

Unveiling the population of massive quenched galaxies at $z \geq 2$ in the COLIBRE simulations – I. Galaxy demographics

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Accepted 2026 July 28. Received 2026 July 28; in original form 2025 December 17

ABSTRACT

The *James Webb Space Telescope* has uncovered a substantial population of Massive ($M_\star > 10^{10} M_\odot$), Quenched Galaxies (MQGs) in the early Universe ($z \geq 2$), whose properties challenge current galaxy formation models. In this series, we examine this population of MQGs within the new COLIBRE cosmological hydrodynamical simulations, which introduce key innovations in their sub-grid physics. In this first paper, we find a dependence of MQG number densities on both mass resolution and the Active Galactic Nucleus feedback implementation, as well as a significant impact from potential observational uncertainties. Using the fiducial $(200 \text{ cMpc})^3$ volume L200m6 simulation, which provides adequate volume, mass, and spatial resolution to study these systems, we report number densities and stellar mass functions in broad agreement with the latest observations. The predicted quenching and formation time-scales are qualitatively consistent with observational inferences, indicating extended formation (medians $t_{50} \approx 0.5\text{--}1.5 \text{ Gyr}$) followed by rapid quenching (medians $t_q \lesssim 0.6 \text{ Gyr}$) with strong starburst episodes. Leveraging the state-of-the-art physics in COLIBRE, the model predicts that MQGs have dust and H_2 fractions more than 1 dex lower than their massive star-forming counterparts; generally consistent with the (scarce) observational estimates. MQGs and massive star-forming systems show broadly similar stellar sizes and kinematics, suggesting that size or morphological transformations occur after quenching in COLIBRE. Our results provide robust predictions for MQGs and show that tensions with observations are reduced when an effective observational uncertainty is forward-modelled.

Key words: methods: numerical – galaxies: evolution – galaxies: formation – galaxies: high-redshift.

1 INTRODUCTION

The *James Webb Space Telescope* (*JWST*) has ushered in a new era in observational astronomy, thanks to its high sensitivity and resolution, providing an unprecedented view of the early Uni-

verse (see e.g. A. Adamo et al. 2025, for a review). The first *JWST* results revealed a surprisingly large population of Massive, Quenched Galaxies (hereafter MQGs) at high redshift ($z > 3$), with stellar masses $M_\star > 10^{10} M_\odot$ and negligible star formation (T. Nanayakkara et al. 2022; A. C. Carnall et al. 2023). Such galaxies had already been detected (J. Dunlop et al. 1996; A. Cimatti et al. 2004; K. Glazebrook et al. 2017; C. Schreiber et al. 2018; F. Valentino et al. 2020; J. R. Weaver et al. 2022), but *JWST* showed

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that their number densities are higher than previously thought, that older MQGs exist and that they are found at even higher redshifts (A. Weibel et al. 2025), implying that this population is not as rare as once believed.

The high number densities inferred from the first *JWST* observations were initially difficult to reconcile with the hierarchical Λ cold dark matter (hereafter Λ CDM) model; these objects appeared too massive for the early epochs at which they are detected and would require implausibly high star formation efficiencies (M. Boylan-Kolchin 2023). However, as observational samples have grown, through large photometric surveys (e.g. W. M. Baker et al. 2025c; S. D. Stevenson et al. 2026) and spectroscopic confirmations (e.g. T. Nanayakkara et al. 2025; Y. Zhang et al. 2026) extending to $z \gtrsim 2$, the inferred number densities have consistently decreased, easing much of the tension. In fact, the initially reported high number densities by A. C. Carnall et al. (2023) have since been revised downward in light of more recent analyses. However, they remain more than a factor of 2 higher than earlier ground-based estimates. New surveys are beginning to unveil the diverse properties of MQGs, extending stellar mass and star formation rate (SFR) measurements to include dust content (M. M. Lee et al. 2024), sizes (L. Kawinwanichakij et al. 2026) and kinematics (R. G. Pascalau et al. 2026), and they are enabling comparisons with lower- z counterparts.

The short time-scales on which MQGs form and quench are also puzzling. Spectroscopic observations indicate that some quenched systems must have formed rapidly, as early as when the Universe was about or even less than one Gyr old (with examples at $z \approx 11$; K. Glazebrook et al. 2024). These studies suggest that strong starburst episodes drive this early mass assembly (B. Forrest et al. 2020). In the local Universe, feedback processes explain the quiescent state of galaxies (e.g. A. Man & S. Belli 2018); these include internal mechanisms such as supernova (SN) and active galactic nucleus (AGN) feedback and external influences such as interactions with, and regulation by, the environment. SN feedback is insufficient to quench massive systems and predominantly affects lower-mass galaxies (A. J. Benson et al. 2003), even at high redshifts (e.g. V. Gelli et al. 2023); while it is believed that environment is already important at high redshifts (e.g. S. Jin et al. 2024), its role in quenching massive galaxies seems to be minor (e.g. S.-K. Lee et al. 2015; M. Shuntov et al. 2026). Given the short quenching time-scales of MQGs, AGN feedback is therefore considered the most plausible mechanism. This process involves the injection of energy and momentum by central supermassive black holes (BHs) into their surroundings and is supported by growing observational evidence of AGN activity in these systems (M. Martínez-Marín et al. 2024; F. D'Eugenio et al. 2024; M. Park et al. 2024; S. D. Stevenson et al. 2026; W. M. Baker et al. 2025a).

The last decade has witnessed a remarkable growth in galaxy formation simulations that model statistical samples of galaxies within cosmological volumes, capable of producing population properties that are in broad agreement with observations of galaxies in the local Universe (e.g. J. Schaye et al. 2015; A. Pillepich et al. 2018). They accomplish this by calibrating parametrized sub-grid models for, e.g. BH growth and feedback, to recover particular sets of observational data (e.g. R. A. Crain et al. 2015; E. Chaikin et al. 2026a), typically from low-redshift galaxy surveys, while still enabling genuine predictions for other galaxy properties. Such simulations provide an ideal framework to test what role AGN feedback plays in quenching MQGs at high redshift, and to connect them to their low- z descendants, a link that is

difficult to establish observationally (see e.g. the reviews by R. S. Somerville & R. Davé 2015; R. A. Crain & F. van de Voort 2023).

