiabatic for a time-scale of $t_{\text{adi}}$. Although $t_{\text{adi}} = 10^7$ yr is reasonable for a single SN explosion, we adopt a much longer $t_{\text{adi}}$ of $\sim 10^9$ yr. This is mainly because multiple SN explosions can occur for a gas particle with a mass of $10^5 M_\odot$ in these galaxy-scale simulations, and $t_{\text{adi}}$ can be different for multiple SN explosions in a small local region owing to complicated interaction between gaseous ejecta from different SNe. Such interaction of multiple SN explosions would make the adiabatic phase significantly longer in real ISM of galaxies.

### 2.4 IMF

We adopt a canonical stellar initial mass function (IMF) proposed by Kroupa (2001), which has three different slopes at different mass ranges. Our recent study (Bekki 2013b, hereafter B13b) have shown that if the IMF depends on local physical properties of ISM (e.g. gas density and metallicity), then galaxy evolution, in particular, the time evolution of $H_2$ and dust contents, can be significantly influenced by the time-varying IMF. Since the main purpose of this study is not to demonstrate how the $H_2$ contents of disc galaxies can be influenced by a time-varying IMF, we assume that the IMF is fixed at the adopted Kroupa IMF in the present study. It is our
future works to clarify the roles of time-varying IMFs in controlling H$_2$ properties in galaxies with different masses and Hubble types.

2.5 Evolution of dust and metals

2.5.1 Chemical enrichment

Since the present model for chemical enrichment processes of galaxies is exactly the same as that used in B13a, we briefly describe the model here. Chemical enrichment through SF and metal ejection from Type Ia supernova (SNIa), Type II supernova (SNIII), and AGB stars is self-consistently included in the chemodynamical simulations. We investigate the time evolution of the 11 chemical elements of H, He, C, N, O, Fe, Mg, Ca, Si, S, and Ba in order to predict both chemical abundances and dust properties in the present study. We consider the time delay between the epoch of SF and those of SN explosions and commencement of AGB phases (i.e. non-instantaneous recycling of chemical elements).

We adopt the ‘prompt SNIa’ model in which the delay time distribution (DTD) of SNeIa is consistent with recent observational results by extensive SNIa surveys (e.g. Mannucci, Della Valle & Panagia 2006). In this prompt SNIa model, there is a time delay ($t_d$) between the SF and the metal injection for SNIa and the range of $t_d$ is 0.1 ≤ $t_d$ ≤ 10 Gyr. The fraction of the stars that eventually produce SNIa for 3–8 M$_\odot$ have not been observationally determined. In the present study, $f_o = 0.05$ is assumed. We adopt the nucleosynthesis yields of SNeII and SNIa from Tsujimoto et al. (1995, hereafter T95) and AGB stars from van den Hoek & Groenewegen (1997, hereafter VG97) in order to estimate chemical yields in the present study.

2.5.2 Dust model

Since the dust model adopted in the present study is the same as those in B13a and B14, we here briefly describe the model. We calculate the total mass of $i$th component ($j = C, O, Mg, Si, S, Ca, and Fe$) of dust from $k$th type of stars ($k = I, II, and AGB$ for SNIa, SNIII, and AGB stars, respectively) based on the methods described in B13a that is similar to those adopted in Dwek (1998). We consider that the key parameter in dust accretion is the dust accretion time-scale ($\tau_d$). In the present study, this parameter can vary between different gas particles and is thus represented by $\tau_{d,i}$ for $i$th gas particle. The mass of dust component ($j = C, O, Mg, Si, S, Ca, and Fe$) of dust for $i$th gas particle at time $t$ ($d_{i,j}(t)$) can increase owing to dust accretion processes. The mass increase is described as

$$\Delta d_{i,j}(t) = \Delta t_i d_{i,j}(t)/\tau_{d,i},$$

where $\Delta t_i$ is the individual time step width for the $i$th gas particle and $f_{dust,i,j}$ is the fraction of the $j$th chemical element that is locked up in the dust. Owing to this dust growth, the mass of dust component that is not locked up in the dust ($z_{i,j}(t)$) can decrease, which is simply given as

$$\Delta z_{i,j}(t) = -\Delta t_i (1 - f_{dust,i,j}) d_{i,j}(t)/\tau_{d,i}.$$  

As is clear in these equations, the total mass of $j$th component in $i$th gas particle ($m_{i,j}(t)$) is $z_{i,j}(t) + d_{i,j}(t)$. Dust grains can be destroyed through SN blast waves in the ISM of galaxies (e.g. McKee 1989) and the destruction process is parametrized by the destruction time-scale ($\tau_{d,i}$) in previous one-zone models (e.g. Lisenfeld & Ferrara 1998; Hirashita 1999). Following the previous models, the decrease of the mass of $j$th component of dust for $i$th gas particle at time $t$ due to dust destruction process is as follows:

$$\Delta d_{i,j}^{\text{dest}}(t) = -\Delta t_i d_{i,j}(t)/\tau_{d,i},$$

where $\tau_{d,i}$ is the dust destruction time-scale for $i$th particle. The dust destroyed by SN explosions can be returned back to the ISM, and therefore the mass of $j$th chemical component that is not locked up in the dust increases as follows:

$$\Delta z_{i,j}^{\text{dest}}(t) = \Delta t_i d_{i,j}(t)/\tau_{d,i}.$$  

Thus the equation for the time evolution of $j$th component of metals for $i$th gas particle are given as

$$z_{i,j}(t + \Delta t) = z_{i,j}(t) + \Delta z_{i,j}^{\text{dest}}(t) = \Delta z_{i,j}^{\text{acc}}(t) + \Delta z_{i,j}^{\text{dest}}(t).$$

Likewise, the equation for dust evolution is given as

$$d_{i,j}(t + \Delta t) = d_{i,j}(t) + \Delta d_{i,j}^{\text{acc}}(t) + \Delta d_{i,j}^{\text{dest}}(t).$$

Dust is locked up in stars as metals are done so, when gas particles are converted into new stars.

2.5.3 Variable dust accretion models

We investigate the variable dust accretion (‘VDA’) model in which $\tau_d$ is different between different particles with different gaseous properties and changes with time according to the changes of gaseous properties. We need to introduce a few additional parameters in VDA in order to describe the possible dependences of $\tau_d$ of gas particles on the gas densities, temperature, and chemical abundances. Our previous simulations with VDA (B14) clearly show the importance of dust accretion and destruction in the evolution of $D$ and $f_{dust}$. The details of the VDA model is given in (B14), which discusses the comparison between the VDA and the constant dust accretion model in which $\tau_d$ is constant for all particles throughout simulations.

We adopt the following dependence of $\tau_d$, on the mass density and temperature of a gas particle in the VDA:

$$\tau_d = \tau_0 \left( \frac{\rho_{g,i}}{\rho_{g,i,0}} \right) \left( \frac{T_{g,i}}{T_{g,i,0}} \right)^{0.5},$$

where $\rho_{g,i}$ and $T_{g,i}$ are the gas density and temperature of a $i$th gas particle, respectively, $\rho_{g,0}$ (typical ISM density at the solar neighbourhood) and $T_{g,0}$ (temperature of cold gas) are set to be 1 atom cm$^{-3}$ and 20 K, respectively, and $\tau_0$ is a reference dust accretion time-scale at $\rho_{g,0}$ and $T_{g,0}$. The dust destruction time-scale, $\tau_d$, for each gas particle is described as follows:

$$\tau_d = \beta_d \tau_{d,i},$$

where $\beta_d$ controls the time-scale ratio of dust destruction to dust growth. In our previous studies (B13a, B14), $\beta_d = 2$ is demonstrated to reproduce the observed dust properties of galaxies. We therefore consider that $\beta_d$ should be adopted a reference value in the present dust model.

In the present study, the dust-to-metal ratio of a galaxy is defined as follows:

$$f_{dust} = \frac{M_{\text{dust}}}{M_Z},$$

where $M_{\text{dust}}$ and $M_Z$ are the total amount of dust and metals in the galaxy, respectively. Although the initial value of $f_{dust}$ could be different in different galaxies, we mainly adopt the standard value of 0.4 (corresponding to the value of the solar neighbourhood) and
thereby investigate the evolution of dust and H$_2$. We briefly discuss how the present results depend on the initial $f_{\text{dust}}$ by changing $f_{\text{dust}}$ from 0.1 to 0.4.

### 2.6 H$_2$ formation and dissociation

The model for H$_2$ formation and dissociation in the present study is exactly the same as those used in B13a: H$_2$ formation on dust grains and H$_2$ dissociation by FUV radiation are both self-consistently included in chemodynamical simulations. The temperature ($T_p$), hydrogen density ($\rho_{\text{H}_2}$), dust-to-gas ratio ($D$) of a gas particle, and the strength of the FUV radiation field ($\chi$) around the gas particle are calculated at each time step so that the fraction of molecular hydrogen ($f_{\text{H}_2}$) for the gas particle can be derived based on the H$_2$ formation/destruction equilibrium conditions. Thus the H$_2$ fraction for ith gas particle ($f_{\text{H}_2,i}$) is given as

$$f_{\text{H}_2,i} = F(T_p,i, \rho_{\text{H}_2,i}, D_i, \chi_i).$$

(15)

where $F$ is a function of $f_{\text{H}_2,i}$ determination.

