# INGREDIENTS FOR 21CM INTENSITY MAPPING

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## ABSTRACT

Current and upcoming radio telescopes will map the spatial distribution of cosmic neutral hydrogen (HI) through its 21cm emission. In order to extract the maximum information from these surveys, accurate theoretical predictions are needed. We study the abundance and clustering properties of HI at redshifts  $z \leq 5$  using TNG100, a large state-of-the-art magneto-hydrodynamic simulation of a  $75 h^{-1}$ Mpc box size, which is part of the IllustrisTNG Project. We show that most of the HI lies within dark matter halos and we provide fits for the halo HI mass function, i.e. the mean HI mass hosted by a halo of mass M at redshift z. We find that only halos with circular velocities larger than  $\simeq 30$  km/s contain HI. While the density profiles of HI exhibit a large halo-to-halo scatter, the mean profiles are universal across mass and redshift. The HI in low-mass halos is mostly located in the central galaxy, while in massive halos HI is concentrated in the satellites. Our simulation reproduces the DLAs bias value from observations. We show that the HI and matter density probability distribution functions differ significantly. Our results point out that for small halos the HI bulk velocity goes in the same direction and has the same magnitude as the halo peculiar velocity, while in large halos differences show up. We find that halo HI velocity dispersion follows a power-law with halo mass. We find a complicated HI bias, with HI becoming non-linear already at  $k = 0.3 h \text{Mpc}^{-1}$  at  $z \gtrsim 3$ . The clustering of HI can however be accurately reproduced by perturbative methods. We find a new secondary bias, by showing that the clustering of halos depends not only on mass but also on HI content. We compute the amplitude of the HI shot-noise and find that it is small at all redshifts, verifying the robustness of BAO measurements with 21cm intensity mapping. We study the clustering of HI in redshift-space, and show that linear theory can explain the ratio between the monopoles in redshift- and real-space down to 0.3, 0.5 and 1  $h \text{Mpc}^{-1}$  at redshifts 3, 4 and 5, respectively. We find that the amplitude of the Fingers-of-God effect is larger for HI than for matter, since HI is found only in halos above a certain mass. We point out that 21 cm maps can be created from N-body simulations rather than full hydrodynamic simulations. Modeling the 1-halo term is crucial for achieving percent accuracy with respect to a full hydro treatment.

Keywords: large-scale structure of universe – radio lines: general – methods: numerical

#### 1. INTRODUCTION

The  $\Lambda$ CDM model describes how the initial quantum perturbations in the primordial Universe grow and give rise to the cosmic web: large accumulations of matter in the form of dark matter halos accrete material through filaments and sheets that surround enormous diffuse regions in space. This model has been successful in explaining a very diverse set of cosmological observables, including, among others, the anisotropies in the cosmic microwave background (CMB), the spatial distribution of galaxies, the statistical properties of the  $Ly\alpha$ -forest, the abundance of galaxy clusters, and correlations in the

shapes of galaxies induced by gravitational lensing.

The ACDM model has free parameters that describe physical quantities such as the geometry of the Universe, the amount of cold dark matter (CDM) and baryons, the sum of the neutrino masses, the expansion rate of the Universe, the nature of dark energy, and the initial conditions of the Universe. The current quest in cosmology is to determine the values of these parameters as precisely as possible, by exploiting the fact that they influence the spatial distribution of matter. Thus, by examining the statistical properties of matter tracers such as galaxies and cosmic neutral hydrogen, the spatial distribution of matter can be inferred and the value of the cosmological parameters can be constrained.

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The amount of information that can be extracted from cosmological surveys depends on several factors, such as the volume being covered or the range in scales where theoretical predictions are reliable. For example, in the case of the CMB, theoretical predictions are extremely precise, because the radiation we observe was produced when the fluctuations were in the linear regime. Tracing the large-scale structure of the Universe at low redshifts, through spectroscopic galaxy surveys, represents a complementary approach for extracting cosmological information, where much larger volumes can be surveyed but the theoretical predictions are more uncertain. For galaxy surveys the volume that can be probed also limits the method, because at high redshifts galaxies are fainter and their spectroscopic detection is challenging.

A different way to trace the matter field is through 21cm intensity mapping (Bharadwaj et al. 2001; Bharadwaj & Sethi 2001; Battye et al. 2004; McQuinn et al. 2006; Chang et al. 2008; Loeb & Wyithe 2008; Bull et al. 2015; Santos et al. 2015; Villaescusa-Navarro et al. 2015). The method consists of carrying out a low angular resolution survey where the total 21 cm flux from unresolved sources is measured on large areas of the sky at different frequencies. The emission arises from the hyperfine splitting of the ground state of neutral hydrogen into two levels because of the spin-spin interaction between the electron and proton. An electron located in the upper energy level can decay into the lower energy state by emitting a photon with a rest wavelength of 21 cm. This method has several advantages over traditional approaches. First, given that the observable is the 21 cm line, the method is spectroscopic in nature. Second, very large cosmological volumes can be surveyed in a fast and efficient manner. Third, the amplitude of the signal depends only on the abundance and clustering of neutral hydrogen, so cosmic HI can be traced from z = 0 to  $z \simeq 50^2$ .

Current, upcoming and future surveys such as the Giant Meterwave Radio Telescope (GMRT)<sup>3</sup>, the Ooty Radio Telescope (ORT)<sup>4</sup>, the Canadian Hydrogen Intensity Mapping Experiment (CHIME)<sup>5</sup>, the Five hundred meter Aperture Spherical Telescope (FAST)<sup>6</sup>, Tianlai<sup>7</sup>, BINGO (Baryon acoustic oscillations In Neutral Gas Observations)<sup>8</sup>, ASKAP (The Australian Square Kilometer Array Pathfinder)<sup>9</sup>, MeerKAT (The South African Square Kilometer Array Pathfinder)<sup>10</sup>, HIRAX (The Hydrogen Intensity and Real-time Analysis eXperiment)<sup>11</sup> and the SKA (The Square Kilometer Array)<sup>12</sup> will sample the large-scale structure of the Universe in the postreionization era by detecting 21 cm emission from cosmic neutral hydrogen (Sarkar et al. 2018a; Carucci et al. 2017b; Sarkar et al. 2018b; Marthi et al. 2017; Sarkar et al. 2016b; Choudhuri et al. 2016).

In order to extract information from those surveys, the observational data has to be compared with theoretical predictions. To linear order, the amplitude and shape of the 21 cm power spectrum is given by

$$P_{21\rm cm}(k,\mu) = \bar{T}_b^2 \left[ (b_{\rm HI} + f\mu^2)^2 P_{\rm m}(k) + P_{\rm SN} \right] , \quad (1)$$

where  $\bar{T}_b$  is the mean brightness temperature,  $b_{\rm HI}$  is the HI bias, f is the linear growth rate,  $\mu = k_z/k$ ,  $P_{\rm m}(k)$  is the linear matter power spectrum and  $P_{\rm SN}$  is the HI shot-noise. Here,  $k_z$  is the projection of k along the line-of-sight, which we take to be the z-axis.

At redshifts  $z \in [0, 5]$  we have relatively good knowledge of the abundance of cosmic neutral hydrogen, and therefore, of  $\overline{T}_b$ . On the other hand, little is known about the value of the HI bias and HI shot-noise in that redshift interval. It is important to determine their values since the signal-to-noise ratio and range of scales where information can be extracted critically depends on them. One of the purposes of our work is to measure these quantities at different redshifts. Moreover, it is important to determine the the regime where linear theory is accurate. In this work we investigate in detail at which redshifts and scales the clustering of HI in real-space (i.e. the HI bias) and in redshift-space (Kaiser factor) becomes non-linear.

In order to optimize what can be learned from the surveys mentioned above, theoretical predictions in the mildly and fully non-linear regimes are needed. The halo model provides a reasonably accurate framework for predicting the abundance and clustering of HI from linear to fully non-linear scales. To apply this method, several ingredients are needed for a given cosmological model: 1) the linear matter power spectrum,  $P_{\text{lin}}(k, z)$ , 2) the halo mass function, n(M, z), 3) the halo bias, b(M, z), 4) the average HI mass that a halo of mass M hosts at redshift z,  $M_{\rm HI}(M, z)$ , which we refer to as the halo HI mass function<sup>13</sup> and 5) the mean density profile of neutral hydrogen within halos of mass M at redshift z,  $\rho_{\rm HI}(r|M,z)$ . In addition, the halo model is formulated under the assumption that all HI is confined to dark matter halos. With the above ingredients at hand one can write the fully non-linear HI power spectrum as the sum of 1-halo and 2-halo terms

- <sup>3</sup> http://gmrt.ncra.tifr.res.in/
- <sup>4</sup> http://rac.ncra.tifr.res.in/
- <sup>5</sup> http://chime.phas.ubc.ca/
- <sup>6</sup> http://fast.bao.ac.cn/en/
- <sup>7</sup> http://tianlai.bao.ac.cn
- <sup>8</sup> http://www.jb.man.ac.uk/research/BINGO/

<sup>9</sup> http://www.atnf.csiro.au/projects/askap/index.html

- <sup>10</sup> http://www.ska.ac.za/meerkat/
- <sup>11</sup> https://www.acru.ukzn.ac.za/~hirax/
- <sup>12</sup> https://www.skatelescope.org/

 $<sup>^2</sup>$  At higher redshifts the atmosphere becomes opaque at the relevant wavelengths.

 $<sup>^{13}</sup>$  note that the term "HI mass function" is commonly used to model the abundance of galaxies with different HI masses. Thus, in order to distinguish the two concepts we use "halo HI mass function" to refer to the function that returns the average HI mass inside a halo of mass M at redshift z.

$$P_{\rm HI}(k,z) = P_{\rm HI,1h}(k) + P_{\rm HI,2h}(k)$$
<sup>(2)</sup>

$$P_{\rm HI,1h}(k,z) = \frac{1}{(\rho_c^0 \Omega_{\rm HI}(z))^2} \int_0^\infty dM n(M,z) M_{\rm HI}^2(M,z) \left| u_{\rm HI}(k|M,z) \right|^2 \tag{3}$$

$$P_{\rm HI,2h}(k,z) = \frac{P_{\rm lin}(k,z)}{(\rho_{\rm c}^0 \Omega_{\rm HI}(z))^2} \left[ \int_0^\infty dM n(M,z) b(M,z) M_{\rm HI}(M,z) |u_{\rm HI}(k|M,z)| \right]^2 \tag{4}$$

where  $\rho_c^0$  is the critical density of the Universe today and  $\Omega_{\rm HI}(z) = \bar{\rho}_{\rm HI}(z)/\rho_c^0$ , with  $\bar{\rho}_{\rm HI}(z)$  being the mean HI density at redshift z. u(k|M,z) is the Fourier transform of the normalized HI density profile:  $u(x|M,z) = \rho_{\rm HI}(x|M,z)/M_{\rm HI}(M,z)$ .

Some of the goals of our work are to quantify: 1) the amount of HI outside of halos, 2) the form of the halo HI mass function, and 3) the density profiles of HI within halos.

While the halo model is a powerful analytic framework, it does not model accurately a number of things, e.g. the transition between the 1-h and 2-h terms (Massara et al. 2014). Thus, its accuracy can be severely limited by that. A more precise modeling can be achieved by *painting* HI on top of dark matter halos according the HI halo model ingredients (Villaescusa-Navarro et al. 2014), i.e. more like an HI Halo Occupation Distribution (HOD) modeling.

Since 21cm intensity mapping observations are carried out in redshift-space, modeling the abundance and spatial distribution of HI in halos is not enough. A complete description also requires to know the distribution of HI velocities. In this work we investigate the HI bulk velocities, the velocity dispersion of HI inside halos and the amplitude of the Fingers-of-God in the power spectrum.

The standard halo model does not account for various complexities expected in the real Universe, e.g. whether the HI density profiles depend not only on mass but on the galaxy population (blue/red) of the halo, whether the clustering of halos depends not only on mass but also on environment, and so forth. These questions can however be addressed with hydrodynamic simulations, and in this paper we investigate them in detail.

We also study some quantities that can help us to improve our knowledge on the spatial distribution of HI: the probability distribution function of HI, the relation between the overdensities of matter and HI, the contribution of central and satellites galaxies to the total HI mass content in halos, the HI column density distribution function and the DLAs cross-section.

We carry out our analysis using the IllustrisTNG Project, state-of-the-art hydrodynamic simulations that follow the evolution of billions of resolution elements representing CDM, gas, black holes and stars in the largest volumes ever explored at such mass and spatial resolution. Given the realism of our hydrodynamic simulations, we always aim to connect our results to the underlying physical processes. We note that previous works have studied the HI content of simulated galaxies in detail (Crain et al. 2017; Bahé et al. 2016; Davé et al. 2013; Bird et al. 2014; Lagos et al. 2014; Faucher-Giguère et al. 2016; Marinacci et al. 2017; Zoldan et al. 2017; Xie et al. 2017).

We also show that once the most important ingredients

for modeling the abundance and clustering properties of HI have been calibrated using full hydrodynamic simulations, less costly dark mater-only simulations, or approximate methods such as COLA (Tassev et al. 2013), PEAK-PATCH or PINOCCHIO (Monaco et al. 2002; Munari et al. 2017), can be used to generate accurate 21 cm maps. Those maps can then be used to study other properties of HI in the fully non-linear regime, such as the 21 cm bispectrum or the properties of HI voids. In this work we investigate the accuracy achieved by creating 21cm maps from N-body with respect to full hydrodynamic simulations.

This paper is organized as follows. In section 2 we describe the characteristics of the IllustrisTNG simulations and the method we use to estimate the mass of neutral hydrogen associated with each gas cell. We consider different properties of the abundance of HI in sections 3 to 12:

- In section 3 we compare the overall HI abundance in our simulations to observations.
- In section 4 we quantify the fraction of HI within halos and galaxies.
- In section 5 we study the halo HI mass function.
- In section 6 we investigate the density profiles of HI inside halos.
- In section 7 we quantify the fraction of the HI mass in halos that is in the central and satellites galaxies.
- In section 8 we examine the probability distribution function (pdf) of the HI density and compare it with the total matter density pdf.
- In section 9 we compute the HI column density distribution function for the absorbers with high column density and quantify the DLAs cross-section and bias.
- In section 10 we consider the bulk velocities of HI inside halos.
- In section 11 we investigate the velocity dispersion of HI inside halos and compare it against matter.
- In section 12 we quantify the relation between the overdensity of matter and HI.

We investigate HI clustering in sections 13 to 16:

- In section 13 we present the amplitude and shape of the HI bias and investigate how well perturbation theory can reproduce the HI clustering in real-space.
- In section 14 we show that the clustering of dark matter halos in general depends on their HI masses for fixed halo mass.

- In section 15 we quantify the amplitude of the HI shotnoise.
- In section 16 we study the clustering of HI in redshift-space.

In section 17 we estimate the accuracy that can be achieved by simulating HI through a combination of Nbody simulations with the results derived in the previous sections rather than through ful hydrodynamic simulations. Finally, we provide the main conclusions of our work in section 18. During the course of the discussion, we provide fitting formulae that can be used to reproduce our results.

#### 2. Methods

## 2.1. The IllustrisTNG simulations

The simulations used in this work are part of the IllustrisTNG Project (Springel et al. 2017; Pillepich et al. 2017a; Nelson et al. 2018; Naiman et al. 2017; Marinacci et al. 2017). We employ two cosmological boxes that have been evolved to z = 0, TNG100 (which is the same volume as the Illustris simulation; Vogelsberger et al. 2014a,b; Genel et al. 2014) and TNG300, with 75  $h^{-1}$ Mpc and 205  $h^{-1}$ Mpc comoving on a side, respectively. In particular, we use their high-resolution realizations that evolve baryonic resolution elements with mean masses of  $1.4 \times 10^6$  M<sub> $\odot$ </sub> and  $1.1 \times 10^7$  M<sub> $\odot$ </sub>, respectively.

These simulations have been run with the AREPO code (Springel 2010), which calculates gravity using a tree-PM method, magneto-hydrodynamics with a Godunov method on a moving Voronoi mesh, and a range of astrophysical processes described by sub-grid models. These processes include primordial and metal-line cooling assuming a time-dependent uniform UV background radiation, star and supermassive black hole formation, stellar population evolution that enriches surrounding gas with heavy elements or metals, galactic winds, and several modes of black hole feedback. Importantly, where uncertainty and freedom exist for the implementation of these models, they are parametrized and tuned to obtain a reasonable match to a small set of observational results. These include the galaxy stellar mass function and the baryon content of group-scale dark matter halos, both at z = 0. The numerical methods and subgrid physics models build upon Vogelsberger et al. (2013), and are specified in full in Weinberger et al. (2017a,b) and Pillepich et al. (2017b). Accounts of the match between the simulations and observations in a number of diverse aspects, such as galaxy and halo sizes, colors, metallicities, magnetic fields and clustering, are presented in the references above as well as in Genel et al. (2017), Vogelsberger et al. (2017) and Torrey et al. (2017).

In this paper we work mainly with halos identified by the Friends-of-Friends (FoF) algorithm with a linking length of b = 0.2 (Davis et al. 1985). We take the halo center as the position of the most bound particle in the halo. For each FoF halo, we also use the halo's "virial" radius, defined using  $M = 4\pi/3\Delta_c\rho_c R^3$ , where  $\rho_c$  is the Universe critical density at the halo's redshift z and  $\Delta_c = 18\pi^2 + 82x - 39x^2$ , with x = $\Omega_m(1+z)^3/(\Omega_m(1+z)^3 + \Omega_\Lambda) - 1$  (Bryan & Norman 1998). We refer to these objects as "FoF-SO" halos, for 'spherical overdensity,' since a single SO (spherical overdensity) halo is identified for each FoF halo<sup>14</sup>. Unless stated explicitly, we refer for FoF halos when talking generally about dark matter halos. The SUBFIND algorithm (Springel et al. 2001) has been run to identify self-bound substructures in each FoF halos, and those objects are referred to as 'galaxies' in what follows. This class of objects includes both the satellites and the central SUB-FIND subhalos of each FoF halo.

## 2.2. Modeling the hydrogen phases

We now describe the method we use to quantify the fraction of hydrogen that is in each phase (neutral, ionized or molecular) for each Voronoi cell in the simulation.

For non-star-forming gas, we use the division between neutral and ionized mass fractions that is calculated in the IllustrisTNG runs on-the-fly and is included in the simulation outputs. This breakdown assumes primordial chemistry in photo-ionization equilibrium with the cosmic background radiation (Faucher-Giguère et al. 2009), including a density-dependent attenuation thereof to account for self-shielding following Rahmati et al. (2013a).

For star-forming gas, we post-process the outputs of the simulations to account for the multi-phase interstellar medium, including the presence of molecular hydrogen, H<sub>2</sub>. The values stored in the simulation output are based on the mass-weighted temperature between cold and hot phases according to the Springel & Hernquist (2003) model, and are thus expected to underestimate the neutral hydrogen fraction. Instead, we set the temperature of star-forming cells to  $T = 10^4$  K and recalculate the equilibrium neutral hydrogen fraction, also including the self-shielding correction.