Because of this, a plethora of simulation studies has increasingly produced predictions for these passive systems in recent years to help interpret the *JWST* observations. These efforts span a wide range of galaxy formation and evolution models with different sub-grid physics implementations: large-volume hydrodynamical simulations such as ILLUSTRISTNG (A. I. Hartley et al. 2023; S. Kurinchi-Vendhan et al. 2024), MAGNETICUM (L. C. Kimmig et al. 2025; R.-S. Remus & L. C. Kimmig 2025) or SIMBA-C (J. Szpila et al. 2025); zoom-in hydrodynamical simulations such as FLARES (C. C. Lovell et al. 2023; C. Turner et al. 2025) or THESAN (H. G. Chittenden et al. 2026); semi-analytical models such as SHARK v2.0 (C. d. P. Lagos et al. 2024) or GAEA (G. De Lucia et al. 2024; L. Xie et al. 2024); as well as comparisons between multiple modelling approaches (P. Lustig et al. 2023; C. d. P. Lagos et al. 2025; E. J. Weller et al. 2025). These studies reveal substantial differences between models, primarily arising from variations in AGN feedback implementations (C. d. P. Lagos et al. 2025), and in some cases from numerical limitations such as limited statistics due to small simulation volumes and finite spatial resolution. Moreover, these models continue to struggle to reproduce the observational properties of these systems, most notably their abundance, in general underpredicting the observed number densities at $z \gtrsim 4$. Discrepancies also remain in reproducing their stellar mass distribution and other physical properties (e.g. C. d. P. Lagos et al. 2025; W. M. Baker et al. 2025c). Together, these factors have so far limited the ability of current simulations to provide a consistent and comprehensive description of MQGs.

We present here a series of papers, including this work (Paper I), and Á. Chandro-Gómez et al. (2026, hereafter *Paper II*), intended to be read together, where we investigate the properties and origins of MQGs at high redshift in the new COLIBRE cosmological hydrodynamical simulations (E. Chaikin et al. 2026a; J. Schaye et al. 2026). COLIBRE introduces several advances over previous cosmological simulations, including the self-consistent modelling of a cold molecular phase in the interstellar medium (ISM) coupled to live dust grains, together with updated BH growth and AGN feedback prescriptions. E. Chaikin et al. (2026b) show that the evolution of the galaxy stellar mass function (SMF) in COLIBRE is reproduced across the full redshift range ($z = 0 - 12$) for which observational data are available. That work presents the first results on the abundance of MQGs in these simulations, demonstrating good agreement with *JWST* data. In this first paper of the series, we extend this initial investigation with a more comprehensive analysis of the COLIBRE MQGs, providing further details on their abundance and assessing whether the COLIBRE model can reproduce the many other key characteristics of MQGs as revealed by recent *JWST* surveys. We focus on a comprehensive set of galaxy properties, including stellar masses, SFRs, dust and molecular gas content, stellar sizes and kinematics; and compare them with the latest observational constraints. In *Paper II*, we identify the physical mechanisms responsible for their rapid formation and quenching. By tracing the evolutionary histories of individual MQGs, we explore the role of BH growth and their associated AGN feedback, as well as environmental factors in driving quenching of these systems. The tracking is performed down to $z = 0$, enabling us to examine the fate of MQGs after quenching.

The structure of this first paper is as follows. In Section 2, we describe the COLIBRE simulations and their sub-grid physics

models. Section 3 outlines our sample selection, as well as the properties analysed in this work. Predictions across a range of observables, including number densities, SMFs, star formation histories (SFHs), dust and molecular gas fractions, sizes and kinematics, are presented and compared with observations in Section 4. Finally, Section 5 summarizes our results.

2 THE COLIBRE SIMULATION SUITE

For this analysis, we use the new COLIBRE¹ large-volume cosmological hydrodynamical simulations (E. Chaikin et al. 2026a; J. Schaye et al. 2026). The COLIBRE suite comprises several simulations that vary in volume (periodic box size of $L = 25 - 400$ cMpc per side), resolution (mean initial gas particle mass, m_g , and mean DM particle mass, m_{DM} , $\sim 10^5 - 10^7 M_\odot$), and AGN feedback model (either fiducial thermal or hybrid thermal + jet). Table 1 summarizes the simulation set used in this analysis, which allows us to assess how resolution, volume, and feedback variations influence the properties of MQGs. Among these, we adopt the L200m6 simulation as our fiducial choice, as it offers the best compromise between volume ($L = 200$ cMpc per side), sufficient to sample rare MQGs, and resolution (m_g and $m_{DM} \sim 10^6 M_\odot$), adequate to capture their internal structure more accurately. The relatively small gravitational softening lengths (ϵ_{com} and ϵ_{prop}) of this run are important for more reliably analysing galaxy sizes and kinematics, as discussed in Section 4.5 and Appendix E.

2.1 Simulation methods

The initial conditions (ICs) are generated with MONOFONIC (O. Hahn et al. 2020; M. Michaux et al. 2021) and evolved using the SWIFT code (M. Schaller et al. 2024). The density field is sampled with cold DM and baryonic particles, with the latter initially representing gas but able to convert into collisionless stellar or BH particles. To suppress spurious energy transfer between DM and stellar particles, the ICs of the simulations contain four times more DM particles than baryonic ones (A. D. Ludlow et al. 2019). Stellar and gas particles can increase or decrease their mass due to stellar mass-loss. Gas particles exceeding $4 m_g$ are split into two nearly co-spatial equal-mass particles to avoid baryonic particles with very different masses. Gravity is solved with a 4th-order fast multipole method (W. Dehnen 2014) and softened using a kernel with a functional form given by H. Wendland (1995), while hydrodynamics is handled with the SPHENIX implementation of smoothed particle hydrodynamics (SPH) (J. Borrow et al. 2022) using a quartic spline kernel. The simulations are run from $z = 63$ to $z = 0$, adopting the DES Y3 ‘3x2pt + All Ext.’² Λ CDM cosmology (T. M. C. Abbott et al. 2022): $h = 0.681$, $\Omega_\Lambda = 0.693922$, $\Omega_m = 0.306$, $\Omega_{CDM} = 0.256011$, and $\Omega_b = 0.0486$.