Since the detail of the derivation methods of $\chi$, and $f_{\text{H}_2,i}$ (thus $F$) are given in B13a and B13b, we here briefly describe the methods. The SEDs of stellar particles around each ith gas particles (thus ISRF) are first estimated from ages and metallicities of the stars by using stellar population synthesis codes for a given IMF (e.g. Bruzual & Charlot 2003). Then the strength of the FUV part of the ISRF is estimated from the SEDs so that $\chi$ can be derived for the ith gas particle. Based on $\chi$, $D$, and $\rho_{\text{H}_2,i}$ of the gas particle, we can derive $f_{\text{H}_2,i}$ (see fig. 1 in B13a). Thus each gas particle has $f_{\text{H}_2,i}$, metallicity (Fe/H), and gas density, all of which are used for estimating the IMF slopes for the particle (when it is converted into a new star).

The ages of stars ($t_s$) are assumed to be 5 and 2 Gyr for the models with $z = 0$ and 2, respectively. The results of the present models are influenced by the choice of $t_s$ only for the very early phase of disc evolution ($T < 0.1$ Gyr), if $t_s$ is rather short (~0.1 Gyr). The influences of $t_s$ is very limited, because the photodissociation of H$_2$ by stars can be very efficient when gas is surrounded by very young stars and thus irradiated by the strong UV radiation fields. We therefore discuss only the results of the models with $t_s$ adopted above.

A number of previous theoretical models of H$_2$ formation (e.g. Hidaka & Sofue 2002) adopted the phase transition theory proposed by Elmegreen (1993), in which H$_2$-to-H$_2$ transition in ISM is determined basically by gas pressure and radiation field. Elmegreen (1993) already showed that the observed H$_2$ mass function ($\propto M^{-1.5}$) can be understood by his theory and also suggested that spiral density waves can convert H$_2$ into H$_2$. We do not adopt his phase transition theory but instead try to reproduce the observed H$_2$ properties using a different model based on H$_2$ formation on dust grains.

### 2.7 Gravitational dynamics and hydrodynamics

One of key ingredients of the code is that the gravitational softening length ($\epsilon$) is chosen for each component in a galaxy (i.e. multiple gravitational softening lengths). Thus the gravitational softening length ($\epsilon$) is different between dark matter ($\epsilon_{\text{dm}}$) and gas ($\epsilon_g$) and $\epsilon_{\text{dm}}$ is determined by the initial mean separation of dark matter particles. The gravitational softening length for stars ($\epsilon_s$) is set to be the same as that for gas. Initial $\epsilon_s$ is set to be significantly smaller than $\epsilon_{\text{dm}}$ owing to rather high number density of gas particles. The softening length for new stars formed from gas is set to be the same as $\epsilon_g$. Furthermore, when two different components interact gravitationally, the mean softening length for the two components is applied for the gravitational calculation. For example, $\epsilon = (\epsilon_{\text{dm}} + \epsilon_g)/2$ is used for gravitational interaction between the values of $\epsilon_{\text{dm}}$ and $\epsilon_g$ (=$\epsilon_s$) are 2.1 and 0.2 kpc, respectively, for the fiducial MW-type disc model.

We consider that the ISM in galaxies can be modelled as an ideal gas with the ratio of specific heats ($\gamma$) being 5/3. The gaseous temperature ($T_p$) is set to be 10$^4$ K initially in all models. The basic methods to implement SPH in the present study are essentially the same as those proposed by Hernquist & Katz (1989). We adopt the predictor-corrector algorithm (that is accurate to second order in time and space) in order to integrate the equations describing the time evolution of a system. Each particle is allocated an individual time step width ($\Delta t$) that is determined by physical properties of the particle. The maximum time step width ($\Delta t_{\text{max}}$) is 0.01 in simulation units, which means that $\Delta t_{\text{max}} = 1.41 \times 10^6$ yr in the present study. Although a gas particle is allowed to have a minimum time step width of $1.41 \times 10^3$ yr in the adopted individual time step scheme, no particle actually has such a short time step width ($\sim 10^4$ yr) owing to conversion from gas to star in high-density gas regions. The radiative cooling processes are properly included by using the cooling curve by Rosen & Bregman (1995) for $100 \leq T < 10^4$ K and the MAPPING III code for $T \geq 10^4$ K (Sutherland & Dopita 1993).

### 2.8 Tidal interaction model

In order to investigate how external tidal perturbation can influence the physical properties of H$_2$ in disc galaxies, we investigate tidal interaction models in which two disc galaxies strongly interact with each other. One of the two galaxies (‘primary galaxy’) is represented by the disc galaxy model described above whereas the interacting companion galaxy is represented by a point-mass particle. Although the mass ratio of the companion to the primary can be a free parameter represented by $m_2$, we present the results only for the models with $m_2 = 1$ in which the influences of tidal interaction on H$_2$ properties can be clearly seen.

In all of the simulations of tidal interaction, the orbit of the two discs is set to be initially in the $x$–$y$ plane and the distance between the centre of mass of the two discs is set to be 10$R_d$ (corresponding to 175 kpc for the MW-type disc model) for most models. The pericentre distance, represented by $r_p$, is set to be $3R_d$. The eccentricity is set to be 1.0 for all models of galaxy interaction, meaning that the encounter of galaxy interaction is parabolic. The spin of the primary galaxy in an interacting pair is specified by two angle $\theta$ and $\phi$ (in units of degrees), where $\theta$ is the angle between the $z$-axis and the vector of the angular momentum of a disc and $\phi$ is the azimuthal angle measured from $x$-axis to the projection of the angular momentum vector of a disc on to $x$–$y$ plane.

In the present study, we present the results of the following four tidal interaction models: (i) prograde (‘PR’) model with $\theta = 0$, $\phi = 0$, and $r_p = 3R_d$; (ii) retrograde (‘RE’) model with $\theta = 180$, $\phi = 0$, and $r_p = 3R_d$; (iii) highly inclined model with $\theta = 30$, $\phi = 60$, and $r_p = 3R_d$; and (iv) distant interaction model with $\theta = 0$, $\phi = 0$, and $r_p = 4R_d$.

### 2.9 A parameter study to solve key questions

We investigate numerous models to try to answer the following key questions related to the origin of H$_2$ in disc galaxies: (i) how can H$_2$ gas distribute within discs?; (ii) what determines the molecular gas (H$_2$) fractions in disc galaxies?; (iii) what are the roles of galactic...
bulges in controlling H$_2$ properties of disc galaxies?; (iv) can dust evolution influence the evolution of H i and H$_2$ in galaxies?; (v) does galaxy interaction enhance H$_2$ contents of galaxies?; (vi) is there any threshold gas density (or threshold galaxy mass) beyond which H$_2$ formation is possible?; and (vii) can high-$z$ disc galaxies can contain larger fractions of H$_2$ within discs? It should be noted here that these are selected, because the present numerical code allows us to investigate these: other questions such as the influences of AGN and dust size evolution on H$_2$ evolution cannot be addressed in the present study.

In order to address these questions, we mainly describe the results of the selected 34 models in the present study. We indeed investigated more than 34 models, in particular, for low-mass disc models in order to understand whether there can be a threshold halo mass beyond which H$_2$ formation is possible. However, we discuss only these results, because these representative models can more clearly show how the results depend on model parameters. The values of parameters adopted in these models are given in Table 2. In order to discuss the importance of dust evolution in H$_2$ evolution of galaxies, we investigate the models with different basic dust parameters. The parameter values for dust models and chemical evolution are summarized in Table 3. We first describe the results of the ‘fiducial model’ (M1) that corresponds to a disc galaxy similar to the MW (thus referred to as MW-type disc model). Then we discuss how the key model parameters control the H$_2$ properties of disc galaxies in detail.

### 2.10 A method to estimate H$_2$ surface density distribution (H2SDD)

The present chemodynamical models do not have enough spatial resolution to resolve the sub-pc-scale central cores of GMCs with H$_2$. We therefore cannot discuss whether and where self-gravitating molecular clouds are formed in galactic gas disc. Instead of investigating the molecular cloud mass function (MCMF), we try to derive the H2SDD, which would be useful in discussing the origin of MCMFs of galaxies. We estimate the H2SDD in a disc galaxy as follows. We first divide the simulated stellar disc region ($R_d = 17.5$ kpc for the MW model) of a disc galaxy into 200 $\times$ 200 or 400 $\times$ 400 small meshes and thereby estimate the total mass of H$_2$ ($m_{H_2,\text{mesh}}$).

We count the number of meshes ($N_{H_2}$) with $m_{H_2,\text{mesh}}$ within a given mass range so that we can estimate the H2SDD. The mesh size can be as small as $\sim$90 pc for the MW-type disc models, which
Table 3. Description of the basic parameter values for the models of SF, dust, and chemical evolution.

| Parameters       | Adopted values | The standard value adopted in most models |
|------------------|----------------|------------------------------------------|
| $\tau_0$ a       | 0.1, 0.2, 0.4, 2 Gyr | 0.2 Gyr                                  |
| $\beta_d$ b      | 1, 2, 4         | 2                                        |
| $f_{dust}$ c     | 0.1, 0.4        | 0.4                                      |
| Dust yield       | B13a (fixed)    | –                                         |
| Chemical yield   | T95 for SN, VG97 for AGB | –                                      |
| $\alpha_d$ d     | 0, −0.04        | 0                                        |
| $\rho_{th}$ e    | 1 cm$^{-3}$ (fixed) | –                                        |
| IMF              | Kroupa (fixed)  | –                                        |

*a* The dust growth time-scale for a gas density of 1 atom cm$^{-3}$ for the adopted variable dust accretion model. *b* The ratio of dust destruction time-scale of a gas disc. *c* The initial dust-to-metal ratio to dust growth time-scale. *d* The initial metallicity gradient (of the gas disc) in units of dex kpc$^{-1}$. *e* $\rho_{th}$ is the threshold H$_2$ gas density for SF for each gas particle.

can be enough to discuss the mass of each individual H$_2$ gas clouds in a local region of a disc galaxy. Although this method is not exactly the same as that used in the observational estimation of MCMF, we consider that the derived H2SDD could be quite useful in discussing the origin of the observed MCMF in a qualitative manner (e.g. discussing the slope of the MCMF). We mainly check whether the simulated slope of H2SDD can be similar to the observed slope of the Galactic MCMF.