The above procedure gives the fraction of hydrogen which is neutral:  $M_{\rm NH}/M_{\rm H}$ , with  $M_{\rm NH} = M_{\rm HI} + M_{\rm H_2}$ . We then compute the H<sub>2</sub> fraction,  $f_{\rm H_2} = M_{\rm H_2}/M_{\rm NH}$  employing the KMT model (Krumholz et al. 2008, 2009; McKee & Krumholz 2010; see also Sternberg et al. 2014), which we briefly review here.

The molecular hydrogen fraction,  $f_{\text{H}_2}$ , which we assume non-zero only for star-forming gas, is estimated through

$$f_{\rm H_2} = \begin{cases} 1 - \frac{0.75s}{1 + 0.25s} & \text{if } s < 2\\ 0 & \text{if } s \ge 2 \end{cases}$$
(5)

where s is given by

$$s = \frac{\log(1 + 0.6\chi + 0.01\chi^2)}{0.6\tau_c} , \qquad (6)$$

and

$$\chi = 0.756(1 + 3.1Z^{0.365}) \tag{7}$$

$$\tau_c = \Sigma \sigma_d / \mu_{\rm H} \ . \tag{8}$$

In the above equations Z represents the gas metallicity in units of solar metallicity (Allende Prieto et al. 2001),  $\sigma_d$  is the cross-section of dust, which we estimate from  $\sigma_d = Z \times 10^{-21}$  cm<sup>2</sup>,  $\mu_{\rm H}$  is the mean mass per hydrogen nucleus,  $\mu_{\rm H} = 2.3 \times 10^{-24}$  g, and  $\Sigma$  is the surface density of the gas, which we compute as  $\Sigma = \rho R$ , where  $\rho$  is the gas density and  $R = (3V/4\pi)^{1/3}$  with V being the volume of the Voronoi cell.

 $^{14}$  Notice that a pure SO algorithm may identify several SO halos inside a single FoF halo (see appendix C).



Figure 1. Spatial distribution of neutral hydrogen (left) and gas (right) in slices of 5  $h^{-1}$ Mpc depth at redshift z = 1. The upper panels show the distribution in the entire simulation volume of TNG100, while the middle and bottom panels display a zoom-in into the regions marked with a white square in the upper and middle panels, respectively. While the HI in the Ly $\alpha$ -forest occupies most of the volume, the HI in galaxies represents the majority of its total mass.

It is possible that our treatment may underestimate the  $H_2$  fractions since: 1) the molecular hydrogen fractions go to zero at low densities in the KMT model, 2) we assign molecular hydrogen only to star-forming cells, and 3) it is pessimistic to estimate the surface density from the cell radii. However, we believe that a more precise treatment of  $H_2$  will not affect our results, as its overall abundance is small and therefore not much HI will be transformed into  $H_2$ . In order to test this more explicitly we have considered two extreme cases in which: 1) no  $H_2$ is modeled and 2) all hydrogen in star-forming cells is in molecular form. We have computed the value  $\Omega_{\rm HI}(z)$  (see section 3) and did not find significant changes. We thus believe that our conclusions are robust against our  $H_2$ treatment.

We note that in our approach we have considered ionization only from the UV background. In other words, we are neglecting the contribution of ionizing photons from, e.g., local sources (Miralda-Escudé 2005; Schaye 2006; Rahmati et al. 2013b) or X-ray heating from the intracluster medium (Kannan et al. 2015).

Fig. 1 shows the z = 1 spatial distribution of HI and gas in slices of 5  $h^{-1}$ Mpc depth through the entire TNG100 simulation box as well as in zoomed-in regions thereof. We see that the Ly $\alpha$ -forest dominates the abundance of HI in terms of volume, but the HI inside galaxies dominates in terms of mass.

#### 3. OVERALL HI ABUNDANCE: $\Omega_{\rm HI}(z)$

Here, we study the overall abundance of neutral hydrogen in the IllustrisTNG simulations. In Fig. 2 we show the value of  $\Omega_{\rm HI}(z)$  from TNG300 (solid black) and TNG100 (dashed black). In this plot we also indicate measurements from different observations (Zwaan & Prochaska 2006; Rao et al. 2006; Lah et al. 2007; Songaila & Cowie 2010; Martin et al. 2010; Noterdaeme et al. 2012; Braun 2012; Rhee et al. 2013; Delhaize et al. 2013; Crighton et al. 2015).

The agreement between the results from our simulations and observations is good, although the simulations tend to overpredict the amount of HI at redshifts z < 0.5and underpredict the HI abundance at 2 < z < 3.5. Compared to earlier studies with hydrodynamic simulations (e.g. Davé et al. 2013; Bird et al. 2014) and semianalytic models (Lagos et al. 2014), however, our results agree better with observations at z > 1 and comparable to the agreement found by (Rahmati et al. 2015).

The overall HI mass in the simulations depends on resolution, such that the simulation with higher resolution, TNG100, contains between  $\simeq 2.5\%$  and  $\simeq 40\%$  more HI in the redshift interval z = 0-5 than TNG300. This is a consequence of the fact that the stellar mass function is not yet converged (Pillepich et al. 2017a). For example, in TNG100 there is HI in halos with masses that TNG300 cannot resolve (see section 5). This can be seen in Fig. 4, where we show the HI mass within halos versus total halo mass. In TNG300, halos with masses only above  $2 \times 10^9 \ h^{-1} M_{\odot}$  can be resolved, assuming a minimum of 50 CDM particles in a halo. From Fig. 4 we see that the amount of HI in halos below that mass is not negligible at high-redshift, thus we would expect that  $\Omega_{\rm HI}$  will be lower at high-redshift in TNG300 in comparison with TNG100, as we find.

In this paper we examine the most important prop-



Figure 2.  $\Omega_{\rm HI}(z) = \rho_{\rm HI}(z)/\rho_{\rm c}^0$  from observations (colored points) and from the simulations (black lines) as a function of redshift. Our highest resolution simulation, TNG100, reproduces well the abundance of cosmic HI in the post-reionization era, although it slightly overpredicts/underpredicts the HI abundance at  $z = 0/z \in$ [2-3.5]. A simulation with even higher mass resolution would likely yield an increased HI abundance.

erties of cosmic neutral hydrogen over a wide range of redshifts. Not being able to resolve the HI that is contained within the smallest halos impacts our results in several ways. For example, the values of the HI bias, HI shot-noise, the HI halo mass function or the amplitude of the HI Fingers-of-God effect will be affected by this. For this reason, from now on we focus our analysis to the TNG100 simulation.

## 4. HI FRACTION IN HALOS AND GALAXIES

The fraction of the total HI mass that resides within halos is an important ingredient for theoretical frameworks that aim at modeling the abundance and clustering properties of cosmic neutral hydrogen, such as the halo model (Cooray & Sheth 2002; Barnes & Haehnelt 2014; Villaescusa-Navarro et al. 2014; Padmanabhan et al. 2016; Padmanabhan & Refregier 2017; Padmanabhan et al. 2017). In particular, these methods make the assumption that all HI is confined within halos, whose properties, such as spatial distribution or abundance, are well-described by analytic models and/or numerical simulations.

In contrast to the gas in halos, the properties of the gas in the intergalactic medium (IGM) are more difficult to model analytically (see however Iršič & McQuinn 2018). The standard approach has been to characterize the gas in the IGM using numerical simulations. If a significant amount of HI is found outside halos, any standard HI halo model will need to be complemented with either simulations or further analytic ingredients. Below, we determine the amount of HI that is outside of halos, to quantify the limitations of standard HI halo models.

We have computed the HI mass inside each FoF, FoF-SO and galaxy in the simulation at several redshifts. In Fig. 3 we show, for each of these object types, the fraction of the total HI mass in the simulation that resides inside all objects combined.

We find that at redshifts  $z \leq 2$  more than 99% of



Figure 3. The fraction of total HI mass that is inside FoF halos (solid red lines), FoF-SO halos (dashed red lines) and galaxies (blue lines) as a function of redshift. At low redshift nearly all HI is located within FoF halos and galaxies, while at high-redshift the amount of HI outside FoF halos/galaxies can be 10%/20%. There is a significant amount of HI in the outskirts of FoF halos: the fraction of HI inside FoF-SO halos ranges from 90% at z = 0 to 67% at z=5.

all HI is contained within FoF halos. While a significant fraction of the baryons lie outside these regions, the IGM is highly ionized at these times. At these redshifts, the fraction of HI within galaxies is larger than 95%. We note that SUBFIND may not identify any subhalo/galaxy within a FoF halo. This could happen for several reasons, like low-density or virialization not having been reached. Thus, we conclude that at these redshifts  $\simeq 5\%$  of the cosmic neutral hydrogen is outside galaxies<sup>15</sup> but inside halos.

The fraction of HI within FoF halos and galaxies decreases monotonically with redshift. At redshift z = 5the HI inside FoF halos only accounts for 88% of the total HI, while the mass within galaxies is 80%. These results are in qualitative agreement with Villaescusa-Navarro et al. (2014), who studied the HI outside halos using a different set of hydrodynamic simulations. Morever, we find that our results are not significantly affected by mass resolution, since the same analysis carried out for the TNG300 simulation gives similar results.

We consider our finding that the fraction of HI outside halos increases with redshift to be reasonable. At highredshift the gas in the IGM is denser and the amplitude of the UV background is lower, and so it is easier for that gas to host higher fractions of neutral hydrogen (see Appendix A for further details).

The fraction of HI outside FoF-SO halos is not negligible, varying from 10% at z = 0 to 33% at z = 5. On average, the ratio of HI mass in FoF-SO halos to that in FoF halos is similar to the ratio between their total masses. Thus, FoFs host more HI that FoF-SO halos simply because they are larger and more massive. This also tells us that the regions beyond the virial radius of typical halos are neither HI poor nor HI rich, while when this is examined specifically in massive halos we find these regions to be HI rich (see appendix C for further details).

We thus conclude that while the standard assumption that all HI lies within halos is reasonable at  $z \leq 2$ , at high redshift it begins to break down since a small fraction is located outside halos ( $\sim 10\%$  at z = 5). The numbers derived here can be used to quantify the limitations of HI halo models that target the distribution of HI at high redshift.

## 5. HALO HI MASS FUNCTION

In the previous section we have shown that most of the HI is inside halos, justifying the use of HI halo models to characterize the spatial distribution of HI. As discussed in the introduction, besides the linear matter power spectrum, halo mass function and halo bias, we need to know the halo HI mass function (i.e. the average HI mass hosted by a halo of mass M at redshift z) and the spatial distribution of HI inside halos. Below, we investigate the former:  $M_{\rm HI}(M, z)$ .

We emphasize the paramount importance of this function by noting that knowing it is sufficient for predicting the amplitude and shape of the 21 cm power spectrum to linear order (see Eq. 1):

$$P_{21\rm cm}(k,\mu,z) = \bar{T}_b(z)^2 \left[ (b_{\rm HI}(z) + f(z)\mu^2)^2 P_{\rm m}(k,z) + P_{\rm SN}(z) \right] ,$$

where  $\overline{T}_b(z)$ ,  $b_{\rm HI}(z)$  and  $P_{\rm SN}(z)$  can all be derived from  $M_{\rm HI}(M,z)$  as

$$\bar{T}_b(z) = 189h\left(\frac{H_0(1+z)^2}{H(z)}\right)\Omega_{\rm HI}(z) \text{ mK}$$
(9)

$$\Omega_{\rm HI}(z) = \frac{1}{\rho_{\rm c}^0} \int_0^\infty n(M, z) M_{\rm HI}(M, z) dM$$
 (10)

$$b_{\rm HI}(z) = \frac{1}{\rho_{\rm c}^0 \Omega_{\rm HI}(z)} \int_0^\infty n(M, z) b(M, z) M_{\rm HI}(M, z) dM$$
(11)

$$P_{\rm SN}(z) = \frac{1}{(\rho_{\rm c}^0 \Omega_{\rm HI}(z))^2} \int_0^\infty n(M, z) M_{\rm HI}^2(M, z) dM , \qquad (12)$$

where n(M, z) and b(M, z) are the halo mass function and halo bias, respectively. Knowledge of this function can be used to understand the impact of different phenomena on the amplitude and shape of the 21cm power spectrum such as neutrino masses (Villaescusa-Navarro et al. 2015), warm dark matter (Carucci et al. 2015) or modified gravity (Carucci et al. 2017a).

For each dark matter halo in the simulation we have computed its enclosed HI mass. In Fig. 4 we show the HI mass versus halo mass for each single FoF halo in the simulation at redshifts 0, 1, 2, 3, 4 and 5. The color indicates the number of halos in each bin. We show this map rather than the  $M_{\rm HI}(M, z)$  function since the former contains more information, such as the scatter in  $M_{\rm HI}(M, z)$ .

The halo HI mass function increases monotonically with halo mass. Two trends can be identified: 1) in the high-mass end  $M_{\rm HI}(M, z)$  can be approximated by a power law, and 2) in the low-mass end it has a sharp

<sup>&</sup>lt;sup>15</sup> We emphasize that the term "galaxy" should be considered in our framework, not in the traditional observational definition. For instance, gas far away from the center of a halo but gravitationally bound to it will still be considered as belonging to that galaxy.



Figure 4. Halo HI mass function. For each FoF halo of the simulation TNG100 we compute the total HI mass it hosts. The plots show the HI mass versus halo mass, color coded by the number of halos in each bin. The blue vertical lines show the mass corresponding to a halo that hosts 50 dark matter particles, which we adopt a rough mass resolution threshold. We take narrow bins in halo mass and compute the total HI mass in each of them. The top part of each panel shows the ratio between the total HI mass in the bin and the total HI mass in all halos. Our results can be well reproduced by the fitting formula  $M_{\rm HI}(M, z) = M_0 x^{\alpha} e^{-1/x^{0.35}}$ , with  $x = M/M_{\rm min}$ . The best fits are shown with green lines at each redshift.

		Fo	ъF	FoF-SO				
z	$\alpha$ $M_0$		$M_{\min}$	M <sub>hard</sub>	α	$M_0$	$M_{\min}$	$M_{\rm hard}$
		$[h^{-1}M_{\odot}]$	$[h^{-1}M_{\odot}]$	$[h^{-1}M_{\odot}]$		$[h^{-1}M_{\odot}]$	$[h^{-1}M_{\odot}]$	$[h^{-1}M_{\odot}]$
0	$0.24\pm0.05$	$(4.3 \pm 1.1) \times 10^{10}$	$(2.0 \pm 0.6) \times 10^{12}$	$1.5 \times 10^{10}$	$0.16\pm0.05$	$(4.1 \pm 1.0) \times 10^{10}$	$(2.4 \pm 0.7) \times 10^{12}$	$1.3 \times 10^{10}$
1	$0.53\pm0.06$	$(1.5 \pm 0.7) \times 10^{10}$	$(6.0 \pm 2.9) \times 10^{11}$	$6.9 \times 10^9$	$0.43\pm0.06$	$(1.8 \pm 0.8) \times 10^{10}$	$(8.6 \pm 4.2) \times 10^{11}$	$6.1 \times 10^{9}$
2	$0.60\pm0.05$	$(1.3 \pm 0.6) \times 10^{10}$	$(3.6 \pm 1.6) \times 10^{11}$	$3.1 \times 10^{9}$	$0.51\pm0.05$	$(1.5 \pm 0.7) \times 10^{10}$	$(4.6 \pm 2.1) \times 10^{11}$	$2.5 \times 10^{9}$
3	$0.76\pm0.05$	$(2.9 \pm 2.0) \times 10^9$	$(6.7 \pm 4.0) \times 10^{10}$	$9.9 \times 10^{8}$	$0.69\pm0.06$	$(3.7 \pm 2.6) \times 10^9$	$(9.6 \pm 6.0) \times 10^{10}$	$7.6 \times 10^{8}$
4	$0.79\pm0.04$	$(1.4 \pm 1.0) \times 10^9$	$(2.1 \pm 1.3) \times 10^{10}$	$3.9 \times 10^8$	$0.61\pm0.06$	$(4.5 \pm 2.7) \times 10^9$	$(7.6 \pm 4.4) \times 10^{10}$	$2.3 \times 10^8$
5	$0.74\pm0.04$	$(1.9 \pm 1.2) \times 10^9$	$(2.0 \pm 1.2) \times 10^{10}$	$2.7 \times 10^{8}$	$0.59\pm0.07$	$(4.1 \pm 2.8) \times 10^9$	$(5.4 \pm 3.6) \times 10^{10}$	$1.7 \times 10^{8}$

Table 1We fit our results for the  $M_{\rm HI}(M,z)$  function to the form  $M_0 x^{\alpha} \exp(-1/x^{0.35})$ , where  $x = M/M_{\rm min}$ . This table shows the best-fit value of the free parameters, for FoF and FoF-SO halos, at different redshifts. The column  $M_{\rm hard}$  indicates the value of our hard cutoff mass, which is defined so that halos with masses  $M \ge M_{\rm hard}$  host 98% of all HI in halos. For FoF-SO halos we can express  $M_{\rm hard}$  in terms of circular velocities, giving 34, 35, 31, 24, 19 and 18 km/s at redshifts 0, 1, 2, 3, 4 and 5, respectively.

cutoff. A good fit to our results is given by

$$M_{\rm HI}(M,z) = M_0 \left(\frac{M}{M_{\rm min}}\right)^{\alpha} \exp(-(M_{\rm min}/M)^{0.35}) .$$
(13)

The free parameters are  $M_{\min}$ , which sets the cutoff mass in  $M_{\rm HI}(M, z)$ ,  $\alpha$ , which controls the slope of the function at the high-mass end, and  $M_0$ , which determines the overall normalization and represents  $\simeq 40\%$  of the HI mass of a halo of mass  $M_{\min}$ . We have fitted our results to this function and give the best fitting values for both FoF and FoF-SO halos in Table 1. The green lines in Fig. 4 indicate the best fits at each redshift.

At redshifts  $z \ge 3$  for FoF halos  $\alpha$  is  $\simeq 0.75$ , while it declines at lower redshifts:  $\alpha = 0.60$  at z = 2,  $\alpha = 0.53$  at z = 1 and  $\alpha = 0.24$  at z = 0. We interpret this as a result of several physical processes such as AGN feedback, ram pressure and tidal stripping being more efficient at removing gas from galaxies at low redshift than at higher redshifts.

The value of  $M_{\rm min}$  decreases monotonically with redshift, from  $\simeq 2 \times 10^{12} h^{-1} M_{\odot}$  at z = 0 to  $2 \times 10^{10} h^{-1} M_{\odot}$ at z = 5. This indicates that as the redshift increases, lower mass halos host HI. In the appendix B we discuss the physical origin of the cutoff in the halo HI mass function and the relative importance of supernova feedback, gas stripping and the UV background for this.

Similar conclusions can be reached when computing  $M_{\rm HI}(M, z)$  using FoF-SO halos (see Table 1). The derived values of  $\alpha$ ,  $M_0$  and  $M_{\rm min}$  are roughly compatible, within the errors, between FoF and FoF-SO halos. There are, however, systematic differences between the best fit values from FoF and SO, which is because the total amount of HI in a given halo is sensitive to its definition as we will see below.