Between $z = 30$ and $z = 0$, the simulations output 36 full snapshots and 92 reduced ‘snapshots’ (which record only BH properties and a limited subset of gas and stellar properties). Haloes are

first identified with a friends-of-friends (FoF) algorithm that links DM particles separated by less than 0.2 times the mean interparticle distance, with baryonic particles attached to the nearest DM neighbour. FoF groups with fewer than 32 particles are discarded. Subhaloes are then identified using the HBT-HERONS code (V. J. Forouhar Moreno et al. 2025), an extension of HBT + (J. Han et al. 2018), which tracks the most bound particles of each structure from the time it was first identified. This explicit temporal tracking improves detection of substructures near halo centres (V. J. Forouhar Moreno et al. 2025) and prevents unphysical mass fluctuations in merger trees (Á. Chandro-Gómez et al. 2025). Finally, the SOAP code (R. McGibbon et al. 2025) computes halo, subhalo and galaxy properties across multiple 3D and projected apertures, defined either by fixed sizes (e.g. 1, 10, 50 pkpc) or overdensity thresholds (e.g. 200 times the mean density of the Universe, 200 or 500 times the critical density of the Universe), using all or only the bound particles.

2.2 Sub-grid prescriptions

Compared to other large-volume hydrodynamical simulations, COLIBRE introduces key innovations in its sub-grid prescriptions, which capture processes occurring below the simulation’s spatial resolution. These improvements are briefly outlined below, although we refer the reader to J. Schaye et al. (2026) and the individual papers describing each sub-grid model for a detailed discussion. The parameters of these models are calibrated (E. Chaikin et al. 2026a; F. Huško et al. 2026) to reproduce the $z = 0$ galaxy SMF (S. P. Driver et al. 2022), galaxy sizes (J. A. Hardwick et al. 2022), and BH masses (A. W. Graham & N. Sahu 2023). The hybrid AGN feedback model additionally incorporates the $z = 0.2$ bolometric AGN luminosity function (X. Shen et al. 2020) as a calibration constraint. Each COLIBRE resolution and AGN feedback model uses a separate calibration (see table 1 in J. Schaye et al. 2026).

(i) *Radiative cooling*: unlike most other hydrodynamical simulations that impose an effective equation of state to model the ISM, COLIBRE explicitly tracks the chemical processes in the cold ISM, allowing gas to cool down to ≈ 10 K using the HYBRID-CHIMES model (S. Ploekinger et al. 2025). HYBRID-CHIMES uses the CHIMES reaction network (A. J. Richings, J. Schaye & B. D. Oppenheimer 2014a, b) to compute radiative cooling and heating rates, treating hydrogen and helium in full non-equilibrium and metals in equilibrium with corrections for non-equilibrium free electrons.

(ii) *Dust*: the formation and evolution of dust grains is modelled directly on-the-fly, explicitly tracking three grain species and two grain sizes (J. W. Trayford et al. 2026). Grains are nucleated in the ISM by ejecta from asymptotic giant branch (AGB) stars (F. Dell’Agli et al. 2017), as well as by core collapse SNe (CCSNe; S. Zhukovska, H. P. Gail & M. Tieloff 2008). In the ISM, grains grow by accretion (H. Hirashita & N. V. Voshchinnikov 2014), primarily in molecular clouds, and are destroyed through sputtering (J. C. Tsai & W. G. Mathews 1995), astration, and feedback shocks. Grain sizes evolve via coagulation (S. Aoyama et al. 2017) and shattering (G. L. Granato et al. 2021). The dust model is coupled to the radiative cooling module, so that reactions and cooling rates account for dust presence and properties.

(iii) *Star formation*: star formation follows the local gravitational instability criterion from F. S. J. Nobels et al. (2024). SFRs of gas particles that satisfy this criterion are calculated using

¹<https://colibre-simulations.org/>

²Maximum-posterior likelihood values from the Dark Energy Survey year three (DES Y3) assume a spatially flat universe and combine constraints from three two-point correlation functions: cosmic shear, galaxy clustering, and galaxy-galaxy lensing, with external data from baryon acoustic oscillations (BAO), redshift-space distortions, type Ia SNe, and Planck observations of the Cosmic Microwave Background (CMB) (including CMB lensing), big bang nucleosynthesis, and local measurements of the Hubble constant.

Table 1. COLIBRE hydrodynamical simulations used in this work. L : the periodic box size in comoving Mpc (cMpc); N_b : the initial number of baryonic particles in the volume; N_{DM} : the number of DM particles in the volume; m_g : the mean initial gas particle mass in $M_\odot$; m_{DM} : the mean DM particle mass in $M_\odot$; ϵ_{com} : the gravitational softening length in ckpc; ϵ_{prop} : the maximum gravitational softening length in proper kpc (pkpc); and the type of AGN feedback implemented (thermal or hybrid including thermal + jet); $N_{MQ}(z=3)$: the number of MQGs selected at $z=3$ using the criteria defined in Section 3.1. We highlight in bold the simulation adopted as fiducial in this work.