3 RESULTS

3.1 Fiducial MW model

3.1.1 Spatial distributions of hydrogen gas and H$_2$ surface density distribution

Figs 1 and 2 describe how the spatial distributions of stars, H$\text{I}$, H$_2$, and dust evolve with time during the dynamical evolution of the gas disc with spiral arms and a central bar in the fiducial MW-type disc model (M1). Numerous spiral arms can be developed at $T = 0.6$ Gyr owing to gravitational instability, and they can influence the conversion from H$\text{I}$ to H$_2$ in the gas disc after their formation. The locations of high-density H$_2$ regions at $T = 0.6, 0.8,$ and $1.1$ Gyr appear to be roughly coincident with the locations of H$\text{I}$ spiral arms of the gas disc. However, H$_2$ shows a very clumpy distribution along spirals arms, which is in a striking contrast with the relatively smooth distribution of H$\text{I}$ along spiral arms. This implies that only the high-density parts of the gaseous spiral arms can be the possible formation sites of H$_2$ in galactic discs. Numerous H$_2$ clumps can be active star-forming regions in the present SF model based on H$_2$ gas densities. Although the projected distribution of interstellar dust follows the spiral-like distribution of H$\text{I}$ gas, it does not show clump-like structures as H$_2$. Interstellar dust can become less clumpy, because it can be efficiently destroyed by star formation (i.e. SNe) which can occur in high-density gas clumps.

Figure 1. The time evolution of the projected mass densities for stars ($\Sigma_*$, left four) and H$\text{I}$ ($\Sigma_{\text{H}\text{I}}$, right four) for the fiducial MW-type disc model (M1). The time $T$, which represents the time that has elapsed since the simulation started, is shown in the upper left-hand corner for each panel. The mass densities are derived from the distributions of particles projected on to the x-y plane of the disc. The projected density fields are smoothed by using a Gaussian kernel with a smoothing length of 875 pc.
The physical roles of spiral arms in the formation of GMCs have been already discussed in a number of recent theoretical works based on high-resolution numerical simulations of gas disc evolution in disc galaxies (e.g. Dobbs, Burkert & Pringle 2011; Wada, Baba & Saitoh 2011; Halle & Combes 2013). Although these previous works did not self-consistently model the H2 formation on dust grains and the time evolution of dust, they have already shown projected H2 distributions in galactic discs (e.g. fig. 14 in Halle & Combes 2013). The derived distributions of H2 along spiral arms in the present MW-type disc model are similar to those reported in Halle & Combes (2013). The clumpy H2 distributions derived in the present study are not so clearly seen in previous works, which could reflect the differences in the models of SF and SN feedback effects between the present and other works.

Fig. 3 shows the spatial distributions of H i and H2 and the mass function of H2 gas clouds (referred to as MCMF) in the gas disc at T = 1.1 Gyr in the fiducial MW-type disc galaxy model with f_H2 = 0.09. The simulated H2 distribution is more centrally concentrated than H i gas within the disc owing to the more efficient formation of H2 on dust grains in the inner part of the disc where both gas density and D can be higher during the disc evolution. The spatial distribution of H2 gas shows small-scale clumpy structures within gaseous spiral arms where gas density can become rather large. Clearly, there is an outer truncation (R ~ 13 kpc) beyond which no/little H2 gas can be found in this model. The projected radial density profile of H2 is steeper than that of H i in this model.

The central part of the disc is dominated by H2 gas and most of the gas particles there have rather high f_H2 (>0.5), which implies that molecular hydrogen can be systematically more massive. The simulated H2SDD has a slope of ~−1.5 for log (Σ_H2) < 2.4 M⊙ pc−2, which means that the simulated slope is similar to the observed slope of MCMF that is approximated as N_{gas} ~ m_{gas}^{−1.5} for the MW and M31 (e.g. fig. 4 in Fukui & Kawamura 2010). This implies that the present model of H2 formation on dust grains is realistic and reasonable for H2 formation in disc galaxies. Although the MCMF can be shifted towards higher masses if a coarser mesh size (n_{mesh} = 200^2) is used for the MCMF derivation, the slope of the MCMF does not change significantly.

This MW-type fiducial model can develop a central stellar bar owing to bar instability and the stellar bar can influence the formation process of H2 significantly. The formation process of the stellar bar in the central 2 kpc and its influence on gas for T ≤ 1.1 Gyr are given in Appendix A. Fig. 4 shows that the gas disc has a very strong concentration of H2 in the central 200 pc at T = 2.3 Gyr. This H2 concentration corresponds to the formation of nuclear H2 gas disc due to the dynamical action of the central stellar bar on the surrounding gas. Owing to the rather high concentration of H2 in the disc, the SFR can be significantly increased, in particular, in the central region of this barred disc galaxy. Furthermore, the H2 fraction can be significantly increased (from f_{H2} ~ 0.1 to ~0.3). Thus these results clearly demonstrate that stellar bars can play a vital role in converting H i to H2 in disc galaxies.

Fig. 5 describes how the simulated H2SDDs depend on the model parameters for metallicity gradient and dust growth/destruction. The slopes of the H2SDDs do not depend strongly on the parameters, though some models (with steep metallicity gradient and longer dust accretion/destruction time-scales) show the overproduction of high-density H2 regions with log Σ_{H2} > 2.4 M⊙ pc−2 within their discs. The larger number of high-density H2 regions is due largely to the stronger central concentration of H2 gas in the inner regions of the gas discs. As shown in Fig. 4, a central region of a galaxy is dominated by high-density H2 gas so that almost all of the meshes in the central region can have high Σ_{H2}. As a result of this, the simulated H2SDDs can have a bump around log Σ_{H2} = 2.6–2.8 M⊙ pc−2. It is a bit surprising that the simulated H2SDDs are less sensitive to the adopted dust model.
3.1.2 The fraction of molecular hydrogen

Fig. 6 describes the physical correlations between molecular fraction \( R_{\text{mol}} \), which is defined as the mass ratio of H\(_2\) to H\(_i\), and \( P_g k_B^{-1} \), where \( P_g \) is the gas pressure of a particle and \( k_B \) is the Boltzmann constant, in the gas disc of the fiducial MW model with different initial metallicity gradients \( \alpha = 0 \) and \(-0.04\) dex kpc\(^{-1}\) at \( T = 1\) Gyr. It should be stressed that this \( R_{\text{mol}} \) is not exactly the same as \( f_{\text{H}_2} \) \((= M_{\text{H}_2}/(M_{\text{H}_i} + M_{\text{H}_2}))\), which is often shown in figures of this paper. The observed correlation of \( R_{\text{mol}} \propto P_g^{0.95} \) (e.g. Blitz et al. 2007; Fukui & Kawamura 2010) can be used as a key observational constraint for the present H\(_2\) formation model. Although the dispersion in \( R_{\text{mol}} \) at each bin appears to be large, the two models show a clear positive correlation between \( R_{\text{mol}} \) and \( P_g \) (i.e. higher \( R_{\text{mol}} \) for higher gaseous pressure). This result implies that the present model for H\(_2\) formation, which does not explicitly assume a dependence of H\(_2\) formation efficiency on gaseous pressure, does a good job in predicting \( R_{\text{mol}} \) and its dependence on gaseous pressure.

Although the two models with different slopes of gaseous metallicity gradients \( \alpha = 0 \) and \(-0.04\) have the slopes of the \( R_{\text{mol}}-P_g \) that are similar to the observed one \( R_{\text{mol}} \propto P_g^{0.95} \), the model with a steep negative gradient of gaseous metallicity \( \alpha = -0.04 \) can have the slope more similar to the observed one. The model with \( \alpha = -0.04 \) shows a lower H\(_2\) formation efficiency at \( P_g k_B^{-1} < 10^5 \) (cm\(^{-3}\) K) in comparison with the model with \( \alpha = 0 \), mainly because the model with a negative metallicity gradient has a significantly lower dust-to-gas-ratio (i.e. lower metallicity) at the outer region of the disc.
The H2SDD in different five MW-type disc models (M1): relation in the model with shorter dust relation. It is clear from Fig. at higher τ describes the simulated − in disc galaxies (e.g. Wong and similar to the observed one as long as τ β = 2 = R = 1 = R = 2 = R = 7 = 6 = R β P 444, 1 and 4 (magenta long-dashed), and formation efficiency caused by the formation efficiency (τ α = 0.2 Gyr) cannot reproduce the observed τ mol P g relation on initial metallicity gradients implies that the slopes can be quite similar between different galaxies with different metallicity gradients.