For FoF-SO halos we can relate halo masses to circular velocities through  $V_{\text{circ}} = \sqrt{GM/R}$ , where G is the gravitational constant and M and R are the halo mass and radius. Expressing  $M_{\text{min}}$  in terms of circular velocities we obtain:  $V_{\text{circ}}(M_{\text{min}}) \simeq 180 \pm 20 \text{ km/s}$  for  $z \in [0, 2]$  and  $V_{\text{circ}}(M_{\text{min}}) \simeq 120 \pm 20 \text{ km/s}$  for  $z \in [3, 5]$ . This suggests that the minimum halo mass that can host HI depends primarily on the depth of its gravitational potential and that at lower redshifts the potential has to be deeper since astrophysical processes such as AGN feedback, tidal stripping, and so forth are more effective at removing gas from small halos.

Since our parametrization of the halo HI mass function does not have a "hard" cutoff, the value of  $M_{\rm min}$ only represents a mass scale at which the halo HI mass function changes its trend. In other words, halos with masses around  $M_{\rm min}$  host a significant amount of HI. It is also very interesting to quantify the cutoff in the halo HI mass function more rigidly, i.e. so that halos below a certain mass contain a negligible amount of HI.

We have calculated the halo mass at which 98% of all HI in halos is above that mass, and only 2% is in smaller halos. We term this halo mass as a "hard cutoff mass",  $M_{\rm hard}$ ,

ъ*л* 

$$\frac{\int_{0}^{M_{\text{hard}}} n(M,z) M_{\text{HI}}(M,z) dM}{\int_{0}^{\infty} n(M,z) M_{\text{HI}}(M,z) dM} = 0.02$$
(14)

and we show corresponding values in Table 1. For FoF-SO halos we obtain:  $1.3 \times 10^{10}$ ,  $6.1 \times 10^9$ ,  $2.5 \times 10^9$ ,  $7.6 \times ^8$ ,  $2.3 \times 10^8$  and  $1.7 \times 10^8 \ h^{-1} M_{\odot}$  at redshifts 0, 1, 2, 3, 4 and 5, respectively. These can be transformed to circular velocities, giving: 34, 35, 31, 24, 19 and 18 km/s at redshifts 0, 1, 2, 3, 4 and 5, correspondingly. The values we infer do not change much if we use a threshold equal to 99%. We thus conclude that at redshifts  $z \leq 2$  only halos with circular velocities above about 30 km/s host HI, while at redshifts  $z \geq 3$  the HI is only in halos with circular velocities above  $\sim 20 \text{ km/s}$ .

A more conventional parametrization of the halo HI mass function

$$M_{\rm HI}(M,z) = M_0 \left(\frac{M}{M_{\rm min}}\right)^{\alpha} \exp(-M_{\rm min}/M) \ . \tag{15}$$

also reproduces our results. The fit in Eq. 13 is, however, preferred for our results since at high-redshift  $M_{\rm HI}(M,z)$ falls more slowly for very low halo masses than the standard profile. In order to facilitate the comparison with works using the above parametrization (e.g. Bagla et al. 2010; Castorina & Villaescusa-Navarro 2017; Obuljen et al. 2017a; Villaescusa-Navarro et al. 2017; Pénin et al. 2018a; Padmanabhan et al. 2017) we also provide the best-fit values for the more conventional fit in the Appendix D.

#### 6. HI DENSITY PROFILE

Another important ingredient in describing the spatial distribution of cosmic neutral hydrogen using HI halo models is the density profile of HI inside halos (see Eqs. 2, 3, 4). In this section we investigate the spatial distribution of HI inside simulated dark matter halos.

Since FoF halos can have very irregular shapes, we have computed the HI profiles inside FoF-SO halos. For each FoF-SO halo we have computed the HI mass within narrow spherical shells up to the virial radius, and from them the HI profile. Fig. 5 shows individual HI profiles for halos in a narrow mass bin at different redshifts with grey lines. The large halo-to-halo scatter is surprising, and highlights that individual HI profiles, as opposed to dark matter ones, are far from universal.

The scatter is particularly large towards the centers of massive halos, as discussed below, as well as for halos with masses around or below the cutoff we observe in Fig. 4. This is expected as the halo HI mass function also exhibits large scatter in that range. As we will see later in section 14, the clustering of halos in that mass range depends significantly on their HI mass. Thus, it is likely that the HI content of these halos is influenced by their environment, so small halos around more massive ones may have lose or gain a significant fraction of their HI mass due to related effects.

The scatter generally tends to be lower at higher redshifts, and, in particular, is small in halos with masses above  $10^{10} h^{-1} M_{\odot}$  at redshift z = 5. This is related to the lower scatter we find at high redshift in the halo HI mass function,  $M_{\rm HI}(M, z)$  (see Fig. 4). We speculate that this originates from a reduced role that AGN feedback and environmental gas stripping play at earlier times.

The blue lines in Fig. 5 show the mean and the standard deviation of the HI profiles from all halos that lie in each mass bin and redshift, while the red lines display the median. Clearly, in some cases they differ substantially. This behavior can be partially attributed to the HI profiles arising from two distinct populations: i.e. HI-rich blue galaxies versus HI-poor red ones (Nelson et al. 2018). This can clearly be seen in the panel in Fig. 5 corresponding to halos in the mass range  $M \in [1-2] \times 10^{12} h^{-1} M_{\odot}$  at z = 0. In this range, some halos have a core in their HI profiles while others do not. The reason is that the central galaxy of some halos is experiencing AGN feedback (those with holes in the profile) and are therefore becoming red, while the



Figure 5. Density profiles of HI for halos of different masses in different rows (see labels in the left column) at redshifts z = 0 (left), z = 1 (middle-left), z = 2 (middle-right) and z = 5 (right). In each panel we display up to 50 individual profiles (grey lines), the mean profile and the standard deviation (blue lines) and the median profile (red lines). Empty panels correspond to situations with either no halos (top-right) or with halos far below the cutoff mass  $M_{\min}$ . In contrast to dark matter, HI density profiles are not universal, and they exhibit, in most of the cases, a very large scatter. The HI-H<sub>2</sub> transition saturates the amplitude of the profiles in the core, while processes such as AGN feedback create HI holes in the core of the most massive halos. The mean and the median can be quite different, indicating that the distribution is asymmetric. In some cases, that asymmetry is due to the presence of two different populations such as blue and red galaxies.

![](_page_10_Figure_2.jpeg)

Figure 6. To better understand the features in the HI profiles of Fig. 5, we have chosen halos with HI profiles close to the mean. The images show the HI column density for halos of mass ~  $10^{14} h^{-1} M_{\odot}$  at z = 0 (left), ~  $10^{13} h^{-1} M_{\odot}$  at z = 0 (top-right), ~  $10^{12} h^{-1} M_{\odot}$  at z = 1 (bottom-middle) and ~  $10^{11} h^{-1} M_{\odot}$  at z = 0 (bottom-right). The center of galaxy clusters is typically occupied by HI poor ellipticals, whereas HI rich spirals reside in the centers of lower mass halos. Processes such as tidal-stripping and ram pressure efficiently remove gas from galaxies near the centers of galaxy clusters. In small halos ( $\leq 10^{12} h^{-1} M_{\odot}$ ) gas can cool and accumulate in the center while in groups AGN feedback produces holes in the core of the HI profile (see top-right panel). The "cuspyness" of the HI profiles increases with decreasing halo mass, but saturates due to the formation of H<sub>2</sub>.

galaxies in the other halos are not yet being affected by AGN feedback, remaining blue (Nelson et al. 2018).

We find that the HI density profiles of small halos  $(M \lesssim 10^{12} h^{-1} M_{\odot})$  increase towards their halo center. We note, however, that the amplitude of the HI profile tends to saturate; i.e. the slope of the profiles declines significantly towards the halo center. For example, at z = 0 and z = 1 and for halos with masses larger than  $10^{11} h^{-1} M_{\odot}$ , the mean HI profiles change slope around ~ 20  $h^{-1}$ kpc. This is expected since neutral hydrogen at high densities will turn into molecular hydrogen and stars on short time scales. For higher halo masses  $(M \simeq 10^{13} \ h^{-1} M_{\odot})$  the HI density profile exhibits a hole in the center. This is caused by AGN feedback in the central galaxy of those halos. We notice that higher densities in the center of halos can give rise to the formation of molecular hydrogen, that can produce a similar effect (Marinacci et al. 2017). Holes, which extend even further than in groups, are also found in the HI profiles of galaxy clusters, which we however do not show here since there are only a few of them and only at low redshift.

We illustrate these features of the HI profiles in Fig. 6, where we show the spatial distribution of HI in and around four individual halos with masses  $10^{11}$ ,  $10^{12}$ ,  $10^{13}$  and  $10^{14} h^{-1} M_{\odot}$  at redshifts 0 or 1. We have selected these halos by requiring that their HI density profiles are close to the mean. It can be seen that HI is localized in the inner regions of small halos, while for groups, the

central galaxy exhibits a hole produced by AGN feedback. For galaxy clusters the central regions have little HI. This happens because the central galaxy is an HI poor elliptical, and ram-pressure and tidal stripping are very efficient in removing the gas content of galaxies passing near the center. The analysis of this section suggests that analytical approaches to the distribution of Damped Lyman- $\alpha$  systems employing a universal HI profile, *e.g.* (Padmanabhan et al. 2017), will not be able to reproduce observations.

In order to quantitatively investigate what is the effective average HI density profile across different halo masses and redshift, we use the mean measured HI density profile and test two models of HI density that both include an exponential cutoff on small scales.

First we consider a simple power law with an exponential cutoff on small scales — Model 1:

$$\rho_{\rm HI}(r) = \frac{\rho_0}{r^{\alpha_\star}} \exp(-r_0/r), \qquad (16)$$

where  $\rho_0$  is the overall normalisation,  $\alpha_{\star}$  is the slope parameter and  $r_0$  is the inner radius at which the density drops and the profile changes its slope.

Second, we consider an altered NFW profile (Maller & Bullock 2004; Barnes & Haehnelt 2014), found to be a good fit to the multiphase gas distribution at high redshifts in hydrodynamical simulations, with an exponen-

	Model 1 — power law + exponential cutoff: $\alpha_{\star}$ , $\log_{10} r_0 [h^{-1} \text{Mpc}]$											
z	$z \qquad M_h = 10^9 \left[ h^{-1} M_{\odot} \right]$		$M_h = 10^{10} \left[ h^{-1} M_{\odot} \right]$		$M_h = 10^{11} \left[ h^{-1} M_{\odot} \right]$		$M_h = 10^{12}  [h^{-1} M_{\odot}]$		$M_h = 10^{13}  [h^{-1} M_{\odot}]$		$M_h = 10^{14}  [h^{-1} M_{\odot}]$	
0			$3.04^{+0.04}_{-0.03},$	$-3.59^{+0.85}_{-0.92}$	$3.03^{+0.03}_{-0.02},$	$-2.8^{+0.5}_{-1.2}$	$3.02^{+0.03}_{-0.03},$	$-2.32^{+0.33}_{-1.15}$	$3.00^{+0.04}_{-0.04},$	$-1.71\substack{+0.09\\-0.12}$	$2.92^{+0.03}_{-0.03},$	$-1.91\substack{+0.11 \\ -0.14}$
1	$3.3^{+1.3}_{-0.7},$	$-2.5^{+1.1}_{-1.6}$	$3.05^{+0.02}_{-0.02},$	$-3.72\substack{+0.77\\-0.84}$	$3.02^{+0.02}_{-0.02},$	$-3.3^{+0.7}_{-1.1}$	$3.00^{+0.03}_{-0.02},$	$-2.32\substack{+0.16 \\ -0.28}$	$2.99^{+0.03}_{-0.03},$	$-1.77\substack{+0.09\\-0.11}$		—
2	$3.07^{+0.10}_{-0.08},$	$-3.2^{+0.9}_{-1.2}$	$3.03^{+0.01}_{-0.02},$	$-3.64\substack{+0.78 \\ -0.89}$	$3.01^{+0.01}_{-0.01},$	$-2.75\substack{+0.26 \\ -0.68}$	$3.00^{+0.02}_{-0.02},$	$-2.18\substack{+0.09 \\ -0.12}$	$2.98^{+0.02}_{-0.01},$	$-1.74\substack{+0.04\\-0.05}$		—
3	$3.05^{+0.02}_{-0.02},$	$-3.63\substack{+0.85\\-0.93}$	$3.02^{+0.02}_{-0.02},$	$-3.1^{+0.5}_{-1.1}$	$3.00^{+0.01}_{-0.01},$	$-2.52\substack{+0.13 \\ -0.20}$	$3.00^{+0.02}_{-0.02},$	$-2.09\substack{+0.06\\-0.07}$				
4	$3.04^{+0.02}_{-0.02},$	$-3.3^{+0.7}_{-1.0}$	$3.00^{+0.01}_{-0.01},$	$-2.46\substack{+0.15 \\ -0.24}$	$3.00^{+0.01}_{-0.01},$	$-2.32\substack{+0.07 \\ -0.08}$	$2.99^{+0.01}_{-0.01},$	$-2.04\substack{+0.03 \\ -0.04}$		_		_
5	$3.03^{+0.02}_{-0.02},$	$-2.9^{+0.5}_{-1.2}$	$3.00^{+0.01}_{-0.01},$	$-2.28\substack{+0.09\\-0.12}$	$3.00^{+0.01}_{-0.01},$	$-2.18\substack{+0.04 \\ -0.05}$	$3.00^{+0.01}_{-0.01},$	$-2.02\substack{+0.03\\-0.03}$	_	_		
		Mo	odel 2 —	altered NI	FW + exp	ponential o	cutoff: log	$g_{10} r_{\rm s} [h^{-1}]$	$Mpc], log_1$	$_{10} r_0 [h^{-1} M$	[pc]	
0	_	—	$-4.0^{+0.7}_{-0.7},$	$-3.8^{+0.8}_{-0.8}$	$-3.7^{+0.6}_{-0.9},$	$-3.4^{+0.7}_{-1.0}$	$-3.2^{+0.7}_{-1.1},$	$-3.1^{+0.8}_{-1.3}$	$-3.0^{+1.0}_{-1.3},$	$-1.8^{+0.1}_{-1.0}$	$-2.3^{+0.5}_{-1.7},$	$-2.6\substack{+0.7\\-1.6}$
1	$-2.8^{+1.8}_{-1.5},$	$-3.3^{+1.2}_{-1.1}$	$-4.0^{+0.5}_{-0.6},$	$-3.7^{+0.6}_{-0.8}$	$-3.9^{+0.6}_{-0.7},$	$-3.6\substack{+0.7\\-0.9}$	$-3.0^{+0.4}_{-1.2},$	$-2.9^{+0.6}_{-1.4}$	$-2.2^{+0.3}_{-1.6},$	$-2.4^{+0.6}_{-1.7}$		—
2	$-3.7^{+0.9}_{-0.8},$	$-3.7\substack{+0.9 \\ -0.9}$	$-3.8^{+0.5}_{-0.7},$	$-3.5^{+0.5}_{-0.9}$	$-3.6^{+0.5}_{-0.9},$	$-3.3^{+0.6}_{-1.1}$	$-2.8^{+0.3}_{-1.3},$	$-2.6\substack{+0.4\\-1.5}$	$-1.8^{+0.1}_{-0.2},$	$-3.0^{+0.8}_{-1.3}$	_	_
3	$-3.8^{+0.6}_{-0.8},$	$-3.5\substack{+0.6 \\ -0.9}$	$-3.6^{+0.5}_{-0.8},$	$-3.3^{+0.5}_{-1.1}$	$-3.3^{+0.4}_{-1.0},$	$-3.0\substack{+0.5 \\ -1.3}$	$-2.8^{+0.4}_{-1.3},$	$-2.4^{+0.3}_{-1.4}$		—	—	—
4	$-3.6^{+0.5}_{-0.9},$	$-3.2^{+0.5}_{-1.1}$	$-3.2^{+0.4}_{-1.1},$	$-3.0^{+0.5}_{-1.3}$	$-2.9^{+0.3}_{-1.3},$	$-2.7^{+0.4}_{-1.4}$	$-2.6^{+0.3}_{-1.4},$	$-2.4^{+0.3}_{-1.2}$				
5	$-3.4^{+0.5}_{-1.0},$	$-3.1^{+0.5}_{-1.1}$	$-2.7^{+0.2}_{-1.1},$	$-3.1^{+0.7}_{-1.3}$	$-2.5^{+0.1}_{-1.1},$	$-3.3^{+1.0}_{-1.2}$	$-2.2^{+0.1}_{-0.4},$	$-3.1^{+0.8}_{-1.2}$				

Table 2

Best-fit values of the parameters determining the HI density profiles. We show the resulting parameters for the two different models considered (see text): an altered NFW profile with an exponential cutoff on small scales (top) and a simple power law with an exponential cutoff on small scales (bottom), as a dependence on the halo mass (columns) and redshift (rows).

tial cutoff on small scales — Model 2:

$$\rho_{\rm HI}(r) = \frac{\rho_0 r_s^3}{(r+3/4r_s)(r+r_s)^2} \exp(-r_0/r), \qquad (17)$$

where  $\rho_0$  is the overall normalisation and  $r_s$  is the scale radius of the HI cloud. In both cases the overall normalisation —  $\rho_0$ , is fixed such that the volume integral of the model density profile integrated up to the virial radius of a given halo matches the mean total HI mass obtained from the density profile found in simulations (blue lines in Fig. 5). We are then left with two free parameters for each model: { $\alpha_{\star}, r_0$ } and { $r_s, r_0$ }. We fit these models to the measured mean HI density profiles limiting our analysis only to the scales above  $r \geq 2h^{-1}$ kpc. For the uncertainties in the density profiles we use the scatter among different galaxies (blue error-bars in Fig. 5) and assume that these uncertainties are uncorrelated between different scales.

The best-fit values along with the 68% confidence intervals are presented in table 2, while in Fig. 30 in Appendix E we show the best-fit results for the Model 1. Based on the resulting best-fit  $\chi^2$ , we find that both Model 1 and 2 are good fits for all the considered redshifts and halo masses, except for the most massive halo bin  $M_h = 10^{14} [h^{-1} M_{\odot}]$  at z = 0. We find that the difference in the best-fit  $\chi^2$  between the two models to be negligible. This is to be expected since the models are rather similar and have the same slope on large scales. In the case of Model 1, we find the HI density profile slope to be consistent with a value of  $\alpha_{\star} = 3$  for all the halo masses and redshifts. The inner radius  $r_0$  depends on the halo mass and is larger for larger halo masses at a fixed redshift, while at a fixed halo mass, it increases with increasing redshift. For example, for halos with  $M_h \leq 10^{11} h^{1-}$  Mpc and  $z \leq 2$ ,  $r_0$  is below the minimum scale considered and the uncertainties are rather large. In the case of Model 2, we find a similar behaviour. The inferred values of  $r_0$  are consistent between two models, with Model 2 having larger uncertainties which is due to the degeneracy between parameters  $r_0$  and  $r_s$ .

We note that other observational and simulation studies have found that the HI surface density profile of galaxies can be reproduced by an exponential profile (Wang et al. 2014; Obreschkow et al. 2009). Based on these studies, other spherically averaged density models have been used in the literature, e.g. an exponential profile (Padmanabhan et al. 2017). We find that using an exponential profile for the spherically averaged profile does not reproduce our mean data very well.