COLIBRE sim.	$L/cMpc$	N_b	N_{DM}	$m_g/M_\odot$	$m_{DM}/M_\odot$	$\epsilon_{com}/ckpc$	$\epsilon_{prop}/pkpc$	AGN feedback model	$N_{MQ}(z=3)$
L050m5	50	1504 ³	4×1504^3	2.30×10^5	3.03×10^5	0.9	0.35	thermal	2
L100m5	100	3008 ³	4×3008^3	2.30×10^5	3.03×10^5	0.9	0.35	thermal	12
L100m6	100	1504 ³	4×1504^3	1.84×10^6	2.42×10^6	1.8	0.7	thermal	79
L200m6	200	3008³	4×3008^3	1.84×10^6	2.42×10^6	1.8	0.7	thermal	470
L200m7	200	1504 ³	4×1504^3	1.47×10^7	1.94×10^7	3.6	1.4	thermal	1527
L400m7	400	3008 ³	4×3008^3	1.47×10^7	1.94×10^7	3.6	1.4	thermal	12359
L100m6h	100	1504 ³	4×1504^3	1.84×10^6	2.42×10^6	1.8	0.7	hybrid (thermal + jet)	5
L200m7h	200	1504 ³	4×1504^3	1.47×10^7	1.94×10^7	3.6	1.4	hybrid (thermal + jet)	310

a M. Schmidt (1959) law with a fixed efficiency of gas-to-stars conversion per free-fall time of 1 per cent. This model reproduces the Kennicutt–Schmidt relation (R. C. Jr Kennicutt 1998) self-consistently at kpc scales, without explicit tuning to that relation; including the observed scatter and its dependence on local properties such as stellar surface density and gas metallicity (C. d. P. Lagos et al. 2026).

(iv) *Chemical enrichment*: yields have been updated with data from the literature to account for stellar mass from AGB stars, massive stars, Type Ia SNe, and CCSNe. Abundances of key elements for radiative cooling, along with s-process elements (Ba, Sr) important in AGB stars and the r-process element (Eu) important in neutron star mergers, common-envelope jets SNe and collapsars, are tracked to enable more realistic ISM enrichment. Turbulent diffusion is included to capture small-scale mixing of metals and dust. These updates are described in C. A. Correa et al. (2026).

(v) *Stellar feedback*: early stellar feedback is implemented through stellar winds, radiation pressure, and H II regions (A. Benítez-Llambay et al. 2026). The model for CCSN feedback is based on E. Chaikin et al. (2023), with 90 per cent of the energy injected thermally (by heating gas particles stochastically, driving galactic winds; C. Dalla Vecchia & J. Schaye 2012) and the remaining 10 per cent injected kinetically (through low-velocity kicks, driving turbulence in the ISM). SN energy injections are distributed statistically isotropically around young stellar particles, following E. Chaikin et al. (2022).

(vi) *BH growth*: supermassive BHs are modelled, including seeding, growth via mergers and gas accretion, and repositioning to account for dynamical friction (V. Springel, T. Di Matteo & L. Hernquist 2005; Y. M. Bahé et al. 2022). Gas accretion can exceed the Eddington rate by a factor of 100, but is regulated by radiative feedback in the thermal model, and by a combination of radiation, accretion disc winds, and jets in the hybrid model. In the hybrid case, mass-loss between the outer accretion disc and the BH horizon is also included, while the accretion disc state (set by the BH accretion rate) determines distinct regimes with different accretion and feedback efficiencies. Further details are provided in F. Huško et al. (2026) and Paper II.

(vii) *AGN feedback*: the fiducial purely thermal model is based on C. M. Booth & J. Schaye (2009) (in which the BH injects energy thermally by increasing the temperature of gas particles) while several simulations adopt a hybrid model that combines a thermal component, modelling winds, and radiation, with kinetic jets (in which the BH injects energy kinetically, giving a velocity kick to gas particles). The jets are regulated by the BH spin, which also

determines their directions and feedback efficiencies (F. Huško et al. 2026). A more detailed description is provided in Paper II, which focuses on analysing the effect of AGN feedback in MQGs.

3 GALAXY PROPERTIES AND SAMPLE SELECTION

Galaxies in COLIBRE are embedded within subhaloes, and so determining galaxy properties is intimately linked to identifying subhaloes and quantitatively characterizing their contents. Subhaloes in COLIBRE are identified with HBT-HERONS, which tracks particles across time-steps. Galaxy properties are then measured using SOAP in different apertures centred on the most bound particle. Throughout this paper, we adopt a fiducial 50 pkpc spherical aperture to analyse high- z MQGs, considering only particles bound to the subhalo, as in J. Schaye et al. (2026). Unless otherwise stated, this aperture is used.

We also test other aperture radii (e.g. 1 and 10 pkpc). For reference, *JWST* observations typically employ apertures of ≈ 10 ckpc to measure colours for MQGs (see section 2.3 in C. d. P. Lagos et al. 2025), corresponding to $\approx 1 - 3$ pkpc over the redshift range $z = 2 - 8$. We find that the measured properties converge for the 10 pkpc aperture and, to a lesser extent, for the 1 pkpc aperture. In the latter case, we obtain slightly higher number densities, likely because this selection excludes star-forming outskirts in more extended star-forming systems (Appendix A). This reflects the compact nature of MQGs at high redshift (see Section 4.5) and confirms that the galaxy properties we use are robust to the fiducial choice of aperture.

Below, we summarize the main galaxy properties and definitions used throughout the paper.

- *Stellar mass* (M_*): computed as the sum of all stellar particles.
- *SFR*: calculated as the sum of the SFRs of gas particles flagged as star-forming (i.e. locally gravitationally unstable; F. S. J. Nobels et al. 2024). We adopt this measure of instantaneous SFR. We verify that using a 10 Myr averaged SFR does not significantly affect the results, whereas a 100 Myr average has a noticeable impact on the number densities at $z > 3$ (see Appendix A). These averaged estimates are more directly comparable to observational tracers (R. C. Kennicutt & N. J. Evans 2012). In particular, photometric studies are typically sensitive to time-scales of order ~ 100 Myr (e.g. S. Albers et al. 2024; W. M. Baker et al. 2025c), while spectroscopic analyses can probe shorter time-scales of around ~ 10 Myr (e.g. Y. Zhang et al. 2026).