Fig. 7 describes the simulated R mol−P g relations in models with different model parameters for dust growth and destruction. These models have the parameter values being less realistic (e.g. rather long dust accretion time-scale) in comparison with the models used in Fig. 6 so that we can discuss how the dust modelling is important for reproducing the observed R mol−P g relation. It is clear from Fig. 7 that the simulated R mol−P g relation in the model with shorter dust growth-time scale (τ α = 0.1 Gyr) is less consistent with the observed one owing to rather small R mol at higher P g (>10^5 k_B) in the model. The model with a shorter dust destruction time-scale (β d = 1 and τ α = 0.2 Gyr) cannot reproduce the observed R mol−P g relation so well either. These results imply that both dust accretion and destruction time-scales should be carefully chosen for reproducing the observed R mol−P g relation.

The models with longer dust accretion time-scale (τ α = 0.4 and 2 Gyr) show R mol−P g similar to the observed one as long as β d = 2 is adopted. However these models cannot reproduce the observed R mol−P g better than the models in Fig. 6, which implies that not only β d but also τ α can be a key parameter for reproducing the observed R mol−P g. The slope of the simulated R mol−P g in the model with a longer dust destruction time-scale (β d = 4 and τ α = 0.2 Gyr) can better match the observed one except for rather high gaseous pressure (P g ∼ 10^5 k_B). The model with an initially lower dust-to-metal ratio (f dust = 0.1) shows R mol−P g relation similar to those in Fig. 6, though R mol at higher P g is systematically smaller than those in Fig. 6 owing to the lower H2 formation efficiency caused by the lower dust-to-gas ratio.

The models with no dust evolution show significantly shallower R mol−P g relations, irrespective of the slopes of the initial radial metallicity gradients (α = 0 and −0.04). This result implies that the time evolution of dust abundances in disc galaxies needs to be included for the self-consistent reproduction of the observed R mol−P g relation. The models without SN feedback and those without chemical evolution show significant deviation from the observed R mol−P g, which strongly suggests that dust growth and destruction processes caused by chemical enrichment and SN explosions need to be carefully included in reproducing the observed R mol−P g relation in a quantitative manner. Thus these results demonstrate that as long as the H2 formation processes on dust grains are included in hydrodynamical simulations of galaxy formation and evolution, the dust growth and destruction processes, which can be influenced by chemical enrichment and SN explosions, should be carefully considered in discussing the origin of the observed R mol−P g relation.

### 3.1.3 Radial gradients of molecular fraction

The observed radial gradients of R mol in disc galaxies (e.g. Wong & Blitz 2002) can be an additional constraint for any model for
The plots of gas particles on the $R_{\text{mol}}$-$P_\text{g}$ plane in M1, where $R_{\text{mol}}$ is the mass ratio of $H_2$ to $H_1$ and $P_\text{g}$ is gaseous pressure. Here $P_\text{g} k_B^{-1}$ rather than $P_\text{g}$ is plotted for each gas particle so that the simulated correlation can be compared with the observed one (black dotted line) by Blitz et al. (2007). The red big circles indicate the mean $R_{\text{mol}}$ for each $P_\text{g}$ bin and the error bar shows the dispersion in $R_{\text{mol}}$. The models with $\alpha = 0$ (flat metallicity gradient) and $-0.04$ (steeper one) are shown in the left- and right-hand panels, respectively.

**Figure 6.** The plots of gas particles on the $R_{\text{mol}}$-$P_\text{g}$ plane in M1, where $R_{\text{mol}}$ is the mass ratio of $H_2$ to $H_1$ and $P_\text{g}$ is gaseous pressure. Here $P_\text{g} k_B^{-1}$ rather than $P_\text{g}$ is plotted for each gas particle so that the simulated correlation can be compared with the observed one (black dotted line) by Blitz et al. (2007). The red big circles indicate the mean $R_{\text{mol}}$ for each $P_\text{g}$ bin and the error bar shows the dispersion in $R_{\text{mol}}$. The models with $\alpha = 0$ (flat metallicity gradient) and $-0.04$ (steeper one) are shown in the left- and right-hand panels, respectively.

$H_2$ formation in galaxy-scale simulations. We here estimate $R_{\text{mol}}$ at each radius in a simulated disc galaxy by calculating the ratio of $\Sigma_\text{H}_2$ (i.e. the projected surface mass density of $H_2$) to $\Sigma_\text{H}_1$ at each radius in Fig. 8. Although individual gas particles corresponding to individual local gaseous regions in a disc galaxy have vastly different $R_{\text{mol}}$ (ranging from 0 to 10), the slopes of the radial $R_{\text{mol}}$ profiles in the two models with different $\alpha$ appear to be similar to the observed one ($R_{\text{mol}} \propto R^{-1.5}$). The model with $\alpha = 0$ can slightly better reproduce the observed slope than the model with $\alpha = -0.04$. Thus, the simulated slopes similar to the observed $R_{\text{mol}} \propto R^{-1.5}$ demonstrate that the present model for $H_2$ formation on dust grains is quite reasonable and realistic in discussing the global (galaxy-scale) distributions of neutral and molecular hydrogen in disc galaxies (as long as a reasonable set of model parameters for dust is adopted).

3.1.4 $H_2$ scaling relations

A number of recent observational studies have found intriguing correlations between physical properties of dust, gas, and stars in galaxies (e.g. Corbelli 2012; Cortese et al. 2012; Boselli et al. 2014). It is therefore essential for the present study to provide some comparisons between these observations and the corresponding simulation results. Fig. 9 shows that the $H_2$ fractions ($f_{\text{H}_2}$) are more likely to be larger for local regions with higher stellar surface densities ($\Sigma_*$), in particular, for $\Sigma_*$ > 10^2 $M_\odot$ kpc$^{-2}$. There is a large dispersion in $f_{\text{H}_2}$ for a given $\Sigma_*$, which reflects the fact that SF histories and chemical enrichment processes (thus dust growth/destruction processes) are quite different in different local regions. The local regions with higher $\Sigma_*$ can have higher gas densities so that conversion from $H_1$ to $H_2$ can occur more efficiently. This is a physical reason for the simulated trend of $f_{\text{H}_2}$ with $\Sigma_*$ in Fig. 9.

There is a positive correlation between the mass ratio of $H_2$ to stars and $\Sigma_*$, though the correlation cannot be simply described as a power-law profile owing to the flatter slope in the simulated relation at $\Sigma_*$ > 10^2 $M_\odot$ kpc$^{-2}$. A large dispersion in $M_{\text{H}_2}/M_*$ can be seen, which again reflects the diverse histories of SF and chemical enrichment in different local regions. The simulated relation between $\Sigma_{\text{H}_2}$ and $\Sigma_{\text{dust}}$ is relatively tight in comparison with other two correlations and can be described roughly as $\Sigma_{\text{H}_2} \propto \Sigma_{\text{dust}}$. These simulated relations between physical properties of dust, gas, and stars are at least qualitatively consistent with observational results (e.g. Boselli et al. 2014).

3.2 Parameter dependences

The physical properties of $H_2$ such as radial profiles of $R_{\text{mol}}$ and time evolution of $f_{\text{H}_2}$ can be quite diverse in the simulated disc galaxies with different model parameters. Since it is not so meaningful (and much less productive) to describe the results of all models in detail, we here describe only the results that are quite important and thus worth mentioning. In the following subsections, $H_2$ properties (e.g. $f_{\text{H}_2}$) are compared between models with different values of a model parameter (e.g. $f_g$) for a given set of other model parameters (i.e. other model parameters are fixed).
3.2.1 \( \text{H}_2 \) morphology

Although the morphologies of \( \text{H}_2 \) distributions in disc galaxies depend largely on the adopted \( f_b \) and \( f_g \) in disc galaxies, almost all models in the present study show very strong central concentration of \( \text{H}_2 \) and clear coincidence between the locations of gas particles with high \( \text{H}_2 \) fractions and those of spiral arms in the discs. The distributions of \( \text{H}_2 \) along gaseous spiral arms appear to be very clumpy, which reflects the fact that only the high-density parts of the spiral arms can efficiently form \( \text{H}_2 \). These clumpy distributions are in a striking contrast with the \( \text{H} \) distributions in disc galaxies.

Furthermore, the detailed spatial distributions of \( \text{H}_2 \) in the central few kpc of the discs can be controlled by the presence (or the absence) of stellar bars developed from bar instability in the central regions. Fig. 10 shows one of clear examples of the strong influences of the central stellar bars on the spatial distributions of \( \text{H}_2 \) in disc galaxies. Clearly, the disc galaxy in this model (M8) has a very

Figure 7. The same as Fig. 5 but for different 10 MW-type disc models (M1). The left-hand panel shows the models with \( \tau_0 = 0.1 \) Gyr (blue solid), \( \tau_0 = 0.4 \) Gyr (red dotted), \( \tau_0 = 2 \) Gyr (green short-dashed), \( \beta_d = 1 \) (magenta long-dashed), and \( \beta_{\text{dust}} = 4 \) (cyan dot–dashed). The right-hand panel shows the models with \( f_{\text{dust}} = 0.1 \) Gyr (blue solid), no dust evolution with \( \alpha = 0 \) (red dotted), no dust evolution with \( \alpha = -0.04 \) (green short-dashed), no SN feedback effects (magenta long-dashed), and no chemical evolution (cyan dot–dashed).