# 7. HI IN CENTRALS AND SATELLITES GALAXIES

It is interesting to quantify what fraction of HI mass inside halos comes from their central and satellites galaxies. This will help us to better understand the HI density profiles (see section 6) and improves our intuition for the amplitude of the HI Fingers-of-God effect (see section 16).

For each FoF halo we have computed its total HI mass, the HI mass within its central galaxy and the HI mass inside its satellites We emphasize that our definition of central galaxy departs significantly from that used in observations, as we consider the central galaxy to be the most massive subhalo. In general, this subhalo hosts the particle at the minimum of the gravitational potential and is therefore the classical central galaxy, but it also has significant spatial extent and particles far away from the halo center can be associated to this subhalo, unless they are bound to a satellite.

![](_page_12_Figure_1.jpeg)

Figure 7. The black lines show the average HI mass inside halos as a function of mass; i.e. the halo HI mass function, at redshifts 0 (top-left), 1 (top-middle), 2 (top-right), 3 (bottom-left), 4 (bottom-middle), 5 (bottom-right). The red and blue lines represent the average HI mass within central and satellites galaxies as a function of halo mass. The bottom panels display the fraction of the HI mass inside halos that is embedded in centrals and satellites. The HI mass of halos below  $\simeq 5 \times 10^{12} h^{-1} M_{\odot}$  is dominated by HI in the central galaxy, while the HI in satellites dominates the HI content of more massive halos. For small halos, the HI mass in the central and satellites galaxies is less than the total HI mass in halos. This happens because the HI in those halos is small in mass and "diffuse".

We take narrow bins in halo mass and compute the average HI mass, for each of the above quantities. The outcome is shown in Fig. 7. The black lines in the upper panels show the halo HI mass function, while the red and blue ones display the average HI mass inside the central and satellites galaxies as a function of halo mass. The bottom panels show the fraction of HI mass within halos that comes from the central and the satellites galaxies. Aside from very low mass halos  $(M \leq 10^9 h^{-1} M_{\odot})$ ,

Aside from very low mass halos  $(M \leq 10^9 h^{-1} M_{\odot})$ , the fraction of HI in the central galaxy decreases with halo mass, while the fraction of HI in satellites increases, independent of redshift. For small halos, nearly all the HI is located in the central galaxy, as expected. For halos of masses  $\sim 5 \times 10^{12} h^{-1} M_{\odot}$ , the fraction of HI in the central galaxy and in satellites is roughly the same, almost independent of redshift. For more massive halos, the total HI mass is dominated by the HI in satellites galaxies.

At high-redshift, the contribution of satellites to the total HI mass in small  $(M \in [10^{10}-10^{11}] h^{-1}M_{\odot})$  halos is non-negligible:  $\simeq 20\%$ . At z = 0 and for galaxy clusters  $M \ge 10^{14} h^{-1}M_{\odot}$ , the contribution of the central galaxy to the total HI mass is negligible, as expected.

The HI mass in very low mass halos  $(M \leq 10^9 h^{-1} M_{\odot})$  is small, in particular at low-redshift. For some of these

halos, the sum of the HI mass in the central and satellite subhalos is much less than the total HI mass. In such cases, some of the HI mass was determined by SUB-FIND to be unbound. In a fraction of these halos, no bound structure was identified by SUBFIND altogether, rendering the combined HI masses of the central and satellites, which by definition do not exist, to be zero, even if the FoF group contains some HI.

#### 8. HI PDF

We now study other quantities that, although are not ingredients for HI halo models, will help us better understand the spatial distribution of neutral hydrogen. One of those quantities is the density probability distribution function (pdf), which we investigate in detail in this section and compare to that of matter.

We compute the density fields of neutral hydrogen and total matter in the whole simulation volume using cloudin-cell (CIC) interpolation on a grid with 2048<sup>3</sup> cells in real-space, namely  $\approx 36.6 \ h^{-1}$ kpc across each grid cell. We then smooth those fields with top-hat filters of radii 1 and 5  $h^{-1}$ Mpc. We have chosen those values for the smoothing scale, R, as a compromise between large and small scales. On one hand the volumes of our simulations do not allow us to explore values much larger than  $\simeq$ 

![](_page_13_Figure_2.jpeg)

Figure 8. The density fields of HI (top) and matter (bottom) smoothed with a top-hat filter of 1 (left) and 5 (right)  $h^{-1}$ Mpc. This figure shows the pdf of those fields at several redshifts (see legend). Deviations from Gaussianity are larger in the HI field than in the matter field at all redshifts. For small smoothing scales the HI density pdf barely changes with redshift. At high-redshifts both the HI and the matter fields are well described by a log-normal distribution.

5  $h^{-1}$ Mpc, while on the other hand we take 1  $h^{-1}$ Mpc as a representative estimate of the non-linear regime. In Fig. 8 we show the pdfs, computed as the number of cells in a given interval in overdensity, over the total number of cells, divided by the width of the overdensity interval.

While the density pdf of the matter field is highly non-Gaussian at low-redshift, for either of the two smoothing scales we consider here, at high-redshift it becomes more nearly Gaussian, as expected. At redshifts  $z \ge 4$  and for  $R = 5 h^{-1}$ Mpc the matter pdf can be well approximated by a lognormal distribution

$$pdf(\delta) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[\frac{(\log(1+\delta) + \sigma^2/2)^2}{2\sigma^2}\right]$$
(18)

where we consider  $\sigma$  as a free parameter. We find  $\sigma = 0.21$  at z = 5 and  $\sigma = 0.28$  at z = 4. At lower redshifts and for smaller values of the smoothing scale the lognormal function does not provide a good fit to our results, as expected (see e.g. Uhlemann et al. 2016).

The HI density pdf exhibits a different behavior compared to the matter pdf. First, the abundance of large HI overdensities remains roughly constant with redshift, independent of the smoothing scale considered. Second, for a smoothing scale of 1  $h^{-1}$ Mpc, the HI pdf hardly changes with redshift.

For redshifts  $z \ge 3$  a lognormal characterizes our re-

sults relatively well: for R = 1  $h^{-1}$ Mpc  $\sigma \simeq 1.9$  while for for R = 5  $h^{-1}$ Mpc  $\sigma \simeq 1$  at z = 3,  $\sigma \simeq 0.9$  at z = 4and  $\sigma \simeq 0.8$  at z = 5. At lower redshifts, a log-normal distribution does not provide a good match to the simulations.

To understand the physical origin of the differences between the pdfs of HI and matter density it is useful to relate the width of the pdf to the amplitude of the HI power spectrum. This is possible since the amplitude of the HI power spectrum represents a measurement of the variance of the field at a given scale. Low values of the HI power spectrum indicate that HI is distributed homogeneously, while higher values mean that spatial variations in HI density can be large.

One of the reasons that the HI density pdf is roughly similar across redshifts while this is less true of the matter density pdf is that the amplitude of the HI power spectrum depends more weakly on redshift than does the matter power spectrum (see section 13). Thus, the variance of the HI pdf is necessarily smaller than that of the matter pdf. Since the amplitude of the HI power spectrum is larger than that of the matter power spectrum at high redshifts, the variance of the HI pdf is larger than that of the matter pdf at those redshifts, as we find. Finally, in the central region of a void, the matter density will be low, but the HI density will be even lower<sup>16</sup>. Thus, we find that there will be more cells with low HI overdensity than with low matter overdensity.

It can be seen for both HI and matter that the distributions are broader for a smoothing scale of 1  $h^{-1}$ Mpc than for 5  $h^{-1}$ Mpc. This is expected since when smoothing over larger scales, any field will become more homogeneous and therefore the width of its pdf will become smaller. This can also be quantified through the amplitude of the power spectrum, using the same reasoning as above.

#### 9. HI COLUMN DENSITY DISTRIBUTION FUNCTION AND DLAS CROSS-SECTIONS

Another quantity commonly employed to study the abundance of neutral hydrogen in the post-reionization era is the HI column density distribution function (HI CDDF), defined as

$$f_{\rm HI}(N_{\rm HI}) = \frac{d^2 n(N_{\rm HI})}{dN_{\rm HI}dX} ,$$
 (19)

where n is the number of lines-of-sight with column densities between  $N_{\rm HI}$  and  $N_{\rm HI} + dN_{\rm HI}$ , and  $dX = H_0(1 + z)^2/H(z)dz$  is the absorption distance. This quantity can be inferred directly from observations of the Ly $\alpha$ -forest.

Here, we investigate the HI CDDF focusing on absorbers with high column densities: damped Lyman alpha systems (DLAs),  $N_{\rm HI} \ge 10^{20.3}$  cm<sup>-2</sup>. We also examine the DLA cross-sections, which are required both observationally (Font-Ribera et al. 2012; Pérez-Ràfols et al. 2018; Alonso et al. 2017) and theoretically (Castorina & Villaescusa-Navarro 2017).

In Fig. 9 we show an example of the spatial distribution of gas and HI around a massive halo at redshift z = 3. As in this case, DLAs correspond to gas in galaxies, gas recently stripped from galaxies, and gas in streams.

The HI CDDF at redshifts 0, 1, 2, 3, 4 and 5 is computed using the following procedure (we refer the reader to appendix B of Villaescusa-Navarro et al. 2014, for further details). We approximate each Voronoi cell by an uniform sphere with radius equal to  $R = (3V/4\pi)^{1/3}$ , where V is the volume of the cell, and determine the HI column density of a line through it from  $N_{\rm HI} = \rho_{\rm HI} d$ , where  $\rho_{\rm HI} = M_{\rm HI, cell}/V$  and d is the length of the segment intersecting the sphere. The simulation volume is projected along the z-axis and a grid with 20000x20000 points is overlaid. Each point is considered to be a lineof-sight, and the column density along it is estimated as the sum of the column densities of all Voronoi cells contributing to it. Since our box size is relatively small, the probability of encountering more than a single absorber with a large column density along the line of sight is negligible. Thus, if the column density of a given lineof-sight is larger than  $\sim 10^{19}$  cm<sup>-2</sup>, it can be attributed to a single absorber. We repeated the tests carried out in Villaescusa-Navarro et al. (2014) to verify that: 1) the grid is fine enough to achieve convergence in the CDDF, and 2) the results do not change if the CDDF is computed by slicing the box into slabs of different widths.

We show the results in Fig. 10. We find excellent agreement with the observations, which are shown as black points with errorbars, at redshifts [1.8-3.5] (Péroux et al. 2005), [2.0-3.5] (Noterdaeme et al. 2012), [3.5-5.4] (Crighton et al. 2015) and [1.5-5.0] (Zafar et al. 2013). The differences between the observed and simulated CDDFs, e.g. the amplitude of the HI CDDF around  $10^{20} - 10^{21}$  cm<sup>-2</sup>, are related to the mismatch between  $\Omega_{\rm HI}$  from observations and TNG100 (see Fig. 2), since

$$\Omega_{\rm HI}(z) = \frac{m_{\rm H} H_0}{c \rho_c^0} \int_0^\infty f_{\rm HI}(N_{\rm HI}, z) N_{\rm HI} dN_{\rm HI} , \qquad (20)$$

where  $m_{\rm H}$  is the mass of the hydrogen atom and c is the speed of light. In agreement with previous works, we find that the HI CDDF exhibits a weak dependence on red-shift (see e.g. Rahmati et al. 2013a). This self-similarity can be associated with the weak redshift dependence that we observe in the high overdensity tail of the HI density pdf for small smoothing scales (see Fig. 8).

Next, we examine the DLAs cross-section. For each dark matter halo of the simulation the area covered by DLAs with different column densities is computed. Then, all halos within mass bins are selected and the mean and standard deviation of their DLA cross-sections are determined. As shown in Fig. 11 we find that, for fixed column density, the DLA cross-section increases with halo mass, while the cross-section decreases with column density for halos of fixed mass.

The cross-section of the DLAs is well fitted by the following function

$$\sigma(M|N_{\rm HI}, z) = A \left(\frac{M}{h^{-1}M_{\odot}}\right)^{\alpha} \left(1 - e^{-(M/M_0)^{\beta}}\right) .$$
(21)

Here, A is a parameter that controls the overall normalization of function, while  $\alpha$  sets the slope of the crosssection for large halo masses, and  $M_0$  determines the characteristic halo mass where the DLA cross-section exponentially decreases at a rate controlled by  $\beta$ .

We fit our results at redshifts  $z \in [2, 4]$  using the above form and find  $\alpha = 0.82$  in the large majority of the cases, while  $\beta$  is well approximated by  $\beta =$  $0.85 \cdot \log_{10}(N_{\rm HI}/{\rm cm}^{-2}) - 16.35$ . There is also a strong correlation between A and  $M_0$ , given by  $A \cdot M_0 =$  $0.0141 \ h^{-2} {\rm kpc} M_{\odot}$ . The only redshift-dependence enters through  $M_0$ , the value of which is given in Table 3. We find that  $M_0$  decreases with redshift, in agreement with the halo HI mass function which implies that less massive halos can host HI at higher redshifts.

The fits to the simulation results, shown as dashed lines in Fig. 11, are a good approximation for column densities below  $10^{22}$  cm<sup>-2</sup>, but apparently less so at higher column densities; e.g. the fit for column densities above  $10^{22.5}$  cm<sup>-2</sup> and low halo masses is several orders of magnitude below the mean. This is mainly an illusion of the fact that some error bars are larger than the value. The reduced  $\chi^2$  obtained from the fits in all cases is below 0.35. The preferred value for  $\alpha$  is slightly larger at higher redshifts, but the redshift-dependence is so weak that for simplicity we did not use it in our fitting. The largest discrepancy between the fit and our results occurs at z = 2 for the DLAs with column densities larger than  $10^{22}$  cm<sup>-2</sup>. In Castorina & Villaescusa-Navarro (2017) it was suggested that a very good fit to the column den-

<sup>&</sup>lt;sup>16</sup> In order to have a significant amount of HI, self-shielding is required. Thus, in low-density regions, HI will be highly ionized.

![](_page_15_Figure_1.jpeg)

Figure 9. Column density of gas (left panel) and HI (right panel) around a massive halo of mass  $1.5 \times 10^{13} h^{-1} M_{\odot}$  at z = 3. The white circles show the position and radius of dark matter halos.

![](_page_15_Figure_3.jpeg)

Figure 10. HI column density distribution function as a function of the HI column density from the TNG100 simulation at redshifts 0 (solid red), 1 (dashed red), 2 (dot-dashed red), 3 (solid blue), 4 (dashed blue) and 5 (dot-dashed blue). Data from observations are shown as black points with errorbars.

	z = 2	z = 3	z = 4
20.0	10.23	9.89	9.41
20.3	10.34	10.00	9.56
21.0	10.77	10.45	10.14
21.5	11.20	10.91	10.68
22.0	11.83	11.39	11.14
22.5	13.11	12.26	11.87
23.0	13.49	13.34	12.72

#### Table 3

Fits to the DLA cross-section from simulations using Eq. 21. This table shows the value of  $\log_{10}M_0$  at different redshifts and DLA column densities. The value of the other parameters in function 21 are given by  $\alpha = 0.82, \ \beta = 0.85 \cdot \log_{10}(N_{\rm HI}/{\rm cm^{-2}}) - 16.35$  and  $A \cdot M_0 = 0.0141 \ h^{-2} {\rm kpc} M_{\odot}.$ 

sity distribution and the DLA bias can be obtained assuming the differential cross section,  $d\sigma/dN_{\rm HI}$  is roughly independent of column density. This implies that the linear bias of different absorbers will be very similar, and the measurements in the BOSS survey of (Pérez-Ràfols et al. 2018) confirm this simple picture, although with large errorbars. As discussed above, our fit to Eq. 21 indicates the the slope  $\alpha$  to a very good approximation is not a function of column density, and  $N_{\rm HI}$  dependence of  $\beta$  can be moved to the normalization constant A using their tight correlation. If we then look at the expression for the linear bias of a given absorber

$$b_{N_{\rm HI}}(z) = \frac{\int_0^\infty b(M, z) n(M, z) \sigma(M|N_{\rm HI}, z) dM}{\int_0^\infty n(M, z) \sigma(M|N_{\rm HI}, z) dM} , \quad (22)$$

we notice that that A cancels between the numerator and the denominator, and the only column density dependence is left in  $\beta$  and it is rather small. The analytical calculation in Castorina & Villaescusa-Navarro (2017) therefore agrees with the measurements in IllustrisTNG, and future observations will tell us if our current understanding of the cross section is correct or not.

We have used the above expression to estimate the bias of the DLAs. We take the DLAs cross-section (for absorbers with  $N_{\rm HI} > 10^{20}$  cm<sup>-2</sup>) and halo mass function from our simulations and use the formula in Sheth et al. (2001) to compute the halo bias. We obtain values of DLAs bias equal to 1.7 at z = 2 and 2 and z = 3. Considering that the DLAs bias follows a linear relation between z = 2 and z = 3 we obtain  $b_{\rm DLA}(z = 2.3) = 1.8$ , in agreement with the latest observations by Pérez-Ràfols et al. (2018):  $b_{\rm DLAs} = 1.99 \pm 0.11$ . We have repeated the above calculations using our fit for the DLAs cross-section, taking the halo mass function from Sheth & Tormen (2002) or Crocce et al. (2010) and find that our results barely change.

We believe that the above calculation should be considered as a lower bound. In other words, the halo bias may be underestimated when calculated using Sheth

![](_page_16_Figure_1.jpeg)

**Figure 11.** The cross-section of DLAs (dark matter halo area covered by DLAs) with column densities above  $10^{20.3}$  (blue),  $10^{21}$  (green),  $10^{21.5}$ ,  $10^{22}$  (purple),  $10^{22.5}$  (brown) and  $10^{23}$  (orange) cm<sup>-2</sup> at redshifts z = 2 (top), z = 3 (middle) and z = 4 (bottom). The points with error bars are measurements from the TNG100 simulation while the dashed lines represent our fit using Eq. 21.

et al. (2001). The reason is that we obtain a value of the HI bias (see section 13), computed without any assumption, of 2 at z = 2 and 2.56 at z = 3, i.e.  $b_{\rm HI}(z = 2.3) = 2.17$ . Following the theoretical arguments in Castorina & Villaescusa-Navarro (2017) it is reasonable to expect that  $b_{\rm HI} \simeq b_{\rm DLAs}$ . We this conclude that both estimations of the DLAs bias are in agreement with observations.

# 10. HI BULK VELOCITY

In section 4 we showed that nearly all the HI at redshifts  $z \leq 5$  resides within halos. Thus, the elements needed to describe the abundance and spatial distribution of HI in real-space through HI halo models are the halo HI mass function and the HI density profiles. To model the distribution of HI in redshift space, an additional ingredient is required: the velocity distribution of HI inside halos. This quantity can be used in both HI halo models and HI HOD models. The accuracy that can be achieved with the former may not be high, due to the limitations of the formalism itself. On the other hand, HI HOD, i.e. painting HI on top of dark matter halos from either N-body or fast numerical simulations like COLA (Tassev et al. 2013), can produce highly accurate results. Hence, we examine the velocity distribution of HI inside halos, beginning with the HI bulk velocity in this section, and continuing with the HI velocity dispersion in the next section, and, in both cases, comparing with the results for all matter.