- **Dust mass** (M_{dust}): the total dust mass in gas particles (the sum over the 6 species described in Section 2.2).
- **Molecular hydrogen mass** (M_{H_2}): the sum of H_2 mass in gas particles.
- **Stellar half-mass radius** (r_*): the radius enclosing half of the stellar mass, measured in projected 50 pkpc apertures along the x, y, and z-axes, considering bound particles only. The final value is the average of the three projections to mimic the random viewing orientation of observed galaxies.

3.1 Selecting the high- z MQG sample

Multiple definitions for MQGs at high- z exist in the literature. We adopt the following criteria, focusing on systems at $z \geq 2$ where there appears to be various degrees of tension with galaxy formation models and simulations (C. d. P. Lagos et al. 2025).

- **Massive criterion:** $M_* > 10^{10} M_\odot$.
- **Quenched criterion:** $\text{sSFR} < 0.2/t_{\text{age}}$, where the specific star formation rate is defined as $\text{sSFR} = \text{SFR}/M_*$ and t_{age} is the age of the Universe at the redshift of selection. Galaxies above this threshold are classified as star-forming.

The ‘massive’ threshold is defined following common practice. For the definition of quiescence, several approaches exist, including colour–colour cuts, fixed specific sSFR thresholds, or redshift-dependent sSFR thresholds. We opt for a redshift- and mass-dependent cut following M. Franx et al. (2008), since relevant time-scales (e.g. gravitational or cooling times) scale with the Hubble time and gas density; while colour-based methods can be contaminated by obscured star formation or emission lines (C. Schreiber et al. 2018) and may even miss quiescent galaxies that fall outside the traditional strict criteria (E. Merlin et al. 2018). Table 1 shows the number of MQGs identified at $z = 3$ using this definition. A comparison of alternative criteria is presented in Appendix A.

3.2 Computing star formation histories

SFHs are computed from stellar particles gravitationally bound to each galaxy within the fiducial 50 pkpc spherical aperture, using their stellar ages and stellar masses at birth to construct a mass-weighted histogram of formation times. It is important to note that this method does not distinguish between *in situ* (stars formed within the galaxy) and *ex situ* (stars formed outside the galaxy’s main progenitor) star formation. Consequently, star formation bursts could reflect the peak formation of an accreted ex-satellite rather than intrinsic activity in the galaxy itself.

We adopt a bin size of 10 Myr to sample the SFHs, which gives reasonable results, being much longer than the simulation time-step and comparable to observational studies capable of probing SFR variations on similar short time-scales via spectral features (R. C. Kennicutt & N. J. Evans 2012). We also test a 20 Myr bin size, which yields similar results but smooths out variability, making it less effective at capturing short-time-scale features in the SFHs.

Observationally, different SFH features are extracted to characterize key evolutionary events in a galaxy, rather than comparing their overall shapes, which have less quantitative meaning. To enable meaningful comparisons with observations, we focus on a subset of these features, measured in lookback time from the epoch of selection, following common practices in the literature:

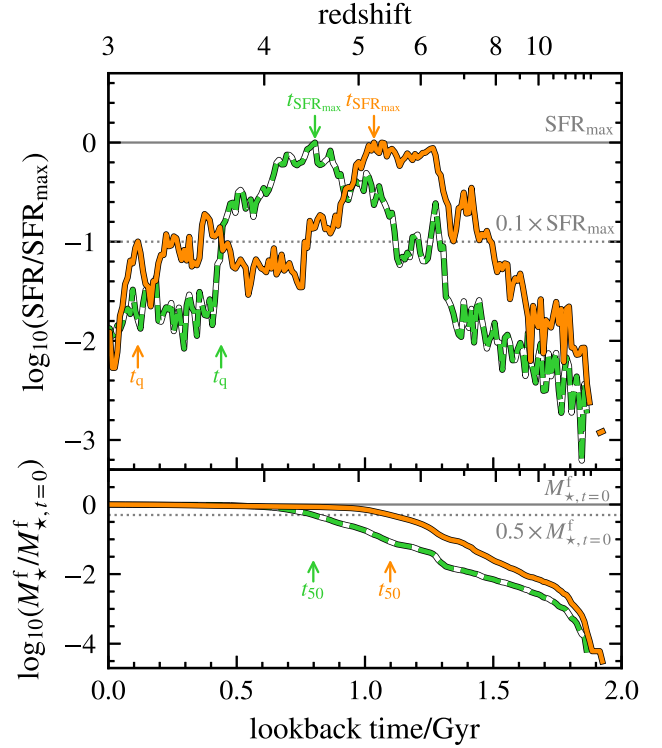


Figure 1. *Top panel:* normalized SFHs ($\text{SFR}/\text{SFR}_{\text{max}}$ versus lookback time, with redshift indicated by the top x-axis) of two example galaxies identified to be massive and quenched at $z = 3$ in L200m6. The horizontal solid line corresponds to the peak SFR value, SFR_{max} , while the dotted line shows the $0.1 \times \text{SFR}_{\text{max}}$ threshold used to define the quenching time-scale, t_q . Arrows indicate t_q for each galaxy, defined as the latest time the galaxy’s SFR drops below this threshold; as well as the SFR peak time, $t_{\text{SFR}_{\text{max}}}$. The green curve represents a galaxy that, once it has crossed the threshold indicated by the dotted line, never rises above it again. The orange curve represents a galaxy that experiences several star formation episodes above the threshold after its SFR peak. *Bottom panel:* normalized stellar mass assembly histories, $M_*/M_{*,t=0}^f$, versus lookback time, with redshift indicated by the top x-axis) for the same galaxies. The horizontal solid line shows the maximum ‘formed’ stellar mass value, $M_{*,t=0}^f$, while the dotted line shows the $0.5 \times M_{*,t=0}^f$ threshold used to define the formation time-scale, t_{50} . Arrows indicate t_{50} .

- The quenching time-scale, t_q , indicates when a galaxy effectively ceases star formation. We define t_q as the lookback time from the selection redshift (not from $z = 0$) when the SFR last dropped below 10 percent of its peak value: $\text{SFR}(t_q) = 0.1 \times \text{SFR}_{\text{max}}$. Our approach is inspired by T. Nanayakkara et al. (2025), although they define quenching as the longest continuous period below this threshold after the peak.