Figure 8. The projected radial distribution of the surface density ratios of \( \text{H}_2 \) to \( \text{H} \) at \( T = 1.1 \) Gyr in the fiducial MW-type disc model (M1) with \( \alpha = 0 \) (left) and \( \alpha = -0.04 \) (right). The observed correlation (\( \Sigma_{\text{H}_2}/\Sigma_{\text{H}} \propto R^{-1.5} \)) by Wong & Blitz (2002) is shown by a dotted line for comparison. The small dots represent the locations of the selected gas particles and the particles with no \( \text{H}_2 \) (i.e. \( f_{\text{H}_2} = 0 \)) are shown at \( \log(\Sigma_{\text{H}_2}/\Sigma_{\text{H}}) = -3 \) for convenience.
Figure 9. The simulated three $H_2$-scaling relations at $T = 1.1$ Gyr in the fiducial MW-type disc model (M1). The left-hand, middle, and right-hand panels show correlations between $f_{H_2}$ and $\Sigma_*$, $M_{H_2}/M_*$ and $\Sigma_*$, and $\Sigma_{H_2}$ and $\Sigma_{dust}$, respectively. Small black dots indicate the physical properties (e.g. $f_{H_2}$) of local regions (represented by gas particles) whereas big red dots indicate the average values at each bin. For comparison, the linear correlations of $M_{H_2}/M_* \propto \Sigma_*$ and $\Sigma_{H_2} \propto \Sigma_{dust}$ are shown by green dotted lines in the middle and right-hand panels, respectively.

Figure 10. The distributions of gas with $f_{H_2} < 0.01$ (blue, $H_I$) and $f_{H_2} \geq 0.01$ (red, $H_2$) projected on to the $x$–$y$ plane at $T = 2.3$ Gyr in the big bulge model with $f_b = 1$ (M8). Clearly, an elongated $H_2$ ring can be seen in this model.

An elongated ring-like structure dominated by $H_2$, which is formed as a result of dynamical action of the central bar on the gas disc. This kind of ‘molecular gas ring’ can be seen in the models in which $f_b$ is not so large and thus stellar bar formation cannot be severely suppressed by the central big bulges.

3.2.2 Time evolution of $f_{H_2}$

The time evolution of $f_{H_2}$ depends strongly on $f_g$, $f_{bary}$, $f_b$, $M_h$, and the formation redshifts of galaxies in the present models. Furthermore, tidal galaxy interaction can significantly change $M_{H_2}$ and $f_{H_2}$ depending on the orbit configurations of interacting two galaxies. The time evolution of 2D $\Sigma_{H_2}$ and $\Sigma_{dust}$ distributions for interacting galaxies is discussed in Appendix B, because the formation process of $H_2$ is quite interesting for interacting galaxies. The final 2D $\Sigma_{H_2}$ and $\Sigma_{dust}$ distributions for a high-$z$ disc model are in a striking contrast with those of low-$z$ discs and thus shown in Appendix B.

Since the time evolution of $M_{H_2}$ and $f_{H_2}$ are very similar in each model, we briefly summarize the derived key seven dependences of $f_{H_2}$ (not $M_{H_2}$) on the model parameters in Figs 11 and 12. First, $f_{H_2}$ can be initially larger in the models with larger $f_g$ for a given set of other model parameters (e.g. $f_b$). The final values of these two quantities ($T = 1$ Gyr) in the model with larger $f_g (= 0.27)$, however, can become rather small owing to rapid $H_2$ gas consumption by SF. As a result of this, the model with larger $f_g$ can have smaller final $M_{H_2}$ and $f_{H_2}$ than the model with smaller $f_g (= 0.09)$. It should be noted that the final $f_g$ in the model with $f_g = 0.27$ can become rather low too.

Secondly, $f_{H_2}$ can be initially smaller in the models with smaller $f_{bary}$ for a given $f_g$ and $M_h$, mainly because formation of non-axisymmetric structures such as bars and spirals can be suppressed in less strongly self-gravitating discs (owing to the dominant dark matter haloes) so that $H_2$ formation efficiency can be lower. The lower surface gas densities in the models with smaller $f_{bary}$ are also responsible for the smaller $f_{H_2}$. The smaller $f_{H_2}$ for smaller $f_{bary}$ can be seen in low-mass models with $M_h = 10^{10} M_\odot$. As shown in the model with smaller $f_{bary}$ (0.02) yet larger $f_g (= 0.33)$, $f_{H_2}$ can be larger than the model with $f_{bary} = 0.03$ and smaller $f_g$. Since gas consumption by SF is slower in these models with smaller $f_{bary}$, the...
The time evolution of $f_{\text{H}_2}$ in the representative 18 isolated and interaction models with different $f_g$, $f_{\text{bary}}$, $M_h$, and $z$. Each panel includes only three models in which only one or two model parameters are different so that the roles of the parameter(s) in controlling the time evolution of $f_{\text{H}_2}$ can be more clearly shown. For example, the top left-hand panel describes how $f_g$ can control $f_{\text{H}_2}$ in disc galaxies.

Initial $f_{\text{H}_2}$ difference in the models (i.e. larger $f_{\text{H}_2}$ for larger $f_g$) can last for a long time-scale.

Thirdly, $f_{\text{H}_2}$ can be initially larger in the models with smaller bulges, because bigger galactic bulges can slow down or suppress the formation of spiral arms and bars so that $\text{H}_2$ formation efficiencies in gas discs can be also severely suppressed by the bulges. Fig. 12 shows that although $f_{\text{H}_2}$ is initially larger in the model with $f_b = 0.17$ (fiducial model with a smaller bulge) than in the model with $f_b = 1$ ($T < 0.2$ Gyr), the $f_{\text{H}_2}$ difference becomes smaller as the time passes by. After the formation of a stronger bar in the central region of the fiducial model, the bar dynamically acts on the gas disc so that a larger amount of gas can be transferred to the central region, where $\text{H}_2$ formation is enhanced. Consequently, $f_{\text{H}_2}$ can become significantly larger at $T > 1.5$ Gyr. This kind of $f_{\text{H}_2}$ enhancement by the dynamical action of a bar can occur to a lesser extent in the big bulge model with $f_b = 1$ in which only a weak stellar bar can be formed.

It should be stressed here that the models (M9 and M12) with rather large $f_b$ (2 and 4), initial $f_{\text{H}_2}$ is rather low ($<0.05$). However, the $\text{H}_2$ consumption by SF is much less efficient in the models so that $f_{\text{H}_2}$ can keep slowly rising (owing to the higher gas densities). As a result of this, these models can finally show larger $f_{\text{H}_2}$ ($>0.1$) at $T = 1.1$ Gyr. Therefore, we cannot claim that discs with bigger bulges show smaller $f_{\text{H}_2}$ in the present study. Fourthly, low surface brightness (LSB) disc galaxies can have initially smaller $M_{\text{H}_2}$ and $f_{\text{H}_2}$ owing to their low gas densities. It should be stressed that owing
The long-term evolution of $M_{H_2}$ (upper) and $f_{H_2}$ (lower) in the two comparative models with $f_b = 0.167$ (M1, blue solid, smaller bulge) and $f_b = 1$ (M8, red dotted, bigger bulges). The discs with smaller bulges are more likely to develop stronger bars in their central regions owing to global bar instability in the present study. The stronger bars can dynamically act on gas discs so that a significant amount of gas can be transferred to the inner regions, where high-density $H_2$ regions can form. The later increase of $f_{H_2}$ in the fiducial model with $f_b = 0.167$ is due to the central gas concentration in the disc caused by dynamical action of the bar (see also Fig. 4).

to much less rapid gas consumption and chemical enrichment, the LSB model can finally have $M_{H_2}$ and $f_{H_2}$ similar to those of the fiducial model.

Fifthly, galaxy interaction between two disc galaxies can significantly increase $f_{H_2}$ after the pericentre passage. This enhancement of $H_2$ formation in discs can be more clearly seen in the PR tidal interaction model in which the spin axes of two discs are roughly parallel to those of their orbital angular momentum. This enhancement of $H_2$ formation, however, cannot be clearly seen in other interaction models (RE or distant encounter models), which implies that not all of interacting galaxies show significantly large $f_{H_2}$ in comparison with isolated field disc galaxies. Galaxy interaction can also change the distribution of $H_2$ and the MCMF, in particular, for the central region. The MCMFs of interaction models are discussed in Appendix A.

Sixthly, less massive disc galaxies can have smaller $f_{H_2}$ first, because the formation of bars and spirals arms can be severely suppressed in the galaxies (owing to the stronger concentration of dark matter and smaller $f_{H_2}$), and secondly because the dust-to-gas ratios ($D$), which are key factors for $H_2$ formation models of the present study, can be lower in the discs. The chemical enrichment processes by SNe and AGB stars in these low-mass models are so slow (owing to low SFRs) that $D$ cannot increase during the dynamical evolution of the discs. Therefore, the formation efficiencies of $f_{H_2}$ can be kept lower in these models. The low-mass model with $M_b = 10^{10} M_\odot$ and smaller $f_{H_2} = 0.01$ shows rather small $f_{H_2}$, which means that this low-mass disc galaxy is almost $H_2$-less. The baryonic fraction ($f_{H_2}$) is particularly important in determining the time evolution of $f_{H_2}$ for low-mass disc galaxies.