For each dark matter halo in the simulation we have computed the HI bulk velocity as

$$\vec{V}_{\rm HI} = \frac{\sum_i M_{\rm HI,i} \vec{V}_{\rm HI,i}}{\sum_i M_{\rm HI,i}} , \qquad (23)$$

where the sum runs over all gas cells belonging to the halo and  $M_{\rm HI,i}$  and  $\vec{V}_{\rm HI,i}$  are the HI mass and peculiar velocity of cell *i*, respectively. The peculiar velocity of halos,  $\vec{V}_h$ , is computed in a similar manner, but summing over all resolution elements in the halo (gas, CDM, stars and black holes) and weighting their velocities by their corresponding masses.

Here, we examine: 1) whether the peculiar velocity of the HI points in the same direction as the halo peculiar velocity, and 2) whether the modulus of the HI peculiar velocity is the same as that of the halo peculiar velocity. The first point is addressed by computing the angle between the peculiar velocities of HI and the halo from

$$\cos(\alpha) = \frac{\vec{V}_{\rm HI} \cdot \vec{V}_h}{|\vec{V}_{\rm HI}||\vec{V}_h|} \tag{24}$$

for each halo in the simulation. We do not consider halos with total HI masses below  $10^5 h^{-1} M_{\odot}$ , since we expect the HI peculiar velocities of those halos to be uncorrelated with halo peculiar velocity. For example, the HI in such halos mass can be from a single cell that is partially self-shielded and not bound to the halo. Moreover, in the limit where the HI mass is close to zero, the HI velocity dispersion is not well defined. Thus, in order to avoid such circumstances, we adopt the above threshold, which corresponds to the mass of  $\simeq 1/5$  of a completely selfshielded gas cell. However, we find that this threshold does not have a significant impact on our results. Choosing a different value hardly changes our results, with the only consequence being that the scatter of very small halos is affected. We then take narrow bins in halo mass and compute the mean value of  $\cos(\alpha)$  and its standard deviation. The results are shown in the upper panels of Fig. 12.

For small halos,  $M \lesssim 10^{12} h^{-1} M_{\odot}$ ,  $\cos(\alpha) \simeq 1$ , indicating that the HI and halo peculiar velocities are aligned. This is expected because the HI is mainly located in the inner regions in low-mass halos, which usually traces well the peculiar velocity of the halo. For smaller halos the value of  $\cos(\alpha)$  deviates from 1, with increased scatter. This happens for halo masses below the cutoff scale,  $\sim M_{\rm min}$ . In at least some cases, this is likely due to halos acquiring HI through an unusual mechanism, e.g. by passing through an HI rich filament, so that the HI bulk velocity will not be correlated with the halo peculiar velocity. On the other hand, we find significant misalignments between the HI and halo peculiar velocities for the most massive halos at any redshift. This is because the HI content of these halos is largely contributed by satellites, whose peculiar motions do not necessarily trace that of the halo. We return to this point below.

Further, in the bottom panels of Fig. 12, we show the average and standard deviation of the ratio between the moduli of the HI and halo peculiar velocities,  $|\vec{V}_{\rm HI}|/|\vec{V}_h|$ . This quantity is again calculated in narrow bins in halo mass, for all halos with HI mass larger than  $10^5 \ h^{-1}M_{\odot}$ .

For small halos, the moduli of the HI and halo peculiar velocities are essentially the same. For halos with masses below  $\sim M_{\rm min}$ , the modulus ratio can be larger than 1 and its scatter increases. This is for the same reason as above: the HI content of some of those halos may not be bound to the halos and are instead part of a filament. For massive halos, the modulus of the HI peculiar velocity can be much larger than that of the halo peculiar velocity. As earlier, this is because the HI peculiar velocity is dominated by the HI in satellites, whose peculiar velocities do not perfectly trace the halo peculiar velocity.

To corroborate the assertion that the peculiar velocities of satellites do not trace the halo peculiar velocity in either modulus or direction, we have performed the following test. We compute the peculiar velocities of halo satellites and compared their mean, weighted by the total mass of each satellite, against the peculiar velocity of their host halo. The velocities of the satellites do not have the same modulus or direction as those of the host halo, showing similar trends to those for HI, with differences increasing with halo mass.

Thus, for small halos, where most of the HI is in the central galaxy, the HI bulk velocity traces the halo peculiar velocity well, in both modulus and direction. On the other hand, the contribution of satellites to the total HI mass in halos increases with mass, and since the bulk velocities of satellites do not trace the halo peculiar velocity, the HI bulk velocities will depart, in modulus and direction, from the halo peculiar velocity, with differences increasing with halo mass.

#### 11. HI VELOCITY DISPERSION

For each halo in the simulation we have computed the 3D velocity dispersion of its HI from

$$\sigma_{\rm HI}^2 = \frac{\sum_i M_{\rm HI,i} |\vec{V}_{\rm HI,i} - \vec{V}_{\rm HI}|^2}{\sum_i M_{\rm HI,i}} , \qquad (25)$$

where the sums run over all gas cells belonging to the halo.  $M_{\rm HI,i}$  and  $\vec{V}_{\rm HI,i}$  are the HI mass and velocity of gas cell *i*, and  $\vec{V}_{\rm HI}$  is the HI bulk velocity, computed as in Eq. 24.

We then take narrow bins in halo mass and compute the mean and standard deviation of the HI velocity dispersion. Fig. 13 shows the results, as well as a comparison with matter, whose properties are calculated analogously, but considering all mass elements within halos; i.e. gas, CDM, stars and black holes.

As expected, the velocity dispersion of both HI and CDM increases with halo mass, independent of redshift. The results can be represented by a simple power-law

$$\sigma_v(M) = \sigma_{10} \left(\frac{M}{10^{10} \ h^{-1} M_{\odot}}\right)^{\alpha} , \qquad (26)$$

where  $\sigma_{10}$  and  $\alpha$  are free parameters with best-fit values provided in Table 4.

The mean HI velocity dispersions are always equal to or smaller than the matter velocity dispersions. For large halo masses both exhibit the same amplitude, but for low mass halos the HI velocity dispersion is less than that of matter. The typical halo masses where the velocity dispersions diverge is around  $10^{12} h^{-1} M_{\odot}$ , with higher redshifts exhibiting departures at larger masses. This behavior is embedded in the slope of the  $\sigma_{\rm HI}(M)$ relation, whose value,  $\alpha$ , is larger than that of  $\sigma_{\rm m}(M)$  at all redshifts, and more so at higher redshifts.

For very small halos, and particularly at low redshift, the velocity dispersion of HI is much smaller than that of matter. This in a consequence of several factors. First,  $\sigma_{\rm m}(M)$  is artificially high, as the relation flattens out towards low masses. By comparing to a version of Fig. 13 (not shown) generated from a lower-resolution analogue of the same cosmological volume (TNG100-2; see Nelson et al. 2018), we conclude that this is due to finite numerical resolution, driven by particles in the outskirts of the halos, which does not apply to the HI, which is centrally-concentrated. In addition, we have examined a few individual low-mass halos and found that in some case the HI arises from just a few cells, or even a single one. In those cases, the HI bulk velocity will be set by these few cells and the HI velocity dispersion will be artificially suppressed due to sampling, again from finite resolution. As we move to more massive halos, the contribution of HI from satellites increases, and those satellites trace the underlying matter distribution more closely.

The scatter in the HI velocity dispersion for very lowmass halos is typically much smaller than the scatter in the matter velocity dispersion. One reason for this is that the HI velocity dispersion has been computed only for halos with total HI masses above  $10^5 h^{-1} M_{\odot}$ . Without such a threshold, the scatter in the HI velocity dispersion would be much larger. That is because if the HI mass in a halo is very low, it will often not be bound to the halo, e.g. the halo is crossing a filament that hosts a small amount of HI. In that case, HI velocity dispersions can be

![](_page_18_Figure_1.jpeg)

Figure 12. The upper panels show the average angle between the HI and halo peculiar velocity vectors,  $\cos(\alpha) = \vec{V}_{\rm HI} \cdot \vec{V}_h / (|\vec{V}_{\rm HI}||\vec{V}_h|)$ , as a function of halo mass. The bottom panels display the average ratio between the moduli of the HI and halo peculiar velocity vectors as a function of halo mass. Only halos with total HI mass above  $10^5 h^{-1} M_{\odot}$  are included. We show results at redshift 0 (top-left), 1 (top-middle), 2 (top-right), 3 (bottom-left), 4 (bottom-middle) and 5 (bottom-right). While the HI bulk velocity traces the halo peculiar velocity for small halos in both modulus and direction, there are departures for larger halos. This happens because most of the HI in small halos is in the central galaxy while in larger halos the contribution from satellites becomes more important.

	ma	tter	HI			
z	$\sigma_{10} \; [{\rm km/s}]$	α	$\sigma_{10} \; [\rm km/s]$	α		
0	$49 \pm 5$	$0.28\pm0.01$	$31 \pm 1$	$0.35\pm0.01$		
1	$56 \pm 4$	$0.30\pm0.01$	$34 \pm 1$	$0.37\pm0.01$		
2	$59 \pm 3$	$0.32\pm0.01$	$39 \pm 2$	$0.38\pm0.01$		
3	$64 \pm 3$	$0.33\pm0.01$	$44 \pm 2$	$0.39\pm0.01$		
4	$70 \pm 2$	$0.33\pm0.01$	$51 \pm 2$	$0.39\pm0.01$		
5	$75 \pm 2$	$0.33\pm0.01$	$54 \pm 2$	$0.40\pm0.01$		

#### Table 4

The mean 3D velocity dispersion of both matter and HI inside

halos can be represented by the relation  $\sigma = \sigma_{10} (M/10^{10} \ h^{-1} M_{\odot})^{\alpha}$ . The table gives the best-fits for  $\sigma_{10}$  and  $\alpha$  for matter and HI at different redshifts.

large. For example, several highly ionized unbound gas cells can produce a large, unphysical, velocity dispersion.

## 12. HI STOCHASTICITY

The relation between HI and matter is given, to linear order, by  $\delta_{\rm HI} = b_{\rm HI}\delta_{\rm m} + \epsilon$ , where  $\epsilon$  is the stochasticity. Below, we examine whether or not this relation reproduces our results in real-space and the amplitude of the stochasticity.

As for the density pdfs (see section 8) we compute the density fields of HI and matter on a grid with 2048<sup>3</sup> cells employing the CIC mass-assignment scheme. We then compute the overdensity of each field and smoothed them with a top-hat filter of radius 1 or 5  $h^{-1}$ Mpc. Next, we randomly select a subset of cells and make a scatter plot between the overdensities of HI and matter for each chosen cell. The results are shown in Figs. 14 (R = $1 h^{-1}$ Mpc) and  $15 (R = 5 h^{-1}$ Mpc).

For  $R = 1 h^{-1}$ Mpc two trends can be distinguished. The Ly $\alpha$ -forest shows up as cells with matter overdensities below the mean and very low HI overdensities because the gas there is mostly ionized. For large matter overdensities, the HI within halos is self-shielded. The

![](_page_19_Figure_1.jpeg)

Figure 13. The mean and standard deviation of the 3D velocity dispersion of HI (blue lines) and CDM (red lines) as a function of halo mass at redshifts 0 (top-left), 1 (top-middle), 2 (top-right), 3 (bottom-left), 4 (bottom-middle) and 5 (bottom-right). Our results are well-represented by a simple power law,  $\sigma = \sigma_{10} (M/10^{10} \ h^{-1} M_{\odot})^{\alpha}$ , with best-fit parameter given in Table 4. At low redshift, the velocity dispersion of HI is very similar to that of CDM, while at high-redshift CDM exhibits larger values than HI.

density  $\rho_{\rm m}/\bar{\rho}_{\rm m} \simeq 0.4$  marks a transition from one regime to the other, indicating that HI self-shielding does not take place for lower matter overdensities. In all cases, the HI overdensity increases with matter overdensity.

At higher redshifts the range occupied by matter and HI overdensities is smaller. As the Universe becomes more homogeneous, fluctuations are smaller. This behavior can also be seen in the pdfs of Fig. 8. The scatter in the overdensity relations also decreases towards higher redshift.

The dashed black lines show the predictions from linear theory,  $\delta_{\rm HI} = b_{\rm HI}\delta_{\rm m}$ , where  $b_{\rm HI}$  is the linear HI bias measured from the simulation (see section 13 and Table 5). As expected, linear theory is not accurate in this regime because the bias is not linear on the smoothing scale considered. An exception if for z = 1 where linear HI bias reproduces the results reasonably well. This is because the HI bias is relatively flat at that redshift (see Fig. 16).

As we move to a larger smoothing radius, the morphology of the results changes, as can be seen in Fig. 15, where  $R = 5 h^{-1}$ Mpc. Now, the HI and matter overdensities extend over a smaller range, because the smoothing is over a larger scale, making the field more homogeneous. In addition, the Ly $\alpha$  forest is no longer visible because in the neighborhood of the highly ionized HI in filaments, i.e. the Ly $\alpha$  forest, there will always be some halo within 5  $h^{-1}$ Mpc that contains self-shielded HI gas.

As above, we find that HI overdensities increase with matter overdensities at all redshifts. However, at high-redshift the slope of the relation becomes more pronounced. This behavior can be partly explained by linear HI bias, shows as dashed black lines. As with  $R = 1 \ h^{-1}$ Mpc, linear bias can explain the results relatively well at z = 1. At other redshifts, linear bias is more accurate than for smaller smoothing scales, as expected, but the agreement is not good for both large and small matter overdensities. Again, the scatter reduces with redshift.

#### 13. HI BIAS

We now examine different aspects of HI clustering in detail. In this section we focus on the amplitude and shape of the HI bias.

The relation between the clustering of HI and that of dark matter involves the HI bias through  $P_{\rm HI}(k) = b_{\rm HI}^2(k)P_{\rm m}(k)$ . The matter power spectrum, the quantity that contains the information on the values of the cosmological parameters, can thus be inferred only if bias is understood (see Pénin et al. 2018b, for a detailed discussion on HI scale-dependence bias). On linear scales the HI bias is constant, but on small scales we expect to see scale-dependence. It is important to determine the scales on which the HI bias is scale-dependent and whether or not analytic models can reproduce that behavior.

We have computed the HI and matter auto-power spectrum and the HI-matter cross-power spectrum of the sim-

![](_page_20_Figure_1.jpeg)

Figure 14. Relations between the HI and matter density fields smoothed with a top-hat filter of radius  $R = 1 h^{-1}$ Mpc, shown as scatter plots between the respective overdensities at redshifts z = 0 (top-left), z = 1 (top-middle), z = 2 (top-right), z = 3 (bottom-left) z = 4 (bottom-middle) and z = 5 (bottom-right). The colors indicate the number cells in each hexabin. The presence of the Ly $\alpha$ -forest can be seen at low matter and HI overdensities, while the HI inside halos dominates the behavior of the relation for  $\rho_{\rm HI}/\bar{\rho}_{\rm HI} \gtrsim 0.1$ . The HI-matter relation is tighter at high-redshift than at low-redshift. The dashed black lines show the expectation from linear theory,  $\delta_{\rm HI} = b_{\rm HI}\delta_{\rm m}$ , where  $b_{\rm HI}$  is the large-scale HI bias, taken from table 5.

![](_page_20_Figure_3.jpeg)

Figure 15. Same as Fig. 14 but for a smoothing scale of 5  $h^{-1}$ Mpc.

ulation at redshifts 0, 1, 2, 3, 4 and 5. The HI bias is then obtained using two different definitions:  $b_{\rm HI}(k) = \sqrt{P_{\rm HI}(k)/P_{\rm m}(k)}$  and  $b_{\rm HI}(k) = P_{\rm HI-m}(k)/P_{\rm m}(k)$ . While the latter is "preferred", as it does not suffer from stochasticity, the former is closer to observations. The results are shown in Fig. 16.

The amplitude of the HI bias on large scales increases

with redshift, from  $\simeq 0.85$  at z = 0 to  $\simeq 3.20$  at z = 5. On the largest scales that can be probed with TNG100, the amplitude of the HI bias is independent of the method used to estimate it. We assume that the values on large scales are equal to the linear HI bias, but note that there could be small corrections to those because of box-size. The linear HI bias at different redshifts is given in Table 5. These values can be reproduced from

![](_page_21_Figure_1.jpeg)

Figure 16. HI bias at redshifts 0 (black), 1 (red), 2 (green), 3 (blue), 4 (purple) and 5 (orange) computed as the square root of the ratio between the HI and matter power spectra (left), and as the ratio between the HI-m cross-power spectrum and the matter power spectrum. The value of the HI bias increases with redshift. At high redshift, the HI bias becomes non-linear on scales  $k \gtrsim 0.3 \ h Mpc^{-1}$ .

the halo HI mass function as

$$b_{\rm HI}(z) = \frac{\int_0^\infty n(M, z)b(M, z)M_{\rm HI}(M, z)dM}{\int_0^\infty n(M, z)M_{\rm HI}(M, z)dM} , \qquad (27)$$

and therefore the amplitude of the HI bias is sensitive to the astrophysical parameters  $\alpha$  and  $M_{\min}$  (see section 5). Note, however, that the agreement between the above expression and the simulation results is not perfect because, among other things, our models for the halo mass function and halo bias do not include corrections for baryonic effects.

At z = 0 the HI bias exhibits a scale-dependence even on the largest scales we can probe, due to the fact that the matter power spectrum at the scales probed by TNG100 is not in the linear regime at such low-redshift. It is interesting to notice the dip in the HI bias at  $k \simeq 1 \ h {\rm Mpc}^{-1}$ , that has been also found in observations (Anderson et al. 2018). At z = 1 the bias remains almost constant down to rather small scales,  $k \simeq 1 \ h \text{Mpc}^{-1}$ . These trends agree with the findings of Springel et al. (2017), who studied galaxy bias for different galaxy populations at different redshifts. At high-redshifts,  $z \ge 2$ , the HI bias exhibits a dependence on scale already at  $k = 0.3 \ h \text{Mpc}^{-1}$ , even though these scales are close to linear at those redshifts. Our results are also in qualitative agreement with Sarkar et al. (2016a), who studied the HI bias by painting HI on top of dark matter halos. The scale-dependence of the bias is not necessarily a bad thing, as long we can use perturbative methods to predict the shape of the HI power spectrum. For this purpose we have compared the measurements of the HI power spectrum in TNG100 to analytical calculations using Lagrangian Perturbation Theory (LPT). The first order LPT solution is the well known Zeldovich approximation (ZA) (Zel'dovich 1970; White 2014), for which we can simply write

$$P_{\rm HI} = b_{\rm HI}^2 P_{\rm ZA}(k) + N \tag{28}$$

and then fit for the two free parameters in the above equation. The constant piece takes care of the shot-noise and any other term which is scale independent and uncorrelated with the HI field and therefore can be treated as noise in a cosmological analysis (Seljak & Vlah 2015). Given the small volume of TNG100, a perturbative analysis makes sense only at high redshifts, where linear and mildly non-linear modes are contained in the box, thus we restrict the comparison of Eq. 28 with the measurements in the simulation to  $z \ge 2$ . The upper panel in Fig 17 shows the measurements of the HI power spectrum at different redshift, using the same color scheme of the previous figures. The points with error bars have been shifted horizontally to avoid overlap and facilitate the visual comparison with the theoretical models. The dashed lines display the fit to Eq. 28 including all the modes up to  $k_{\text{max}} = 1 h \text{Mpc}^{-1}$ . The fit is quite accurate, despite its simple functional form, and it confirms the HI distribution as an ideal tracer for cosmological studies. The continuous lines show the next to leading order, *i.e.* 1-loop, calculation in LPT (Modi et al. 2017; Vlah et al. 2016), which includes an improved treatment of non-linearities in the matter fields as well as several non-linear bias parameters. Up to the scale we include in the fit there is no difference between the two approaches, with the 1-loop calculation also working on smaller scales not included in the analysis. The fact that the ZA works so well in describing the simulation measurements could vastly simplify the cosmological analysis and interpretation of 21cm surveys observing at high redshift. For instance, interferometric surveys with large instantaneous field of view like CHIME will be forced to include all the complications arising from the curved-sky, that are very easy to handle in the ZA (Castorina & White 2018a,b).