The top panel of Fig. 1 shows a single-starburst SFH of a $z = 3$ MQG (green line), where the SFR remains below the threshold once crossed. For MQGs with multiple starburst episodes after the peak (orange line), we adopt the last time the galaxy crosses it, reflecting when it finally transitions to quiescence before the selection snapshot. The fraction of galaxies with multiple starbursts after the peak is dominant in general with ≈ 0.76 at $z = 2$, ≈ 0.64 at $z = 3$, ≈ 0.46 at $z = 4$, ≈ 0.09 at $z = 5$, and ≈ 0.50 at $z = 6$ for L200m6. Multiple episodes of SF, before or after the peak, could be connected to ‘mini-quenching’ discussed in the literature (V. Strait et al. 2023; T. J. Looser et al. 2024; W. M. Baker et al. 2025b).

- The formation time-scale describes how rapidly a galaxy assembles its stellar mass. It can be defined in several ways: for example, the time at which 50 per cent (t_{50}) or 90 per cent (t_{90}) of the stellar mass has formed, or the interval $t_{90} - t_{50}$. We adopt t_{50} as the primary measure of formation time, which we compute in lookback time from the selection redshift as follows. Using the SFH, we calculate the cumulative stellar mass by integrating over time bins and estimate when its ‘formed’ mass first exceeds 50 per cent of its integrated mass at selection, $0.5 \times M_{\star, t=0}^f$. This is shown in the bottom panel of Fig. 1. Note that $M_{\star}^f$ ignores stellar mass-loss and may therefore differ from the actual ‘observed’ galaxy stellar mass $M_{\star}^{\text{obs}} = M_{\star}$.

3.3 Kinematic tracer $v_{\star}/\sigma_{\star}$ definition

To characterize the kinematics of a galaxy, we focus on the stellar component and measure $v_{\star}/\sigma_{\star}$ as a tracer. This approach has recently been applied to massive quenched systems (M. Slob et al. 2025; B. Forrest et al. 2026; R. G. Pascalau et al. 2026). Here, $v_{\star}$ represents the stellar rotational velocity, indicating the galaxy’s rotational support, while $\sigma_{\star}$ quantifies the stellar velocity dispersion, indicating the random-motion contribution. This measure differs from the classical spin parameter λ_r , although the two can be converted (M. Cappellari 2016).

To compute these quantities, we must first define a reference frame: (1) measure the galactic centre, and (2) rotate the galaxy to align it with the stellar angular momentum vector. We define our centre as the stellar centre of mass and its corresponding velocity in a 50 pkpc spherical aperture, using only bound particles. Other options are: (i) the stellar centre of mass and its velocity within other apertures such as 10 or 30 pkpc, (ii) the position and velocity of the most massive BH particle within a 50 pkpc spherical aperture, considering only bound particles, or (iii) the most bound particle of the subhalo (subhalo centre) and stellar centre of mass velocity within 10 pkpc. We find that our approach gives more stable results, minimizing the mean position and velocity within our fiducial aperture. Secondly, we rotate the galaxy so that the z -axis aligns with the stellar angular momentum vector of the 10 pkpc core.

Once aligned, we compute the stellar kinematics using cylindrical coordinates for each bound particle (v_r, v_{ϕ}, v_z) in the fiducial 50 pkpc aperture centred on the most bound particle. The rotational velocity is given by the azimuthal component, v_{ϕ} , and the total galaxy’s stellar rotational velocity is computed as the mass-weighted root mean square (RMS):

$$v_{\star} = \sqrt{\frac{\sum_{i \in R} m_i v_{\phi, i}^2}{\sum_{i \in R} m_i}}. \quad (1)$$

The perpendicular component to the plane traces the vertical velocity dispersion in the disc, v_z , and its final value is similarly computed as the mass-weighted RMS:

$$\sigma_{\star} = \sqrt{\frac{\sum_{i \in R} m_i v_{z, i}^2}{\sum_{i \in R} m_i}}. \quad (2)$$

We caution the reader that our $v_{\star}/\sigma_{\star}$ measurements (Section 4.5.1) are not quantitatively comparable to observations because of limitations such as beam smearing and projection effects (K. E. Harborne et al. 2019, 2020), which make our values effectively

upper limits for this ratio.³ Observations measure line-of-sight velocity and velocity dispersion (which differ from our definition) and are sensitive to galaxy orientation, although inclination corrections are applied. Observations also typically measure $v_{\star}/\sigma_{\star}$ within the half-light radius, whereas we use all stellar particles within the aperture.

4 THE DEMOGRAPHICS OF MQGS IN COLIBRE

We present predictions from the COLIBRE model for MQGs (as defined in Section 3.1) at high redshift ($z \geq 2$). Our analysis considers a broad set of properties, including those that can be constrained observationally and others that remain largely theoretical due to current observational limitations.

4.1 Number densities of MQGs

We begin by analysing the evolution of the number density (i.e. number of objects per unit comoving volume) of MQGs. C. d. P. Lagos et al. (2025) have shown that galaxy formation and evolution models face challenges in consistently reproducing the number density of MQGs inferred from *JWST* observations. E. Chaikin et al. (2026b) perform a COLIBRE analysis using only two simulations with the thermal AGN feedback model; here, we extend this study.

4.1.1 Results

The top panel of Fig. 2 presents results from the various COLIBRE simulations listed in Table 1; these differ in volume, resolution, and AGN feedback implementation. Number densities are computed at intervals of 0.5 in redshift over $z = 2 - 8$ (except for L100m5, which is only analysed at integer redshifts). When no galaxies are identified as MQGs at a given redshift, the corresponding redshift bin is omitted; thus, some lines end at $z < 8$. These predictions are compared with the latest *JWST* observational constraints.