Seventhly, disc galaxies at higher $z$ can have larger $f_{H_2}$ than those at $z = 0$, mainly because discs are more compact so that a larger amount of $H_2$ gas can be formed in the high-density gaseous regions of the discs. It should be noted that (i) the simulated MW-type disc with low $f_b = 0.09$ at $z = 2$ can have a larger $f_{H_2}$ ($\sim 0.32$) and (ii) even the less massive disc with $M_b = 10^{11} M_\odot$ can have a larger $f_{H_2}$ ($\sim 0.16$). These results imply that high-$z$ disc galaxies are highly likely to have systematically rather high $H_2$ gas fractions.

The dependences of $M_{H_2}$ and $f_{H_2}$ on $f_b$ and $M_b$ can be seen among the simulated disc galaxies at $z = 2$.

### 3.2.3 Radial density profiles of $H_1$ and $H_2$

Fig. 13 shows that the five MW-type disc models with different $f_b$, $f_{H_2}$, and $f_{H_2}$, and surface stellar densities have qualitatively similar projected radial profiles of $H_1$, $H_2$, and $R_{mol}$, though the absolute magnitudes of these surface mass densities are different between the models. The $\Sigma_{H_2}$ profiles are steeper than $\Sigma_{H_1}$ in the five models, and the radial profiles of $R_{mol}$ ($= \Sigma_{H_2}/\Sigma_{H_1}$) have negative slopes (i.e. higher $R_{mol}$ at smaller $R$). The MW-type disc models with different $f_b$ have the steeper slopes approximated by $R^{-1.5}$, whereas the model with higher $f_b$ ($=0.55$) and smaller $f_{H_2}$ = 0.03 and the LSB model have shallower $R_{mol}$ profiles. The lower $\Sigma_{H_2}$ in the model with larger $f_b$ is due largely to rapid $H_2$ consumption in the inner disc.

Fig. 13 furthermore shows that tidal galaxy interaction can increase both $\Sigma_{H_1}$ and $\Sigma_{H_2}$, significantly owing to the strong gaseous concentration formed in the central regions of the interacting discs and the tidal arms. The strong central $H_2$ concentration is due largely to efficient gas transfer to the nuclear region induced by tidal bar and gaseous dissipation. The formation of $H_2$ is more efficient in the central region and tidal arms during galaxy interaction, which is discussed in more detail in Appendix B. The radial profile of $R_{mol}$ in the interaction model at $R < 1$ kpc is rather flat and there is the lack of $H_2$ gas in the circumnuclear region ($R \sim 2$ kpc) in the model.

The less massive disc models with $M_b = 10^{10}$ and $10^{11} M_\odot$ have shallower $\Sigma_{H_2}$, though this is in contrast with the MW-type disc models. The origin of the low $R_{mol}$ in low-mass disc models is closely associated with weak/no spiral and bar structures (due to the less strongly gravitation discs) and initially low $D$. Fig. 14 clearly demonstrates that if both $f_b$ and $f_{H_2}$ are the same between the fiducial MW-type disc model and the low-mass dwarf disc model (M25 with $M_b = 10^{10} M_\odot$), then $\Sigma_{H_2}$ is dramatically different between the two models. The maximum log $\Sigma_{H_2}$ is only $\sim 3.2$ M$_\odot$ pc$^{-2}$ in the low-mass disc model, which means that even if baryonic fractions are rather high, gas-poor low-mass disc galaxies are unlikely to form $H_2$ efficiently. A more gas-rich dwarf disc model shows a higher $\Sigma_{H_2}$ along S-shaped gaseous region, but $\Sigma_{H_2}$ is much lower than the MW-type disc model. The high-$z$ disc models ($z = 2$) also have shallower $R_{mol}$ profiles in the present study.

As shown in preceding sections, a strong central concentration of $H_2$ can occur in the barred disc galaxies owing to the dynamical action of stellar bars on gas. After the rapid consumption of $H_2$ gas in the centrally concentrated gas in the barred disc galaxies, there can be a deficiency of $H_2$ in their central regions. It is confirmed that the bulgeless disc galaxy with $f_b = 0$ at $T = 2$ Gyr (i.e. after long-term evolution), for which a strong bar can be spontaneously formed owing to global bar instability, can finally show the lack of $H_2$ in its central region after rapid $H_2$ consumption by SF in the central region. This result implies that if gas accretion on to discs is truncated, even the late-type disc galaxies with no/little bulges can show the lack of $H_2$ gas in their central regions.

### 3.2.4 Internal $H_2$-scaling relations

Fig. 15 describes the physical correlations of local properties of $H_2$ with those of dust and stars within galaxies with different model parameters. These ‘internal’ $H_2$-scaling relations will be able to
be compared with ongoing observational studies on H$_2$ properties of disc galaxies (by e.g. ALMA), and thus the predicted scaling relations will be useful for interpreting the observational results. It is clear that the models with different $f_g$, $f_b$, and initial stellar mass densities of the discs have a similar positive correlation between $M_{H_2}/M_*$ and $\Sigma_*$ for $\log \Sigma_* < 8$ M$_\odot$ kpc$^{-2}$. The simulated relatively flat correlation for $\log \Sigma_* \geq 8$ M$_\odot$ kpc$^{-2}$ is due to the strong concentration of H$_2$ in the central regions (where $\Sigma_*$ is high) caused by dynamical action of the stellar bars on gas in the discs.

The tidal interaction model, in which $f_g$ can be enhanced and H$_2$ distribution can be significantly changed, shows a $M_{H_2}/M_*-\Sigma_*$ relation similar to those seen in the isolated MW-type disc models, though the correlation is not so clear owing to the disturbed H$_2$ distribution. The less massive disc models with low $M_h$ also show strong positive $M_{H_2}/M_*-\Sigma_*$ correlations for lower $\Sigma_*$, though the central H$_2$ concentration makes the correlation shallower for higher $\Sigma_*$. The high-z models with $z = 2$ also have clear positive $M_{H_2}/M_*-\Sigma_*$ correlations, which implies that a linear $M_{H_2}/M_*-\Sigma_*$ correlation will be identified in future observations of H$_2$ distributions in high-z disc galaxies.

These 10 models show a much tighter correlation between $\Sigma_{H_2}$ and $\Sigma_{dust}$, which means that local ISM with higher dust surface densities can have higher H$_2$ surface densities in disc galaxies. This simulated almost linear $\Sigma_{H_2}-\Sigma_{dust}$ scaling relation is not so surprising, because H$_2$ formation efficiencies in local ISM are assumed to depend on the dust-to-gas ratios of local ISM in the present study.
Recent observational studies have just started a detailed investigation on the sub-kpc-scale properties of dust in nearby disc galaxies like M31 (e.g. Viaene et al. 2014), which can be combined with the observed sub-kpc-scale properties of H$_2$ to produce a possible dust–H$_2$ scaling relation within galaxies. The observed $\Sigma_{H_2}$ $-$ $\Sigma_{\text{dust}}$ scaling relation within galaxies will be able to be used as a stringent test for any theoretical model of H$_2$ formation on dust grains in galaxies.

### 3.2.5 Maximum possible H$_2$ mass

Fig. 16 describes the dependence of the maximum values of $M_{H_2}$ and $f_{H_2}$ during $\sim$1 Gyr dynamical evolution on the initial halo masses ($M_h$) and dust-to-gas ratios ($D$) in the selected models. It is clear from this figure that the models with larger $M_h$ or larger $D$ are more likely to have larger $M_{H_2,\text{max}}$ and $f_{H_2,\text{max}}$. The low-mass models have initially smaller $D$ due to the adopted mass–metallicity relation, and spiral arms and bars, which are the major driver for efficient H$_2$ formation in discs, cannot be formed owing to the less strongly self-gravitating discs (i.e. more strongly dominated by dark matter). This combination of the low $D$ and the incapability of bar/spiral formation in the low-mass models is the main reason for the derived dependences of $M_{H_2,\text{max}}$ and $f_{H_2,\text{max}}$ on $M_h$ and $D$. It should be stressed here that some models with $M_h \leq 10^{10}$ M$_\odot$ and those with $\log D < -4$ have no H$_2$ in the discs and thus no SF in the present SF models in which new stars can form exclusively from H$_2$ gas. This means that low-mass disc galaxies with very low $D$ are dominated by H i gas and have no SF so that they can be identified as isolated massive H i clouds with no SF (in other words, ‘dark H i galaxies’). The total H$_2$ mass cannot become larger than $10^9$ M$_\odot$ in some of low-mass models with $M_h < 10^{10}$ M$_\odot$, which means that massive star clusters and globular clusters (GCs) are unlikely to be formed from GMCs in low-mass disc galaxies. We will discuss this point later in the Discussion section.

### 4 DISCUSSION

#### 4.1 What determines $f_{H_2}$ ($R_{\text{mol}}$)?

One of the unresolved problems related to H$_2$ contents of galaxies dependent on Hubble types is that Sc/Sd late-type discs have smaller $f_{H_2}$ ($R_{\text{mol}}$) in spite of their having larger gas masses with respect to their dynamical masses ($M_{\text{gas}}/M_{\text{dyn}}$; see figs 4 and 5 in YS91, as an example for this). Although this problem will be able to be better discussed in our forthcoming papers in which ΛCDM galaxy formation models with H$_2$ formation are adopted, we can discuss this problem based on the present new results. Galactic bulges have been demonstrated to suppress H$_2$ formation in ISM only for the early dynamical evolution of disc galaxies, if $f_h$ is quite large (1–4, corresponding to Sa/S0 galaxies). The main reason for this is that spiral arms and bars, which can enhance the H$_2$ formation, can be suppressed by the presence of big bulges. The stronger ISRFs of big and dense bulges can be also responsible for less efficient conversion from H i to H$_2$ in ISM. Such a suppression effect of H$_2$ formation can be seen in models with different $M_h$ and $f_h$.