# 14. SECONDARY HI BIAS

It is well known that the clustering of halos depends primarily on mass. However, mass is not the only variable that determines halo clustering; there is also a dependence on halo age (Sheth & Tormen 2004; Gao et al. 2005), concentration (Wechsler et al. 2006), subhalo abundance (Wechsler et al. 2006; Gao & White 2007), halo shape (Faltenbacher & White 2010), spin (Gao &

![](_page_22_Figure_1.jpeg)

Figure 17. Top panel: HI power spectrum as a function of redshift measured in TNG100 (points with error bars). For visualization purposes only, the data at different redshift have been shifted horizontally to avoid overlap. The dashed lines show the analytical calculation assuming the ZA, whereas the continuous lines correspond to the 1-loop calculation. Both models have been fitted to  $k = 1 h \text{Mpc}^{-1}$ . See text for details. Bottom panel: Ratio of the measured power to the analytical models. Filled points show the 1-loop result, whilst the empty ones the comparison to the ZA.

z	0	1	2	3	4	5
$b_{ m HI}$	0.84	1.49	2.03	2.56	2.82	3.18
$\begin{bmatrix} P_{\rm HI}^{\rm SN} \\ [(h^{-1}{\rm Mpc})^3] \end{bmatrix}$	104	124	65	39	14	7

 Table 5

 Values of the HI bias and HI shot-noise from the simulation at different redshifts.

White 2007), and environment (Salcedo et al. 2018; Han et al. 2018). Here, we identify a new secondary bias, originating from the HI content of halos.

Differently from the previous quantities, which are properties of the dark matter halos, the HI content is more related to the properties of the galaxies inside a halo; e.g. whether galaxies are red or blue. Thus, a study of this kind can only be carried out using hydrodynamic simulations.

To study this issue, we apply the following procedure. First, all halos whose total mass is within a relatively narrow mass bin are selected. The HI mass inside each of those halos and the median value are determined. Next, the halos are split into two categories: HI rich and HI poor, depending on whether the HI content of a particular halo is above or below the median, respectively. Finally, we compute the power spectrum of: 1) all halos, 2) HI rich halos and 3) HI poor halos.

The results are shownin Fig. 18 at redshifts 0, 1, 2, 3 and 4 and for three different mass bins:  $M \in [10^8 - 10^9] h^{-1}M_{\odot}$ ,  $M \in [10^9 - 10^{10}] h^{-1}M_{\odot}$  and  $M \in [10^{10} - 10^{11}] h^{-1}M_{\odot}$ . The black lines indicate the power spectrum of all halos, while the blue and red lines represent the power spectra of the HI rich and HI poor halos, respectively.

Going towards smaller scales, the amplitudes of the different power spectra first flatten and then rise back up. This happens because: 1) we approach the shot-noise limit, and 2) due to aliasing. The shot-noise level of the HI rich/poor halos is different from that of all halos, as the latter contain, by definition, twice more halos than the former. Thus, on small scales, the amplitude of the HI rich and HI poor halos is expected to be the same but higher by a factor of 2 than that of all halos, as is indeed seen.

For all redshifts and mass intervals considered, the clustering of HI rich galaxies is different from that of HI poor ones, showing that halo clustering depends not only on mass but on HI content as well. The difference in the clustering of HI poor and HI rich halos decreases, in general, with halo mass. At z = 0, the amplitude of the halo power spectrum of the HI rich and HI poor can be almost one order of magnitude different for halos in the  $[10^9-10^{10}] h^{-1} M_{\odot}$  mass bin. The largest differences are seen for halos with masses around or below  $M_{\rm min}$  at that particular redshift, namely around the mass scale where the HI content starts being exponentially suppressed (see section 5).

At z = 0, and for the mass bin intervals considered here, the HI poor halos are more strongly clustered than the HI rich halos. On the other hand, at high-redshift the situation is the opposite, and HI rich halos are more strongly clustered than HI poor halos. At z = 1, we find that depending on the halo mass considered, HI rich halos can be more or less clustered than HI poor halos.

Although the halo mass bins are fairly narrow, is not unreasonable to suspect that the most massive halos will have larger HI masses and therefore this could introduce some natural splitting that arises just from halo mass and not from HI secondary bias. In order to test this, we split the halos according to their median total halo mass and repeated the above analysis. We find that the clustering of the two samples is almost indistinguishable,

![](_page_23_Figure_2.jpeg)

Figure 18. We select dark matter halos in narrow mass bins and compute their power spectra, shown with solid black lines. We then compute the HI mass inside each halo and find the median value of all halos in that mass bin. Next, we split the halos in two sets, those with HI mass above (HI rich) or below (HI poor) the median. Finally, we compute the power spectrum of the halos in each set and show the results with blue (HI rich) and red (HI poor) lines. Results are shown at redshifts 0, 1, 2, 3 and 4 from top to bottom and for halo in the  $10^8 - 10^9$  (left column),  $10^9 - 10^{10}$  (middle column) and  $10^{10} - 10^{11} h^{-1}M_{\odot}$  mass bin intervals. The upper part of each panel displays the different halo power spectra while the bottom part shows the same results normalized by the power spectrum of all halos. The clustering of halos depends not only on mass but also on HI content. The magnitude of this effect is generally larger for smaller halos. At low redshift, HI-poor halos are more clustered than HI-rich halos, but at high redshift the trend reverses.

![](_page_24_Figure_2.jpeg)

Figure 19. HI shot-noise. This figure shows the standard HI power spectrum (solid lines) and the power spectrum when the HI inside halos is placed in the halo center (dashed lines) at redshifts z = 0 (black) and z = 4 (purple). For the former we can see both the 1- and 2-halo terms, while for the latter the 1-halo term is just the HI shot-noise.

ruling out the possibility that halo mass is affecting our results.

At low redshift, small halos near big ones are more likely to be stripped of their gas content. Thus, HI poor halos should be more strongly clustered than HI rich halos, as we find. This possibility has been recently suggested to explain the secondary bias that arises from several halo properties in Salcedo et al. (2018); Han et al. (2018).

On the other hand, at high redshift, gas stripping by nearby halo neighbors should be less effective, as the largest halos are not yet very massive and there has been less physical time for these processes to operate. We speculate that at high-redshift, regions around massive halos are richer in HI than other regions. For example, in regions with higher density we would expect the filaments to be slightly more dense and therefore will host more HI. Halos connected by those filaments may thus become HI rich. This naive picture can be seen in Fig. 26, where at high-redshift, the filaments in the denser regions host more HI than in less denser regions.

#### 15. HI SHOT-NOISE

An important consideration in any cosmological survey is shot-noise, as its amplitude determines the maximum scale where cosmological information can be extracted from(see Eq. 1). However, it can also be used to learn about the galaxy population hosting the HI (Wolz et al. 2017, 2018). The purpose of this section is to quantify the amplitude of the HI shot-noise from our simulations.

We now illustrate why computing the HI shot-noise is slightly more complicated than determining the shotnoise for other tracers, such as halos, where the value of the shot-noise is simply given by the amplitude of the power spectrum on small scales.

The solid lines of Fig. 19 show the HI power spectrum at redshifts 0 and 4. It can be seen that those power spectra receive contributions from both the 1- and 2-halo terms; i.e. the power spectrum on very small scales does not become constant, in contrast with the halo power spectrum. This happens simply because there is structure in HI inside halos and galaxies (see Fig. 6).

In order to isolate the contribution of the HI shot-noise, i.e. to avoid the 1-halo term contribution, we do the following. We compute the total amount of HI inside every halo in the simulation and place that HI mass in the halo center. We then compute the HI power spectrum of that configuration. Since in that case there is no HI structure inside halos there is no 1-halo term, and the amplitude of the HI power spectrum on small scales is just the HI shot-noise. The dashed lines in Fig. 19 display the results.

It can be seen that on large scales, the amplitude of the HI power spectrum of the two configurations is essentially identical. The small differences at z = 4 arise from the HI that is outside of halos (see Fig. 3), whose contribution is not accounted for with our procedure. That contribution should, however, have negligible impact on the amplitude of the HI shot-noise. On small scales, the lack of the 1-halo term when we artificially place the HI at the halos center makes possible to isolate the value of the HI shot-noise. We determine the value of the HI shot-noise by averaging the amplitude of the HI power spectrum on scales  $k \in [20 - 30] \ h \text{Mpc}^{-1}$  and show the results in table 5.

The HI shot-noise can also be computed using the halo model framework (assuming all HI is in halos) as (Castorina & Villaescusa-Navarro 2017)

$$P_{\rm HI}^{\rm SN}(z) = \lim_{k \to 0} P_{\rm 1h, \rm HI}(k, z) = \frac{1}{[\rho_{\rm c}^0 \Omega_{\rm HI}(z)]^2} \int_0^\infty n(M, z) M_{\rm HI}^2(M, z) dM = \frac{\int_0^\infty n(M, z) M_{\rm HI}^2(M, z) dM}{\left[\int_0^\infty n(M, z) M_{\rm HI}(M, z) dM\right]^2} .$$
(29)

If we use the Sheth & Tormen (ST) formula (Sheth & Tormen 2002) for the halo mass function in this expression<sup>17</sup> and our fitting formula for  $M_{\rm HI}(M, z)$  (see table 1), we obtain values for the HI shot-noise in agreement with those measured directly in the simulation.

In order to validate our results we have estimated the HI shot-noise by measuring the stochasticity between the

HI and the matter fields (Seljak et al. 2009)

$$P_{\rm HI}(k) - \frac{P_{\rm HI-m}^2(k)}{P_{\rm m}(k)} ,$$
 (30)

which at low enough k should correspond to the uncorrelated part of the HI power spectrum, *i.e.*  $P_{\rm SN}$ . However, the shot-noise amplitudes we obtain in this case are much larger than those found using our fiducial procedure. By repeating the this approach for halos we also find that we

 $<sup>^{17}</sup>$  We find that the halo mass function in Illustris TNG is well reproduced by the ST form.

![](_page_25_Figure_2.jpeg)

Figure 20. An important quantity for BAO studies is  $nP_{0.2}$ , defined as the ratio between the amplitudes of the cosmological signal and the shot-noise level at  $k = 0.2 \ h \text{Mpc}^{-1}$ . In this plot we show this quantity in blue as a function of redshift using TNG100 measurements. We find that it is large at all redshifts, indicating that shot-noise is not important for BAO studies with 21 cm intensity mapping. In order to extract information from small scales it is also crucial to have large nP at high-k. The red line shows that this is indeed the case at  $k = 0.5 \ h \text{Mpc}^{-1}$  for all redshifts considered in our work.

cannot recover the standard  $1/\bar{n}$  result. Our findings are in agreement with other studies, see Hand et al. (2017) and reference therein, and point towards some lack of understanding of the noise properties in low mass halos even in gravity only simulations. For better comparison with previous work, that always considered Poissonian shot-noise, we assume  $P_{\rm SN}$  is given by the fiducial halo model procedure, and defer a study of this unexpected disagreement to future work.

We find that the HI shot-noise is low at all redshifts. This is in broad agreement with the analytical work of Castorina & Villaescusa-Navarro (2017), whose results at high redshift had however a large theoretical error. Our shot-noise values are slightly lower than those in that paper, mostly because values of  $M_{\rm min}$  at high z we find here are lower than those considered in Castorina & Villaescusa-Navarro (2017).

The low values of shot-noise we find have important implications. First, 21 cm intensity mapping experiments that aim at measuring the BAO peak (Obuljen et al. 2017b) position such as CHIME, OOTY, BINGO, HI-RAX, or SKA will barely be affected by shot-noise. We illustrate this in Fig. 20, where we plot, in blue,

$$nP_{0.2}(z) = \frac{P_{\rm HI}(k = 0.2 \ h {\rm Mpc}^{-1}, z)}{P_{\rm SN}(z)}$$
(31)

as a function of redshift. We obtain values of  $nP_{0.2}$  above  $\simeq 15$  at all redshifts, showing that shot-noise contamination on BAO scales is minimal. This is a great advantage over traditional methods such as galaxy surveys.

Second, the shot-noise levels are very low at high redshift. This means that shot-noise does not erase the cosmological information on small scales. The red line shows the value of nP at  $k = 0.5h/\text{Mpc}^{-1}$ , which is still much larger than one and implies these modes can be in principle measured in the cosmic variance limit. With accurate theory predictions as the one described in the previous section, this information can be retrieved and used to reduce errors in the values of the cosmological parameters.

#### 16. REDSHIFT-SPACE DISTORTIONS

21 cm intensity mapping observations probe the spatial distribution of cosmic neutral hydrogen in redshift-space, not in real-space. Thus, it is of utmost importance to understand the impact of peculiar velocities on the clustering of HI. In this section we study the clustering of neutral hydrogen in redshift-space.

Here, we make use of the plane-parallel approximation to displace particles and Voronoi cells positions from real  $(\vec{x})$  to redshift-space  $(\vec{s})$  through

$$\vec{s} = \vec{x} + \frac{1+z}{H(z)}\vec{v}_{||}(\vec{r})$$
 (32)

where  $\vec{v}_{||}(\vec{r})$  is the peculiar velocity of the particle/cell along the line-of-sight. We use the three cartesian axes as different lines-of-sight. Our results represent the mean over the three axes.

We have computed the clustering of HI in redshiftspace and show the results in Fig. 21. While we have computed the HI monopoles, quadrupoles and hexadecapoles, the latter two are too noisy so we restrict our analysis to the monopoles.

We show with red/blue lines the monopoles in real/redshift space in this figure. The two main physical processes governing the effect of peculiar velocities can clearly be seen. On large-scales the clustering of HI in redshift-space is enhanced due to the Kaiser effect (Kaiser 1987). On small scales, peculiar velocities of HI inside halos give rise to Fingers-of-God, suppressing the amplitude of the HI power spectrum.

The bottom part of each panel of Fig. 21 shows the ratio between the monopoles in redshift- and real-space as a solid black line. The black dashed line displays the prediction of linear theory for that ratio, i.e.

$$\frac{P_0^s(k)}{P_0^r(k)} = 1 + \frac{2}{3}\beta + \frac{1}{5}\beta^2 \tag{33}$$

where  $\beta = f/b_{\rm HI}$ , with  $f \simeq \Omega_{\rm m}^{0.545}(z)$  being the linear growth rate. We have estimated  $\beta$  using the values of the linear HI bias from Table 5.

As expected, linear theory is not able to describe our results at low redshift. This is because the scales we probe in TNG100 are too small for linear theory to hold. On the other hand, we find that the Kaiser factor can reasonably well explain the monopoles ratio down to  $k \simeq 0.3, 0.5$  and  $1.0 \ h Mpc^{-1}$  at redshifts, 3, 4 and 5, respectively.

Given the results in Section 13 our findings are not surprising, and we plan to compare the measurements in TNG100 to redshift space LPT analytical predictions in upcoming work.

As an alternate way to visualize the consequences of redshift-space distortions, we show the 2-dimensional power spectrum of cosmic HI in the top 2 rows of Fig. 22, at redshifts from 0 to 5. The Kaiser effect manifests itself as a squeezing of isopower contours along the per-

![](_page_26_Figure_1.jpeg)

Figure 21. Impact of redshift-space distortions on the HI power spectrum at redshifts 0 (top-left), 1 (top-middle), 2 (top-right), 3 (bottomleft), 4 (bottom-middle) and 5 (bottom-right). The upper part of each panel shows the HI power spectrum (monopole) in real-space (red) and redshift-space (blue). The bottom part displays the ratio between the monopoles in redshift- and real-space (solid black) and the prediction of linear theory (dashed black). Redshift-space distortions enhance/suppress power on large/small scales. Linear theory can explain the HI clustering in redshift-space down to very small scales at high-redshift, while it cannot at low redshift on the scales we probe in the simulations.

pendicular direction on large scales. It is apparent down to relatively small scales at high-redshift, as expected.

On small scales, Fingers-of-God arise as isopower contours propagating further in the perpendicular than the radial direction. At low redshift, and on small scales, we find that isopower contours exhibit a very weak dependence on the perpendicular direction, i.e.  $P_{\rm HI}^{s}(k_{||}, k_{\perp}) \simeq P_{\rm HI}^{s}(k_{||})$ .

We show the results for the 2D matter power spectrum in the bottom rows of Fig. 22. It can be seen how: 1) the Kaiser effect is visible down to smaller scales than in the HI field at high-redshift, and 2) the magnitude of the Fingers-of-God is lower in the matter field than in the HI field.

The halo model can be used to understand why the magnitude of Fingers-of-God is higher in HI than in matter. Each dark matter halo will show up in redshift-space not as a sphere, but an ellipsoid, due to internal peculiar velocities. The eccentricity of those ellipsoids will depend primarily on halo mass: the velocity dispersion in large halos will be higher than in small halos, so their eccentricity will be larger. The amplitude of the matter power spectrum on small scales will be dominated by small halos, whose velocity dispersions are not large.

On the other hand, we know for HI that since there is a cutoff in the halo HI mass function, halos below a certain mass will not contribute to the HI power spectrum. Thus, it is expected that the amplitude of the Fingersof-God will be larger in the HI field than in the matter field because: 1) the velocity dispersions of HI and matter/CDM are similar (see section 11), and 2) in the HI field we do not have the contribution of small halos that dominate the amplitude of the power on small scales.

In order to corroborate this hypothesis we have taken all halos with masses above  $10^{10} h^{-1} M_{\odot}$  and we have computed the power spectrum of the matter inside them. In that case, we observe very similar results as those from the HI; i.e. the amplitude of the Fingers-of-God of that particle distribution is much larger than the one for all matter.

![](_page_27_Figure_1.jpeg)

Figure 22. Top 2 rows: 2D power spectrum of HI at redshifts 0 (upper-left), 1 (upper-middle), 2 (upper-right), 3 (bottom-left), 4 (bottom-middle) and 5 (bottom-right). Even though the small volume of our simulation make the 2D power spectrum noisy on large-scales, the Kaiser effect can be seen, particularly at high-redshifts, as isopower contours squeezing in the  $k_{\perp}$  direction. On small scales the 2D power spectrum is dominated by Fingers-of-God, whose amplitude is larger than in the matter field and is more important at low-redshift. Bottom 2 rows: same as above but for matter instead of HI.