Fig. 2 reveals that there is significant variation among the different simulations. At fixed colour, the dashed and solid lines correspond to different simulated volumes at fixed mass resolution. Larger volumes capture rarer galaxies at the highest redshifts, reducing cosmic variance (particularly important for these systems, e.g. S. Lim et al. 2025) and improving number statistics (notably at $z \gtrsim 2$ for the m5 runs, at $z \gtrsim 4$ for m6 runs and at $z \gtrsim 6$ for m7 runs), as well as including longer-wavelength fluctuations that give rise to the largest overdensities capable of forming these galaxies. However, the bump seen in L100m6 around $z \approx 5$ is not solely due to Poisson noise but reflects a pronounced overdensity in the ICs⁴ of the 100 cMpc volume traced at high redshift (final part of appendix A1 in E. Chaikin et al. 2026b).

However, resolution effects are also apparent. Darker (lighter) lines represent lower (higher) mass resolution simulations. There

³The rotational velocity we measure corresponds to the intrinsic rotational component and is therefore typically underestimated in observations, while the velocity dispersion inferred observationally is often overestimated due to observational limitations such as beam smearing or projection effects (see a detailed discussion and demonstration of these in K. E. Harborne et al. 2020).

⁴The ICs are identical for simulations with the same volume, independently of the mass resolution or AGN feedback implementation.

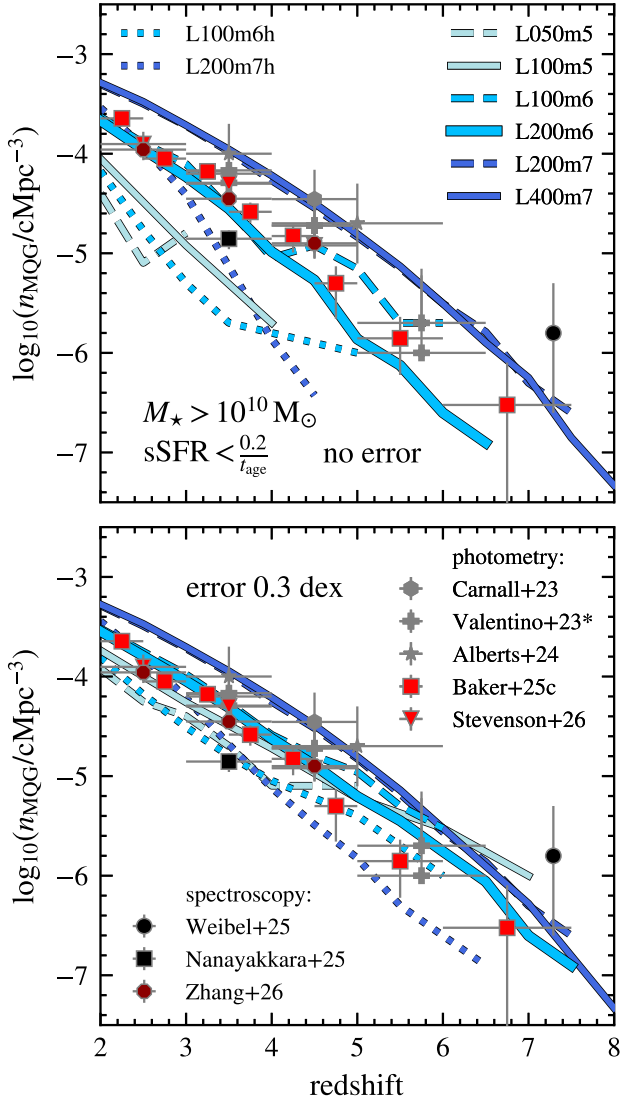


Figure 2. Comoving number density of MQGs, defined by $M_* > 10^{10} M_\odot$ and $s\text{SFR} < 0.2/t_{\text{age}}$, as a function of redshift. Lines represent predictions from various COLIBRE boxes (spanning different volumes, resolutions, and AGN feedback models) in Table 1, with the selection at $2 \leq z \leq 8$. Lines that terminate at $z < 8$ indicate that no galaxies are identified as MQGs beyond those redshifts. These are compared with the latest *JWST* observational estimates: black (smaller area) and dark red (larger area) points show spectroscopic measurements, while grey (smaller area) and red (larger area) points correspond to photometric measurements. Observational data are taken from A. C. Carnall et al. (2023), F. Valentino et al. (2023), S. Alberts et al. (2024), W. M. Baker et al. (2025c), A. Weibel et al. (2025), T. Nanayakkara et al. (2025), S. D. Stevenson et al. (2026), and Y. Zhang et al. (2026). *Top panel:* predicted simulation values. *Bottom panel:* M_* and SFR values in the simulations are convolved independently with a Gaussian distribution (mean 0, standard deviation 0.3 dex) representing a reasonable error budget for these quantities.

is a systematic clear offset between the different resolution simulations, indicating that galaxies in higher-resolution simulations are less quenched, e.g. when comparing L200m6 (solid cyan) and L200m7 (dashed dark blue) or L100m5 (solid light blue) and L100m6 (dashed cyan). Two factors contribute to this trend: (1) at higher resolution, gas particles trace smaller effective vol-

umes, producing denser gas around BHs, and so stronger feedback is required to eject or heat it; (2) AGN feedback becomes less bursty at higher resolution, due to the resolution-dependent nature of the feedback prescriptions (equations 5 and 8 of Paper II). These effects make AGN feedback less effective at higher resolution. Differences in BH seed masses may also play a role, since higher-resolution simulations use lower seed masses, delaying BH growth and the onset of AGN feedback.