However, the larger $f_{H_2}$ in discs with smaller bulges cannot last owing to the more rapid gas consumption by SF. Furthermore, big bulge can severely suppress the SF so that $f_{H_2}$ in discs with big bulges can steadily increase owing to chemical enrichment (i.e. increasing $D$) and finally become significantly larger. This means that although $f_{H_2}$ can be larger in discs with smaller bulges for a fixed $f_h$, such discs do not necessarily continue to show larger $f_{H_2}$ (particularly when there is no external gas supply). Also the initially larger $f_{H_2}$ in discs with smaller bulges appears to be inconsistent with the observed trend of $f_{H_2}$ with Hubble types. Given these
results, it appears difficult to understand the origin of smaller $f_{H_2}$ in late-type Sc/Sd galaxies in the context of the bulge effects on $H_2$ formation.

The central stellar bars formed from global bar instability have been demonstrated to enhance significantly $f_{H_2}$ ($R_{mol}$), in particular, in the central regions of disc galaxies, though such enhancement cannot last long owing to rapid gas consumption by SF. Strong spirals arms have been demonstrated to be where $H_2$ formation is very efficient in the present study. Given that global bar/spiral instability can be prohibited by big bulges, discs with later types (i.e. smaller bulges) are more likely to show larger $f_{H_2}$. This possible trend of $f_{H_2}$ with Hubble types is opposite to the observed trend, which implies that the formation efficiency of stellar bars is not the major factor that determines $f_{H_2}$ in Sc/Sd galaxies.

The present study has also shown that the final $f_{H_2}$ of disc galaxies depends on the initial baryonic mass fractions ($f_{bary}$) such that $f_{H_2}$ can be larger in the models with larger $f_{bary}$ for a given $f_{H_2}$ ($M_h$). Recent observations have shown that $f_{bary}$ can be smaller in galaxies with lower halo masses (e.g. Papastergis et al. 2012). These observations combined with the present results therefore imply that if the late-type Sc/Sd galaxies can be preferentially formed from dark haloes with lower $M_h$, then the observed systematically small $f_{H_2}$ can be more clearly explained. Although the observed luminosity functions for different Hubble types in the local field and the Virgo cluster suggest that Sa+Sb galaxies are systematically brighter than Sc+Sd galaxies (e.g. Binggeli, Sandage & Tammann 1988), observational studies have not yet determined the mass functions of dark matter haloes and baryonic fractions for different Hubble types. Therefore, it is unclear whether the above explanation for the observed small

Figure 15. The simulated $H_2$-scaling relations for the representative 10 models, which are the same as shown in Fig. 13. The left- and right-hand panels show correlations between $M_{H_2}/M_*$ and $\Sigma_*$ and $\Sigma_{H_2}$ and $\Sigma_{dust}$, respectively. For comparison, the linear correlations of $M_{H_2}/M_* \propto \Sigma_*$ and $\Sigma_{H_2} \propto \Sigma_{dust}$ are shown by black dotted lines in the left- and right-hand panels, respectively.
The dependences of the maximum $M_{H_2}$ ($M_{H_2,\text{max}}$, upper) and $f_{H_2}$ ($f_{H_2,\text{max}}$, lower) during 1.1 Gyr dynamical evolution of discs on $M_h$ (left) and dust-to-gas ratio $D$ (right) in the selected 23 models. The models with no $H_2$ formation are plotted as log $M_{H_2} = 3$ and log $f_{H_2} = -4$ just for convenience. It should be noted that some low-mass dwarf models with $M_h \leq 10^{10} \, M_\odot$ have no H$_2$ (thus no SF), which means that these discs can be identified as ‘H I dark galaxies’.

$f_{H_2}$ in Sc/Sd galaxies is really plausible and realistic, though the smaller $f_{\text{bary}}$ in later Hubble types would be a promising scenario.

4.2 Do dark H I galaxies exist?

The present study has shown that low-mass disc galaxies show rather small $f_{H_2,\text{max}}$ (maximum possible H$_2$ fraction) and therefore can be identified as H I-dominated galaxies. The major physical reason for this very low H$_2$ contents is that these low-mass galaxies are extremely dust poor so that they cannot form H$_2$ on dust grains. The possible smaller $f_{\text{bary}}$ in these low-mass galaxies can also contribute to the very low H$_2$ formation efficiency of the ISM. Furthermore, some of the simulated low-mass galaxies with rather high initial $f_2$ (>0.9) can show virtually $f_{H_2,\text{max}} = 0$, if $M_h$ is as low as or lower than $3 \times 10^9 \, M_\odot$. These results imply that there would exist low-mass, and extremely LSB galaxies with only H I gas: these are almost ‘dark’ galaxies.

So far no observational studies have found strong evidence for the presence of isolated (or ‘intergalactic’) dark H I-rich galaxies with total gas masses larger than $10^8 \, M_\odot$ in the nearby universe, though a number of observational studies investigated H I contents of galaxies in group environments (e.g. Kilborn et al. 2005; Pisano et al. 2011). Although most of the detected H I objects have optical counterparts (or tidal origin) in these observations, a few observations so far discovered massive apparently isolated H I gas clouds with masses larger than $10^8 \, M_\odot$ (e.g. Davies et al. 2004; Koribalski et al. 2004). These intriguing massive isolated objects are likely to be just tidal debris rather than dark H I galaxies (e.g. Bekki, Koribalski & Kilborn 2005). If H I-dominated low-mass dark galaxies do not exist, the present study implies that such low-mass galaxies had lost almost all of their gas at their formation epochs or during their evolution owing to some physical processes such as ram pressure stripping and cosmic reionization.

4.3 Implications on the formation of globular clusters at high z

The present study has shown that (i) some low-mass galaxies with $M_h \leq 10^{10} \, M_\odot$ cannot form H$_2$ efficiently owing to their low dust masses and consequently (ii) the total H$_2$ masses are unlikely to exceed $10^7 \, M_\odot$. These results can have the following implications on the formation of massive star clusters, in particular, GCs, the origin of which remains unexplained. As recent theoretical studies of GC formation have demonstrated (e.g. D’Ercole et al. 2008; Bekki 2011), the initial stellar masses of GCs should be $\sim 10^6 \, M_\odot$ even for a high SFE of $\sim 0.2$. 

Although most of the detected H I objects have optical counterparts (or tidal origin) in these observations, a few observations so far discovered massive apparently isolated H I gas clouds with masses larger than $10^8 \, M_\odot$ (e.g. Davies et al. 2004; Koribalski et al. 2004). These intriguing massive isolated objects are likely to be just tidal debris rather than dark H I galaxies (e.g. Bekki, Koribalski & Kilborn 2005). If H I-dominated low-mass dark galaxies do not exist, the present study implies that such low-mass galaxies had lost almost all of their gas at their formation epochs or during their evolution owing to some physical processes such as ram pressure stripping and cosmic reionization.
These theoretical results on GC formation combined with the present results imply that low-mass galaxies with $M_\bullet \leq 10^{10} M_\odot$ are unlikely to form GCs within them owing to the low $H_2$ contents. It would be possible that only low-mass, low-density star clusters can form in their host low-mass galaxies. These low-mass clusters are prone to tidal destruction by their host galaxies so that they can finally become field stars within their hosts. If there exists a threshold halo mass above which GCs can form, then it cannot only explain the observed absence of GCs in some faint dwarf galaxies in the Local Group (e.g. van den Bergh 2000) but also provide a physical basis on the minimum halo mass of GC host galaxies introduced in recent semi-analytic models of GC formation in galaxies based on hierarchical galaxy formation scenarios (e.g. Bekki et al. 2008; Griffen et al. 2010).

5 CONCLUSIONS

We have investigated the physical properties of $H_2$ in disc galaxies with different masses and Hubble types based on our new model for the formation of $H_2$ on dust grains. The basic parameters in this numerical study are $M_\bullet$ (halo mass), $f_\text{gas}$ (baryonic mass fraction), $f_g$ (gas mass fraction), and $f_\text{H_2}$ (bulge-to-disc ratio). We have investigated how the spatial distributions, time evolution, and scaling relations of $H_2$ depend on these parameters both for isolated disc galaxies and for interacting ones. The principal results are as follows.

1. The observed positive correlation between the mass ratio of $H_2$ to $H_1$ ($R_{\text{mol}}$) and gaseous pressure ($P_g$) can be reproduced reasonably well by the present models. However, the $R_{\text{mol}}$–$P_g$ relation ($R_{\text{mol}} \propto P_g^{0.92}$) can be reproduced well only for some ranges of model parameters for dust growth and destruction. These results imply that dust can play a significant role in the formation of the $R_{\text{mol}}$–$P_g$ relation and thus that dust formation and evolution needs to be included in discussing the origin of $H_2$ scaling relations.

2. The simulated $H_2$SDDs in isolated luminous disc galaxies can have the slope of $R_{\text{mol}}$–$P_g$ relation ($R_{\text{mol}} \propto P_g^{0.92}$) and thus that dust formation and evolution needs to be included in discussing the origin of $H_2$ scaling relations.