The impact of redshift-space distortions on the HI power spectrum has recently been studied in Sarkar & Bharadwaj (2018) using N-body simulations. Following their work we have tried to model the 2D HI power spectrum using the following phenomenological expression

$$P_{\rm HI}^s(k,\mu) = (1+\beta\mu^2)^2 P_{\rm HI}^r(k) \frac{1}{\left(1+\frac{1}{2}k^2\mu^2\sigma_p^2\right)^2} ,\quad (34)$$

where  $\beta = f/b_{\rm HI}$ ,  $P_{\rm HI}^r(k)$  is the fully non-linear HI power spectrum and  $\sigma_p$  is a phenomenological parameter that accounts for the Fingers-of-God effect. The reason for using this expression is that even if the HI bias is nonlinear, we will recover the Kaiser factor when computing the monopole ratio (see Fig. 21). at high-redshift, where the amplitude of the Fingers-of-God is small.

By fitting the above expression to our 2D HI power spectrum down to  $k = 1 \ h \text{Mpc}^{-1}$  and assuming Gaussian errors, we find that this approach works reasonably well  $\chi^2/\text{d.o.f} \simeq [1.5 - 2.2]$ , with  $\sigma_p =$ 1.73, 2.09, 1.37, 0.93, 0.34, 0 at redshifts 0, 1, 2, 3, 4 and 5, respectively. However, by computing the monopole from the above expression

$$P_{\rm HI}^0(k) = \frac{1}{2} \int_{-1}^{1} P_{\rm HI}^s(k,\mu) d\mu$$
 (35)

and comparing with our measurements we do not find good agreement.

We have also repeated the above exercise for the models considered in Sarkar & Bharadwaj (2018), concluding that none of those represent a good description of our results. We leave a more detailed analysis of this issue for future work.

## 17. 21CM MAPS

The HI properties studied in this paper can be used to generate mock 21 cm maps. In this section we study: 1) whether less computationally expensive simulations can be used to create 21 cm maps, and 2) the importance of accounting for the 1-halo term when making mocks.

The right column of Fig. 23 shows 21 cm maps created from the spatial distribution of HI in the TNG100 simulation. From top to bottom these maps show: 21 cm map in real-space with 3' angular resolution (top), 21 cm map in redshift-space with 3' angular resolution (top-middle), 21 cm map in real-space with 0.3' angular resolution (bottom-middle), and 21 cm map in redshiftspace with 0.3' angular resolution (bottom). All those maps are centered at a frequency of 710 MHz (z = 1) and have a bandwidth of 1 MHz ( $\simeq 5 h^{-1}$ Mpc).

The procedure used to create these maps is as follows. First, the HI density field is computed by assigning HI masses of gas cells (either in real- or redshift-space) to a grid of 2048<sup>3</sup> cells using the nearest-grid-point (NGP) mass assignment scheme. Then, we select a slice of the HI density field grid whose width is taken to reproduce the desired frequency bandwidth. Next, that slice is projected onto a 2-dimensional grid and HI densities are transformed to brightness temperatures through

$$T_b(\vec{x}) = 189h\left(\frac{H_0(1.0+z)^2}{H(z)}\right)\frac{\rho_{\rm HI}(\vec{x})}{\rho_{\rm c}} \,\,\mathrm{mK} \,\,. \tag{36}$$

Finally, we convolve that grid with a Gaussian filter of

radius  $R = \theta \chi$ , where  $\theta$  is the desired angular resolution and  $\chi$  is the comoving distance to redshift z (or frequency  $\nu$ ).

The 21 cm maps on the left column of Fig. 23 have been created from an N-body simulation that shares the same initial conditions as TNG100; i.e. TNG100-1-DM, but whose computational cost is over an order of magnitude lower. In that simulation, we have placed an HI mass given by  $M_{\rm HI}(M, z)$  from table 1, on the center of each dark matter halo. Then, we have followed the procedure outlined above to create the 21 cm maps. To make 21 cm maps in redshift-space we displace the HI mass that we put in the center of each halo according to the peculiar velocity of that halo.

It can be seen that the qualitative agreement between the maps from the full hydrodynamic simulation and the cheaper N-body one is very good. In Fig. 24 we quantify this visual agreement by computing the HI power spectrum of the hydrodynamic and N-body simulations in real-space at different redshifts.

We find that the amplitude of the two HI power spectra can be significantly different, between 10% and 40%. We attribute these differences to the inaccuracies of our  $M_{\rm HI}(M,z)$  function (e.g. we do not require our fit to reproduce  $\Omega_{\rm HI}(z)$ , to the effects of baryons on the halo mass function and halo clustering, which are neglected in this exercise, and to the omission of the 1-halo term at very high k. For the latter, we emphasize that in this section we do not consider the spatial distribution of HI inside halos, which we leave for future work. However, once the difference in amplitude is taken into account, we find that shapes differ by only  $\simeq 5\%$  from the largest scales down to  $k = 1 \ h \text{Mpc}^{-1}$  at all redshifts. This is rather remarkable considering that the 1-halo term was not accounted for. This exercise demonstrates that populating dark matter halos from a computationally cheap N-body simulation with HI can yield results that are reasonable, at least in shape, at a few percent level in the fully non-linear regime at all relevant redshifts.

In Fig. 25 we show the comparison between the HI power spectra from IllustrisTNG and the N-body simulation in redshift-space at several redshifts. As for the comparison in real-space, the amplitude of the two power spectra can be quite different for the same reasons outlined above. However, even when the normalization offset is taken into account, there are larger shape differences than in real-space. For instance, at z = 1 the discrepancies up to  $k = 1 \ h \text{Mpc}^{-1}$  can be as large as 45%. That difference declines with redshift, so that at z = 5 it is only 6%, very similar to the differences we find in real-space.

The larger differences in redshift-space can be attributed to Fingers-of-God. Here, we did not attempt to model the 1-halo term and, therefore, the HI Fingersof-God are not present in our mock maps, while they are in those created from IllustrisTNG. As we saw in section 16, the HI FoG can propagate to relatively large scales and affect the amplitude and shape of the HI power spectrum. At higher redshift, the magnitude of the FoG is lower, so the agreement between IllustrisTNG and the N-body mocks is expected to improve, as we observe. Finally, the agreement between the different maps also depends on bandwidth. For larger bandwidths the FoG

![](_page_29_Figure_2.jpeg)

Figure 23. 21 cm maps at 710 MHz with 1 MHz bandwidth over an area of  $\sim 4 \text{ deg}^2$ . The upper and bottom pairs of panels show maps with angular resolutions of 3' and 0.3', respectively. Within each pair, the top one was made in real-space and the bottom in redshift-space. The maps on the right column have been generated from the computationally expensive IllustrisTNG simulations, while the maps on the left by painting HI on top of dark matter halos from computationally cheap N-body simulations using the ingredients studied in this paper.

![](_page_30_Figure_1.jpeg)

Figure 24. A comparison of the spatial distribution of HI from IllustrisTNG versus the one obtained by placing HI in the centers of halos in an N-body simulation at redshift 0 (upper-left), 1 (upper-middle), 2 (upper-right), 3 (bottom-left), 4 (bottom-middle) and 5 (bottom-right). The HI mass assigned to each halo in the N-body run is taken from our tabulated  $M_{\rm HI}(M,z)$  of Table 1. We compute the HI power spectrum in real-space for both configurations: N-body (blue) and hydro (green). The black line in the bottom part of each panel shows the ratio between the power spectra. Although the overall normalization can be different (see text for more details), it is more quoted with a number in the bottom part of each panel. This simple procedure allows us to generate mock 21 cm maps whose underlying power spectrum is accurate at  $\simeq 5\%$  down to  $k = 1 \ h Mpc^{-1}$ .

effects will have a smaller impact. We could also argue that beam smoothing in IM surveys will further reduce the effect of FoG in the final measured power spectrum.

We conclude that 21cm intensity mapping maps can be created via less computationally expensive simulations like N-body, or fast simulations, e.g. COLA (Tassev et al. 2013) or Pinocchio (Monaco et al. 2002), instead of expensive hydrodynamic simulations. It is however very important to account for the 1-halo term, as expected, i.e. the FoG, when modeling the distribution of HI in redshift-space.

## 18. SUMMARY AND CONCLUSIONS

A goal of current and upcoming radio telescopes is to map the spatial distribution of matter by detecting 21 cm emission from cosmic neutral hydrogen. The very large volumes that can be sampled through 21 cm intensity mapping observations will place tight constraints on the values of the cosmological parameters (Bull et al. 2015; Villaescusa-Navarro et al. 2015; Obuljen et al. 2017a; Sprenger et al. 2018). In order to extract the maximum information from these surveys, accurate theory predictions are needed.

Theory predictions to linear order are well known. For instance, the amplitude and shape of the 21 cm power spectrum is given by

$$P_{21\rm cm}(k,\mu) = \bar{T}_b^2 (b_{\rm HI} + f\mu^2)^2 P_{\rm m}(k) + P_{\rm SN} , \qquad (37)$$

where  $\overline{T}_b \propto \Omega_{\rm HI}$  is the mean brightness temperature,  $b_{\rm HI}$ is the HI bias, f is the linear growth rate,  $\mu = k_z/k$ ,  $P_{\rm m}(k)$  is the linear matter power spectrum, and  $P_{\rm SN}$  is the HI shot-noise. While the value of  $\overline{T}_b$  is relatively well known from several observations across the redshift range  $z \in [0, 5]$ , little is known about  $b_{\rm HI}$  and  $P_{\rm SN}$ . In this work we have quantified them and studied the scales where linear theory holds, e.g. when the HI bias becomes non-linear.

Accurate theory predictions in the mildly or fully-non linear regimes will allow us to recover the large amount of information embedded in the spatial distribution of HI on small scales. There are several techniques for accomplishing this, such as perturbation theory, HI halo models, or numerical simulations. The purpose of our work has been to study the ingredients that these techniques employ. For example, HI halo models require the halo HI mass function and the HI density profile as inputs.

Our purpose here is not limited to analytic approaches, but is also to understand how HI is distributed across the Universe and how it evolves with time. We have shown that even with a subset of the ingredients studied in this work, one can model the spatial distribution of HI in the fully non-linear regime without the use of computationally expensive hydrodynamic simulations, but using HI HOD models.

We have carried out our analysis using IllustrisTNG

![](_page_31_Figure_1.jpeg)

Figure 25. Same as Fig. 24 but for HI monopole in redshift-space. It can be seen that the distributions of HI in the two configurations differ more significantly than in real-space. The origin of this large discrepancy, more prominent at low-redshift, is the lack of Fingers-of-God in the modeling of HI with the N-body simulations, since we place all HI in the halo center. More realistic 21 cm maps need to account for the HI velocity dispersion inside halos.

(Springel et al. 2017; Pillepich et al. 2017a; Nelson et al. 2018; Naiman et al. 2017; Marinacci et al. 2017), a sophisticated series of cosmological hydrodynamical simulations that have shown to be in broad agreement with many basic observables, run at an unprecedented combination of large volume and high resolution, therefore providing an excellent testbed for accurately investigating the distribution of HI from the disks of spiral galaxies to cosmological scales.

We outline the main conclusions of our work below:

- We find that almost all HI in the Universe is inside halos: from more than 99% at z = 0 to around 88% at z = 5. The fraction of HI outside halos increases with redshift because the gas in the IGM is denser and the amplitude of the UV background decreases with redshift (at z > 2). This justifies the use of halo models to model the distribution of HI in the Universe, but quantifies their limitations at high redshifts. The fraction of HI inside galaxies is slightly lower than in halos. At  $z = 0 \simeq 97\%$  of all HI is inside galaxies while at z = 5 this number declines to  $\simeq 80\%$ .
- We find that the halo HI mass function, i.e. the average HI mass hosted by a halo of mass M at redshift z, is well reproduced by a function like

$$M_{\rm HI}(M,z) = M_0 \left(\frac{M}{M_{\rm min}}\right)^{\alpha} \exp\left(-(M_{\rm min}/M)^{0.35}\right)$$

where  $M_0$ ,  $M_{\min}$  and  $\alpha$  are free parameters. The

best-fit values are given in Table 1 for both FoF and FoF-SO halos. The value of  $\alpha$  increases with redshift, likely indicating that at low redshift processes such as ram-pressure, tidal stripping, and AGN feedback make galaxies in clusters HI poor. We find that  $M_{\rm min}$  decreases with redshift. On the other hand, only halos with circular velocities above around 30 km/s host a significant HI mass fraction. Although the fit is slightly worse, our halo HI mass function can also be well-reproduced by the function

$$M_{\rm HI}(M,z) = M_0 \left(\frac{M}{M_{\rm min}}\right)^{\alpha} \exp\left(-M_{\rm min}/M\right)$$

whose best-fit values are given in Table 6 to facilitate comparison with previous works.

• We find that the HI density profiles inside halos exhibit a large halo-to-halo variation. HI profiles are sensitive to the physical processes that occur in and around halos, such as AGN feedback and tidal stripping. The HI profile of small halos  $(M \lesssim 10^{12} \ h^{-1} M_{\odot})$  is not cuspy, but its amplitude saturates. This is expected as HI at high densities will turn into molecular hydrogen and then stars in short time periods. More massive halos exhibit holes in their centers. For galaxy groups this is mostly due to AGN feedback, while in galaxy clusters the holes are large and generated by a combination of AGN feedback, ram-pressure and tidal

stripping. We find that the average HI density profiles are universal and can be reproduced by an expression like

$$\rho_{\rm HI}(r) = \frac{\rho_0}{r^{\alpha_\star}} \exp(-r_0/r),$$
(38)

or

$$\rho_{\rm HI}(r) = \frac{\rho_0 r_s^3}{(r+3/4r_s)(r+r_s)^2} \exp(-r_0/r), \qquad (39)$$

where  $\rho_0$ ,  $\alpha_*$ ,  $r_0$  and  $r_s$  are free parameters. We fix value of  $\rho_0$  by requiring that  $M_{\rm HI}(M) = \int_0^{R_v} 4\pi r^2 \rho_{\rm HI}(r) dr$ , where  $R_v$  is the halo virial radius. The best-fit values for  $\alpha_*$ ,  $r_0$  and  $r_s$  can be found in table 2.

- We find that the HI mass in small/big halos is mostly located in its central/satellites galaxies. The fraction of the total HI mass in halos that is within the central galaxy decreases with halo mass, while the opposite trend takes place for the satellites. For halos of masses  $\sim 5 \times 10^{12} h^{-1} M_{\odot}$  the HI mass in the central galaxy is similar to that of the satellites, almost independent of redshift. The HI mass fraction in the central galaxy of clusters is negligible at z = 0. At high-redshift,  $z \ge 2$ , the fraction of the halo HI mass in satellites is roughly 20% for small halos  $M \in [10^{10} - 10^{11}] h^{-1} M_{\odot}$ .
- We find that the pdf of the HI density field is quite different from that of the matter field. In general, the HI pdf is broader, indicating that the HI is more clustered than matter. The amplitude of the pdf for low overdensities is higher for HI than for matter, indicating that HI voids are more empty than matter voids. At high-redshift the HI and matter density pdf can be well-reproduced by a lognormal, while at low-redshift the log-normal is not a good description of our results.
- We find that the HI column density distribution function is nearly constant across redshifts, in agreement with previous studies and with observations. In the redshift range  $z \in [2, 4]$  we find that the DLA cross-section depends on both halo mass and HI column density, and its mean value can be well reproduced by

$$\sigma_{\text{DLAs}}(M|N_{\text{HI}}, z) = AM^{\alpha} \left(1 - e^{-(M/M_0)^{\beta}}\right) \qquad (40)$$

where  $\alpha = 0.82$ ,  $\beta = 0.85 \log_{10}(N_{\rm HI}/{\rm cm}^{-2}) - 16.35$ ,  $A \cdot M_0 = 0.0141 \ h^{-2} {\rm kpc} M_{\odot}$  and the best-fit values of  $M_0$  are given in Table 3. We argued that the small dependence of the above relation on column density implies the bias of different absorbers will be very similar. We estimate the DLAs bias using two methods and find agreement with observations in both.

• We find that for small halos,  $M \lesssim 10^{12} h^{-1} h^{-1} M_{\odot}$ , the bulk velocities of HI inside halos trace very well, in modulus and direction, the peculiar velocity of the halos they reside in. On the other hand, for bigger halos,

we observe departures, in modulus and direction, between the HI and halo peculiar velocities. This happens because while for small halos most of the HI is in the central galaxy, for larger halos a significant HI mass is in satellites, whose peculiar velocities do not trace that of the halo.

• We find that the velocity dispersion of HI inside halos can be well reproduced by a simple powerlaw

$$\sigma(M) = \sigma_{10} \left(\frac{M}{10^{10} \ h^{-1} M_{\odot}}\right)^{\alpha}$$
(41)

where  $\sigma_{10}$  and  $\alpha$  are free parameters whose bestvalues are given in Table 4. While at z = 0 the mean velocity dispersions of CDM and HI are similar (for halos above  $\simeq 5 \times 10^{10} \ h^{-1} M_{\odot}$ ), at higher redshifts they depart for small halos, with HI having a lower amplitude than CDM. The mass where they diverge increases with redshift, but is typically around  $10^{12} \ h^{-1} M_{\odot}$ . In general, for fixed mass and redshift the variance in the velocity dispersion of HI is larger than that of CDM, reflecting the larger variation in HI profiles than CDM profiles inside halos.

- We find that the values of the HI bias on the largest scales we can probe is equal to 0.84, 1.49, 2.03, 2.56, 2.82 and 3.18 at redshifts 0, 1, 2, 3, 4 and 5, respectively. While the HI bias is relatively flat down to  $k \simeq 1 \ h \text{Mpc}^{-1}$  at z = 1, it is already non-linear at  $k \simeq 0.3 \ h \text{Mpc}^{-1}$  at  $z \ge 3$ . Our results suggest that the HI bias becomes more non-linear with redshift. This is expected as the value of the linear bias increases with redshift. We have shown the perturbative approaches based on LPT are able to reproduce the clustering measurement up to  $k = 1 h/\text{Mpc}^{-1}$ , therefore making possible, at least in principle, to extract cosmological information from such small scales.
- We identify a new secondary halo bias. Halos of the same mass are clustered differently depending on their HI mass. At low redshift HI-poor halos are more clustered than HI-rich halos. However, at high redshift the situation is reversed and HI richhalos cluster more strongly than HI-poor halos. We believe that this is mainly driven by environment. At low redshift, small halos may lose their gas due to stripping by a larger neighboring halo, so HIpoor halos will be more clustered than field HI-rich halos. On the other hand, at high redshift, gas stripping is likely less effective, so HI-rich halos will be found around larger halos and therefore their clustering will be higher.
- We quantify the amplitude of the HI shot-noise to be 104, 124, 65, 39, 14 and 7  $(h^{-1}\text{Mpc})^3$  at redshifts 0, 1, 2, 3, 4 and 5, respectively. These low levels imply that BAO measurements through 21 cm intensity mapping are hardly affected by shotnoise. Furthermore, the very low shot-noise levels at high redshift suggest that a large amount of cosmological information can be extracted from the clustering of HI on small scales.

- We find that the relation between  $\rho_{\rm m}$  and  $\rho_{\rm HI}$  cannot be explained with linear theory for smoothing scales  $\leq 5 \ h^{-1}$ Mpc at any redshift. The scatter in that relation decreases with redshift, and much larger HI overdensities can be found for the same matter overdensities.
- We find that the Kaiser factor alone cannot explain clustering of HI in redshift-space at low redshift, as expected, given the small volume of our simulations. But, at high redshift the ratio between the monopoles in redshift- and real-space can be explained with linear theory down to 0.3, 0.5 and 1 hMpc<sup>-1</sup> at redshifts 3, 4 and 5 respectively. This is rather surprising taking into account that the HI bias becomes non-linear already at k = 0.3 hMpc<sup>-1</sup> at those redshifts.
- We find that the 2-dimensional HI power spectrum in redshift-space exhibits large differences with respect to the matter field. Those differences arise mainly because the amplitude of Fingers-of-God is higher for HI than for matter. This can be understood taking into account that HI resides only in relatively massive halos. While the amplitude of the matter power spectrum on small scales is dominated by small halos with low velocity dispersion, for HI halos only above  $\simeq M_{\min}$ , i.e. with larger velocity dispersion, can contribute. We find that standard phenomenological models to describe the clustering in 2D in redshift-space are not adequate for reproducing our results.
- We show that accurate 21 cm maps can be created from N-body simulations, rather than full hydrodynamic simulations, by using the ingredients studied in our work. In real-space and without mod-

eling the 1-halo term, the agreement in the shape of the 21 cm power spectrum from N-body and IllustrisTNG is around 5% down to 1 hMpc<sup>-1</sup> at all redshifts. In redshift-space however, the lack of the 1-halo term, i.e. the HI Fingers-of-God, induces much larger errors in the 21cm power spectrum from N-body versus hydro at low redshift, e.g. 45% at z = 1. Modeling the 1-halo term is thus crucial for creating mock 21 cm maps.

The HI properties investigated in this work will help to improve our knowledge of the way neutral hydrogen is distributed across the Universe. The different quantities we have studied can be used as input to analytic approaches like HI halo models or to create very accurate mock 21 cm maps.

The python/cython scripts written to carry out the analysis performed in our work can be found in https://github.com/franciscovillaescusa/ Pylians/tree/master/HI\_Illustris. Our scripts made use of the PYLIANS python routines, publicly available at https://github.com/franciscovillaescusa/ Pylians.

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## APPENDIX

# TIME EVOLUTION OF HI IN THE INTERGALACTIC MEDIUM

In section 4 we found that while at  $z \leq 2$  most of the Universe HI mass is inside halos, at higher redshift an increasing fraction of it is located outside halos. In order to visualize this effect we show in Fig. 26 the spatial distribution of HI in a slice of 5  $h^{-1}$ Mpc width across 10x10 ( $h^{-1}$ Mpc)<sup>2</sup>. We show in that figure HI column density in comoving units to facilitate the comparison across redshifts. We note that our color palette may produce the incorrect impression that at z = 5 there is much more HI than at z = 0. We have explicitly checked that the sum of all column densities across all pixels in our figures give a similar value across redshift, indicating that  $\Omega_{\rm HI}$  is very similar in all panels.

It can be seen that at low redshift, most of the HI mass is inside galaxies, while the hydrogen in the filaments is highly ionized. At higher redshifts, on the other hand, the gas in the intergalactic medium becomes denser and the filaments contain a larger amount of HI. The lower amplitude of the UV background at those redshifts facilitates gas self-shielding. Given these effects it is thus natural that the fraction of HI outside dark matter halos increases with redshift.

## ORIGIN OF THE CUTOFF IN THE HALO HI MASS FUNCTION

We saw in section 5 that the halo HI mass function exhibits a cutoff at low masses. In this appendix we shed light on the physical origin of that feature.

The lack of HI gas in small halos may be due to: 1) a deficit in the abundance of gas in those halos, 2) gas being present but highly ionized, or a mixture of 1) and 2). We quantify the gas content of dark matter halos in TNG100 by computing their gas fraction, i.e. the ratio between the gas mass to the total mass. In the left panel of Fig. 27 we show the average gas fraction as a function of halo mass at different redshifts. In this plot we show results only for halos whose masses are above the mass of 50 CDM particles.

We find that the gas fraction of the smallest halos shown at high redshifts is around  $\sim 0.12$ . As we go to higher halo masses, some stars form and supernova feedback expel the gas of these halos. In even more massive halos the gravitational potential is deeper and hence the mass-loading factors of galactic winds in the TNG model are lower,

![](_page_34_Figure_1.jpeg)

Figure 26. Spatial distribution of HI in a slice of 10x10x5  $(h^{-1}\text{Mpc})^3$  at redshifts 0 (top-left), 1 (top-right), 2 (middle-left), 3 (middle-right), 4 (bottom-left) and 5 (bottom-right). The color indicates the HI column density in comoving cm<sup>-2</sup> units, to facilitate the comparison across redshifts. The region shown is the same as that in Fig. 1 (top and middle panels). At higher gas densities the column densities of HI are higher in the intergalactic medium. It can be seen that some filaments host a significant HI mass at high-redshift, while at low redshift the HI is mostly locked inside galaxies. This explains why the fraction of HI outside halos increases with redshift.

 $h^{-1}{\rm Mpc}$ 

 $h^{-1}{\rm Mpc}$ 

![](_page_35_Figure_1.jpeg)

Figure 27. Average gas fraction (left) and average HI mass to gas mass ratio (right) in halos as a function of their mass at redshifts 0 (blue), 1 (green), 2 (red), 3 (purple), 4 (yellow) and 5 (cyan) in IllustrisTNG. We show results only for halos with masses larger than 50 CDM particles. The stars indicate the hard cutoff mass (i.e. halos below that mass contain *only*2% of all HI inside halos). The gas content of small halos declines with time. The features we observe in the plot are due to: 1) supernova feedback (removes gas form large halos) and 3) the UV background (reduces the gas content of small halos). The dashed black line shows the cosmological baryon fraction,  $\Omega_{\rm b}/\Omega_{\rm m}$ . It can be seen that halos at the hard cutoff mass have a very different gas fraction, while almost all of them have the same HI to gas mass ratio. Thus, the lack of HI gas in small halos is more related to gas being ionized than a lack of gas.

rendering it more difficult for supernova feedback to eject gas from halos. This explains the dip we observe around  $5 \times 10^9 \ h^{-1} M_{\odot}$  halos at high-redshift. In halos with masses above  $\sim 3 \times 10^{11} \ h^{-1} M_{\odot}$ , AGN feedback becomes effective at expelling their gas, explaining the peak at around that mass. Finally, as we go to even higher mass halos, a smaller fraction of the gas can be expelled by AGN feedback since the gravitational potential becomes deeper, explaining the dip around  $3 \times 10^{12} \ h^{-1} M_{\odot}$  halos.

It is interesting to note that the gas fraction of small halos decreases quickly with redshift. We will see below that this is caused by the UV background. At low redshift, the gas fraction of small halos is small, so it is reasonable to expect that very little HI is found in those halos. However, as we go to higher redshifts, the gas fraction of halos at the hard cutoff mass  $M_{\text{hard}}$  (defined such that halos with masses below  $M_{\text{hard}}$  host only 2% of all HI that is in halos, see Eq. 14) is rather large. We show this with colored stars in that figure. Thus, the cutoff in the halo HI mass function cannot be explained, at high-redshift, by the lack of gas in halos. A better explanation is that the gas in these halos is highly ionized.

The average HI mass to gas mass ratio is shown in the right panel of Fig. 27. We find that halos at the hard cutoff mass  $M_{\text{hard}}$  exhibit similarly low HI to gas mass fractions across redshifts:  $\simeq 5\%$ . Thus, while there is a significant amount of gas in these halos at high-redshift, HI formation is impeded, likely due to the gas being at high temperature and diffuse. The low HI to gas mass ratio shows up at all redshifts for low mass halos. However, this is the case particularly at low redshift, where the HI to gas mass fraction of small halos is practically zero, showing how difficult it is to form HI in these halos. We speculate that this is related to the fact that for fixed halo mass, the density of gas and CDM increases with redshift. Thus, for example, while for halos with masses  $\simeq 10^9 h^{-1} M_{\odot}$  the gas fraction increases by only  $\simeq 60\%$  from z = 3 to z = 5, the HI to gas mass ratio changes by more than 400\%, showing how denser gas enables the formation of HI.

We thus conclude that the reason why there is almost no HI in small halos is because the gas in these halos is highly ionized, presumably because its low density and high-temperature prevents HI formation.

It is interesting to understand why the gas fraction of small halos decreases with redshift. We argue that this effect is due to the UV background. In order to demonstrate our claim we have run three hydrodynamic simulations with radiative cooling and star formation but without feedback (neither galactic winds nor AGN). In two of them, no heating by the UV background is included, one with  $2 \times 256^3$  CDM+baryon resolution elements and another with  $2 \times 512^3$  CDM+baryon resolution elements. In the third one, we have heating by the UV background with  $2 \times 512^3$ CDM+baryon resolution elements. In all cases the simulation box is  $25 h^{-1}$ Mpc across.

We have computed the average baryon fraction, i.e. the mass in gas and stars over the total mass, in these simulations and show the results in Fig. 28. The top panel shows the baryon fraction for these simulations and TNG100 at z = 0. We find that in simulations without feedback, the gas content of small halos exhibits a cutoff that occurs at higher masses when the UVB is present.

The bottom panels of Fig. 28 show the time evolution of the average baryon fraction as a function of halo mass. It can be seen that in both types of simulations, with and without UV background, the gas fraction of small halos decreases with redshift. We speculate that in the case of no UV background, many small halos lie in the vicinity of

![](_page_36_Figure_1.jpeg)

Figure 28. We show the average baryon fraction, i.e. the fraction of the mass in baryons (gas+stars) over the total mass in halos, as a function of halo mass. In the upper panel we show results at z = 0 for three different simulations: 1) a simulation with  $2 \times 256^3$  resolution elements and no UV background (green), 2) a simulation with  $2 \times 512^3$  resolution elements and no UV background (blue), and 3) a simulation with  $2 \times 512^3$  resolution elements and UV background (blue). All simulations are in a box of  $25 h^{-1}$ Mpc size and no feedback is incorporated in any of them. The bottom panels display the results for the simulations with  $2 \times 512^3$  with (right) and without (left) at different redshifts. The dashed black line indicates the cosmic baryon fraction,  $\Omega_b/\Omega_m$ . Since the values of the cosmological parameters are slightly different between IllustrisTNG and the other simulations, we show two horizontal lines in the upper panel. It can be seen that the presence of the UV background removes the baryonic, and therefore also the HI, content of small halos. It is interesting that even if the UV background is not present, very small halos exhibit a deficit in their baryon fraction.

massive halos, whose presence can strip the gas from these small halos, and further, that the same mechanism may explain the dependence of halo clustering on HI mass we described in section 14.

The effect of the UV background on the baryon fraction of small halos is more pronounced, as can be seen in the bottom-right panel of Fig. 28. We believe that the reason for this behavior is that the hot intergalactic gas cannot cluster in small halos since their gravitational potential is not deep enough (Okamoto et al. 2008; Bose et al. 2018).

We thus conclude that at low redshift, small halos have a low gas fraction. There are several mechanisms that can remove the gas from such halos, such as tidal stripping by neighbors, the heating of the intergalactic medium by the UV background and supernova feedback. Our results suggest the most effective one for the lowest masses is the presence of the UV background. The little gas inside those halos is highly ionized, so no HI is found within them.

## HI CONTENT IN FOF VERSUS FOF-SO HALOS

We found in section 4 that the HI mass inside FoF and FoF-SO halos is quite different. Here, we determine the reason for this difference.

We have computed the total mass inside FoF and FoF-SO halos, and we find that the former host ~ 9% more mass than the latter at z = 0. This difference is almost equal to the deficit in HI mass we find between FoF-SO and FoF halos at that redshift (see Fig. 3). Similar results hold at higher redshift, where the differences in total mass and HI are slightly larger ( $\simeq 25\%$  at z = 5). This indicates that the deficit in HI mass we find in FoF-SO halos with respect to FoF is simply due to the fact that the latter host a larger total mass, and therefore more HI.

We note however that there are some situations where the difference in HI mass can be much larger than the

![](_page_37_Figure_1.jpeg)

Figure 29. Comparison between the gas and HI content in FoF versus FoF-SO halos. The images show the column density of gas (left) and HI (right) from the cells belonging to a FoF halo of mass  $5 \times 10^{13} h^{-1} M_{\odot}$  at z = 0. The white circle shows the position of the halo center and its SO radius. While the gas content in the FoF and SO halo are similar, the FoF halo has almost a factor of 2 more HI than the SO halo.

		FoF		FoF-SO			
z	$\alpha$ $M_0$		$M_{\min}$	α	$M_0$	$M_{\min}$	
		$[h^{-1}M_{\odot}]$	$[h^{-1}M_{\odot}]$		$[h^{-1}M_{\odot}]$	$[h^{-1}M_{\odot}]$	
0	$0.49\pm0.03$	$(2.1 \pm 0.7) \times 10^9$	$(5.2 \pm 1.3) \times 10^{10}$	$0.42\pm0.03$	$(2.4 \pm 0.8) \times 10^9$	$(5.6 \pm 1.4) \times 10^{10}$	
1	$0.76\pm0.03$	$(4.6 \pm 2.1) \times 10^8$	$(2.6 \pm 1.0) \times 10^{10}$	$0.67\pm0.04$	$(6.5 \pm 3.5) \times 10^8$	$(3.3 \pm 1.5) \times 10^{10}$	
2	$0.80\pm0.03$	$(4.9 \pm 2.1) \times 10^8$	$(2.1 \pm 0.7) \times 10^{10}$	$0.72\pm0.03$	$(5.9 \pm 2.7) \times 10^8$	$(2.4 \pm 0.9) \times 10^{10}$	
3	$0.95\pm0.03$	$(9.2 \pm 4.7) \times 10^7$	$(4.8 \pm 1.9) \times 10^9$	$0.90\pm0.03$	$(1.0 \pm 0.6) \times 10^8$	$(5.5 \pm 2.3) \times 10^9$	
4	$0.94\pm0.02$	$(6.4 \pm 3.7) \times 10^7$	$(2.1 \pm 1.0) \times 10^9$	$0.82\pm0.03$	$(1.6 \pm 0.8) \times 10^8$	$(4.5 \pm 1.9) \times 10^9$	
5	$0.90\pm0.02$	$(9.5 \pm 5.8) \times 10^7$	$(1.9 \pm 1.0) \times 10^9$	$0.84\pm0.04$	$(1.1 \pm 0.9) \times 10^8$	$(2.6 \pm 1.7) \times 10^9$	

## Table 6

We find that an expression like  $M_0 x^{\alpha} \exp(-1/x^{0.35})$ , where  $x = M/M_{\min}$ , reproduces our results well for the halo HI mass function,  $M_{\rm HI}(M, z)$ . In the past, expressions like  $M_0 x^{\alpha} \exp(-1/x)$  have been widely used to model that quantity. In this work we find that the latter reproduces well the high-mass end of  $M_{\rm HI}(M, z)$  but it underestimates the low-mass end. However, that expression still provides a good  $\chi^2$  when fitting our results. In order to help in comparisons with previous works, we provide here the best-fit values for  $\alpha$ ,  $M_0$  and  $M_{\min}$  when fitting our halo HI mass function with  $M_0 x^{\alpha} \exp(-1/x)$ . The left/right part shows the results for the FoF and FoF-SO halos.

difference in total mass. We illustrate one of these situations in Fig. 29. We have selected the gas cells belonging to a FoF halo of mass  $M = 5 \times 10^{13} h^{-1} M_{\odot}$  at redshift z = 0. The total mass inside the FoF and FoF-SO halos are nearly the same, while the HI masses vary by a factor of 2. In Fig. 29 we plot the column density of gas and HI from the gas cells belonging to that halo. In the same plot, we mark the radius of the corresponding FoF-SO halo with a white line. It can be seen that, while most of the gas in the FoF halo is inside the virial radius of the SO halo, the situation is quite different for HI. The HI mass outside the SO radius is almost equal to the one inside. The reason is that the FoF algorithm links the external galaxies to the main halo, and these galaxies are rich in HI. We have found that this situation is usual for the most massive halos at each redshift.

### HALO HI MASS FUNCTION

In section 5 we found that the halo HI mass function,  $M_{\rm HI}(M, z)$ , from IllustrisTNG can be well reproduced by a fitting formula like  $M_0 x^{\alpha} \exp(-1/x^{0.35})$ , where  $x = M/M_{\min}$ . In the literature, however, an expression of the type  $M_0 x^{\alpha} \exp(-1/x)$  has been widely used, (e.g. Bagla et al. 2010; Castorina & Villaescusa-Navarro 2017; Obuljen et al. 2017a; Villaescusa-Navarro et al. 2017; Pénin et al. 2018a; Padmanabhan et al. 2017). We have fit our results to that function, and while the reduced  $\chi^2$  is larger than with our fiducial function, it is still a good fit to the underlying data. We thus provide in Table 6 the best-fit values of the parameters  $\alpha$ ,  $M_0$  and  $M_{\min}$  of the latter expression in order to help in the comparison with previous works. We note that the value of  $M_{hard}$ , i.e. the hard cutoff mass (see section 5), is not affected by using a different parametrization for the halo HI mass function. Thus, the values we quote in Table 1 are valid also here.

#### FIT TO HI PROFILES

The points with error bars in Fig. 30 show the mean HI density profiles within halos of different halo masses at different redshifts (the are the same as the blue lines in Fig. 6). The solid lines represent the best-fit obtained when we fit those results with a HI density profile as

$$\rho_{\rm HI}(r) = \frac{\rho_0 r_s^3}{(r+3/4r_s)(r+r_s)^2} \exp(-r_0/r).$$
(E1)

In each panel of the plot we show the best-fit value of  $r_s$ ,  $r_0$  and the value of the reduced  $\chi^2$ . The value of  $\rho_0$  is fixed by requiring that  $M_{\rm HI} = 4\pi \int_0^{R_v} r^2 \rho_{\rm HI}(r) dr$ , where  $R_v$  is the halo virial radius. REFERENCES

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![](_page_39_Figure_2.jpeg)

Figure 30. Each panel shows the mean and standard deviation of the HI profiles for halos in the mass range indicated in the upperleft part. We fit the results using the form  $\rho_{\rm HI}(r) = \exp(-r_0/r)\rho_0 r_s^3/[(r+3/4r_s)(r+r_s)^2]$ , where  $\rho_0$ ,  $r_s$  and  $r_0$  are free parameters. The best-fit is shown with a solid line. The dashed region represents the error on the fit. The value of  $\rho_0$  is fixed by requiring that  $M_{\rm HI} = 4\pi \int_0^{R_v} r^2 \rho_{\rm HI}(r) dr$ , where  $R_v$  is the halo virial radius. Each panels show the best-fit values of  $r_0$  and  $r_s$  and the value of  $\chi^2$ .

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