3. The simulated radial profiles of the $\Sigma_{H_2}$–$\Sigma_{H_1}$ ratios in isolated luminous disc galaxies can be described as $R^{-1.5}$, which are observed in disc galaxies. This successful reproduction of observations implies that the present dust-regulated $H_2$ models can grasp some essential ingredients of $H_2$ formation in ISM of disc galaxies. The radial gradients can be different between low- and high-mass disc galaxies at low- and high-$z$ and between isolated and interacting galaxies. The simulated $H_2$ distributions are clumpier than $H_1$ in most models. The $H_2$ surface density of a disc galaxy can dramatically drop below a certain radius where $H_2$ formation efficiency becomes rather low owing to the low gas density and the low $D$.

4. The mass ratios of $H_2$ to stars ($M_{H_2}/M_\star$) in individual local regions of a galaxy can anticorrelate with the local surface stellar density ($\Sigma_\star$). This anticorrelation ($M_{H_2}/M_\star \propto \Sigma_\star^{-1}$) can be seen in different galaxy models with different parameters. The $H_2$ surface densities ($\Sigma_{H_2}$) of local individual regions in a galaxy can correlate with the dust surface densities ($\Sigma_{\text{dust}}$) such that $\Sigma_{H_2} \propto \Sigma_{\text{dust}}$. This $H_2$–dust correlation is rather tight in different galaxy models.

5. The initial total masses of dark haloes ($M_\bullet$) can control the $H_2$ mass fractions ($f_{H_2}$) of disc galaxies in such a way that $f_{H_2}$ can be larger for larger $M_\bullet$. This is first because the formation of spiral arms and bars, where $H_2$ formation is rather efficient, can be severely suppressed in smaller $M_\bullet$, and secondly because the dust-to-gas ratios ($D$), which determines the formation efficiency of $H_2$ on dust grains, are lower for smaller $M_\bullet$. Some low-mass galaxies with $M_\bullet \leq 10^{10} M_\odot$ show no/little $H_2$ formation within their discs in the present study.

6. Galactic bulges can strongly suppress the formation of $H_2$ in disc galaxies at the early dynamical evolution of disc galaxies, if $f_\text{H_2}$ is quite large ($\gtrsim 1$). This is mainly because big bulges can prevent global spiral/bar instability from occurring so that efficient $H_2$ formation within spirals and bars can be severely suppressed. This, however, does not necessarily mean that $f_{H_2}$ can continue to be low, because slow gas consumption by SF yet steady chemical enrichment (i.e. increasing $D$) can finally enhance $f_{H_2}$ for some disc models with big bulges in the present study. These results imply that the origin of some late-type disc galaxies (Sc and Sd) with smaller $f_{H_2}$ is not simply due to their small bulges. Some disc models in the present study show the lack of $H_2$ gas in their central regions.

7. Barred disc galaxies are more likely to have larger $f_{H_2}$ owing to the formation of centrally concentrated $H_2$ rings and discs. The central $H_2$ can be rapidly consumed by SF so that higher $f_{H_2}$ in barred galaxies cannot last long without further external gas supply on to the discs. Some of the simulated barred disc galaxies can have elongated $H_2$ rings in their central regions, though such $H_2$ structures are quite short-lived. Bulgeless disc galaxies with central bars can also show the lack of $H_2$ in their central regions after rapid consumption of $H_2$ transferred to the inner few kpc.

8. Disc galaxies at higher $z$ are more likely to have larger $f_{H_2}$ owing to their initially high gas densities in the more compact discs. This result does not depend on other model parameters such as $M_\bullet$. Disc galaxies with smaller $f_{\text{H_2}}$ at higher $z$ can still show higher $f_{H_2}$. For a given $M_\bullet$, $f_{H_2}$, and $z$, disc galaxies with smaller $f_{\text{H_2}}$ have smaller $f_{H_2}$. High-$z$ discs are more likely to have very clumpy $H_2$ distributions with numerous small $H_2$ clouds.

9. The maximum $H_2$ masses ($M_{H_2,\text{max}}$) and fractions ($f_{H_2,\text{max}}$) depend on initial halo masses $M_\bullet$ and dust-to-gas ratios ($D$) such that both can be higher in larger $M_\bullet$ and larger $D$. For low-mass haloes with $M_\bullet \leq 10^{10} M_\odot$, the formation of $H_2$ can be completely suppressed in some models with smaller gas fractions so that no stars can be formed. Some low-mass galaxies with $M_\bullet \leq 3 \times 10^9 M_\odot$ cannot form $H_2$ owing to rather low dust contents even if they are quite gas rich $f_g > 0.9$. These galaxies with no $H_2$ are still very rich in $H_1$ and could be observationally identified as gas-rich extremely LSB galaxies (or almost ‘dark galaxies’).

10. The spatial distributions of $H_2$ in the simulated galaxies are quite diverse depending on initial $M_\bullet$ and Hubble types (e.g. bulge-to-disc ratio, $f_g$). Circumnuclear $H_2$ rings can be formed in barred disc galaxies, and such ring formation can significantly increase $f_{H_2}$ in the galaxies. Radial $H_2$ profiles can be steeper for more luminous disc galaxies in isolation, and tidal interaction can dramatically increase the degrees of central $H_2$ concentration in disc galaxies.

11. The present results have several important implications of SF processes of galaxies. For example, massive star clusters, like old GCs, are unlikely to be formed in low-mass galaxies ($M_\bullet < 3 \times 10^9 M_\odot$), because the maximum possible total $H_2$ masses can be well less than $10^9 M_\odot$ (i.e. owing to the incapability of GMCs to form). This result implies that there would exist a threshold galaxy mass above which old GCs can be formed within galaxies at high $z$. 

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APPENDIX A: THE FORMATION OF A CENTRAL STELLAR BAR

In the present fiducial MW-type disc model (M1), a stellar bar can play a significant role in the formation of H₂ on dust grains and the dynamical evolution of H₂ gas, in particular, in the later evolution of the central region of the gas disc. We here briefly describe the bar formation process in this model. As shown in Fig. A1 on the time evolution of stellar surface density (Σ) of the disc, a stellar bar can start to develop around T = 0.8 Gyr owing to bar instability in this model with a relatively small bulge mass. The formation of a strong nuclear bar can be completed by T = 1.1 Gyr so that the bar can influence the gas dynamics there after its formation (e.g. a massive nuclear H₂ disc can be formed at T = 2 Gyr as a result of dynamical interaction between the bar and H₂ gas, as shown in Fig. 4). The gaseous component (H + H₂) also shows a bar-like distribution in the central region of the disc when the stellar bar forms at T = 1.1 Gyr.

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The time evolution of the projected mass densities for stars ($\Sigma_1$) in the central region of the fiducial MW-type disc model (M1). The formation of a central stellar bar can be developed within less than 1 Gyr in this model so that the bar can influence the formation of $H_2$ there.

**APPENDIX B: INTRIGUING $H_2$ DISTRIBUTIONS IN SELECTED MODELS**

Figs B1 and B2 show intriguing $H_2$ distributions of galactic discs in selected models. In Fig. B1, the initial $\Sigma_{H_2}$ of each mesh at $T = 0$ is calculated by assuming that $H_2$ mass fraction is 0.01 just for convenience, because $H_2$ formation efficiency based ISRF etc. is not calculated at $T = 0$. The formation efficiency of $H_2$ on dust grains can be significantly enhanced in the strong tidal arms of the interacting disc galaxy for the PR interaction model (M16), as shown in Fig. B1 (at $T = 0.6$ Gyr). During the efficient gas infall on to the nuclear regions, both $H_1$ and $H_2$ gas densities can become significantly higher so that SFRs can be high in the nuclear region and the tidal arms. After tidal interaction, the $H_2$ distribution appears to be clumpy with a number of off-centre high-density $H_2$ clumps in the disc. Such off-centre massive gas clumps can be also seen in recent models of gas-rich interacting galaxies by Yozin & Bekki (2014a). Since the number of tidal interaction models investigated in the present study is rather small ($<10$), we cannot conclude whether such a clumpy $H_2$ distribution is a characteristic of post-interacting galaxies. We will investigate this point in our future works by performing a larger number of numerical simulations of interacting galaxies with a much wider range of model parameters for galaxy interaction.

Fig. B2 shows that a gas-rich, more compact disc at $z = 2$ can have a widespread spatial distribution of $H_2$ gas in the model M15. In this model, the baryonic mass fraction is lower than the fiducial MW-disc model (i.e. less strongly self-gravitating) so that the formation of a strong bar can be suppressed. Therefore, a bar-like distribution of gas cannot be clearly seen in this model. Even in the outer part of the gas disc, high-density $H_2$ regions can be seen, which is in a striking contrast with the $H_2$ distribution of the low-$z$ fiducial MW-disc model (M1). The gas disc at $z = 2$ appears to be composed of numerous small $H_2$ clumps, which implies that the MCMF can be significantly different between $z = 0$ and 2. Since the present simulation does not have enough resolution to investigate MCMFs, we will discuss this point in our future numerical works with a much larger number of gas particles.
Figure B1. The time evolution of the projected mass densities for H\textsubscript{I} (\Sigma_{\text{H}1}, left four) and H\textsubscript{2} (\Sigma_{\text{H}2}, right four) for the PR tidal interaction model (M16).

Figure B2. The final projected mass densities for H\textsubscript{I} (\Sigma_{\text{H}1}, left) and H\textsubscript{2} (\Sigma_{\text{H}2}, right) for the high-z MW-type disc model with \(f_g = 0.55\) (M15).