The dotted lines represent simulations that include hybrid AGN feedback, thermal plus jet feedback, instead of purely thermal AGN feedback. This hybrid model produces significantly less quenching. In Paper II, we show that the difference arises because the hybrid model features BHs that grow more slowly in the early Universe compared to the fiducial, purely thermal AGN feedback model. We can see this by considering the ratio, M_{BH}/M_* . The medians are comparable in the thermal L200m7 and hybrid L200m7h simulations at $z = 2$ (~ 0.67); however, at $z = 5$, the medians are 0.70 (thermal) versus 0.64 (hybrid), and 0.70 versus 0.60 at $z = 8$. Moreover, jet feedback appears to take longer to quench galaxies than thermal feedback. At fixed stellar mass and for $z \lesssim 3$, the same cumulative injected BH energy leads to a higher fraction of quenched systems in the thermal feedback model (see fig. 2 of Paper II). These effects do not appear to depend on mass resolution; the same trend is evident in both the m7 and m6 runs, with the pronounced overdensity visible around $z \approx 5$ in L100m6h as well. By $z < 2$, however, hybrid feedback becomes more efficient at quenching because the weaker early feedback allows galaxies to build more stellar mass, which must then converge by $z = 0$ (see fig. 13 in E. Chaikin et al. 2026b).

Ultimately, runs at different resolutions, and within the same resolution, runs with different AGN feedback models (thermal or hybrid), were independently tuned to reproduce $z = 0$ observations. Each run should therefore be seen as a distinct model. We remind the reader that all of them have been calibrated to consistently reproduce the $z = 0$ SMF, the galaxy size–mass relation, and the galaxy BH–mass relation (figs. 12, 14 and 15 in J. Schaye et al. 2026); and additionally the $z = 0.2$ bolometric AGN luminosity function for the hybrid AGN feedback model (fig. 10 in Huško 2026).

Compared with observations, the top panel of Fig. 2 shows that the highest-resolution m5 and m6 COLIBRE thermal AGN feedback runs, as well as the hybrid AGN feedback runs, underpredict the high number densities inferred from *JWST*. However, the tension is significantly alleviated if we consider potential errors associated with the derivation of stellar mass and SFR of galaxies. S. Bellstedt & A. S. G. Robotham (2025) showed that the many decisions behind the derivation of stellar masses and SFRs (i.e. adopted functional form of the star formation and metallicity histories; the choice of stellar population models; the IMF; to mention a few; see C. Conroy 2013, for a review) can lead to differences in the derived stellar masses and SFRs of 0.1–0.2 dex and ≈ 0.2 dex, respectively, in the $z \approx 0$ spectroscopic GAMA survey. We refer the reader to other works for further discussion of these uncertainties (e.g. C. Conroy, J. E. Gunn & M. White 2009; A. S. G. Robotham et al. 2020; R. K. Cochrane et al. 2025; G. T. Jones, C. M. Byrne & E. R. Stanway 2025). The uncertainties reported by S. Bellstedt & A. S. G. Robotham (2025) could be seen as lower limits for the uncertainties one would expect for high- z galaxies with potentially more bursty SFHs, poorer wavelength coverage, and potentially with photometric redshifts only. It is thus natural to expect uncertainties to be even larger at high- z .

To exemplify the impact such an error budget could have, we show in the lower panel of Fig. 2 the number densities after convolving the stellar masses and SFRs of COLIBRE galaxies with a Gaussian centred at 0 with a width of $\sigma = 0.3$ dex. The lack of a systematic shift in the recovered quantities (in a population sense) can be seen as a conservative case, in which the individual uncertainties coming from SED fitting, photometric redshifts, etc., contribute to broadening the scatter of the recovered quantities, consistent with the findings of S. Bellstedt & A. S. G. Robotham (2025) at $z = 0$. A Gaussian error convolution is, however, only an approximate representation, since e.g. observational selections based on colours do not strictly follow this behaviour. We carry out the error convolution for stellar masses and SFRs in an independent manner, which is another simplification, as errors could potentially be correlated. In Appendix B, we explore the impact of adopting different values for the standard deviation (Fig. B1). This procedure produces perturbed values ($M_{\star}^{\text{conv}}$ and SFR^{conv}), to which we then apply the MQG selection (Section 3.1). To reduce stochastic noise introduced by the convolution, the procedure is repeated 100 times, and the median of the resulting measurements is taken. This error convolution is just for reference, and the aim is to make the visual argument that quantifying uncertainties in the observational estimates is crucial to isolate the level of tension between models and the observations. For a more detailed analysis of the impact of errors on the quenched fraction, SMF and number densities of galaxies, we refer the reader to appendix D in E. Chaikin et al. (2026b). A more realistic calibration of observational systematics, based on generating mock photometric and spectroscopic observations of simulated COLIBRE MQGs followed by analysis with modern SED-fitting pipelines under controlled assumptions, is left for future work (Nanayakkara et al., in preparation).

4.1.2 Comparison with observations

For the remainder of Section 4, we primarily focus on the fiducial L200m6 simulation. This run provides a sufficiently large volume to contain dozens of MQGs while also resolving their internal structure more reliably (see Section 4.5 and Appendix E). This run also performs better in reproducing the observed number density evolution after we consider errors. We additionally include results from the L400m7 simulation where relevant. We do not show results from the L200m7h hybrid run henceforth, but confirmed that the results look broadly similar, highlighting the places where this may not be the case.

In Fig. 3, we show the L200m6 predictions (including Gaussian-distributed uncertainties in the stellar masses and SFRs of width 0.3 dex) alongside the same observational data shown in Fig. 2. We have already discussed observational uncertainties arising from some of the choices behind SED modelling. However, there are additional, important caveats, and biases that affect observationally derived number densities that are worth discussing in more detail.

- *Selection criteria:* The observations by A. C. Carnall et al. (2023), W. M. Baker et al. (2025c), and S. D. Stevenson et al. (2026) are most directly comparable to our data; they adopt the same criteria described in Section 3.1 ($M_{\star} > 10^{10} M_{\odot}$ and $\text{sSFR} < 0.2/t_{\text{age}}$). W. M. Baker et al. (2025c) also apply a colour–colour selection to clean their sample. However, other studies use different definitions. For example, S. Alberts et al. (2024) apply a lower stel-

lar mass cut ($M_{\star} \geq 10^{9.5} M_{\odot}$), while F. Valentino et al. (2023)⁵ use a UVJ or NUVUVJ colour–colour selection in addition to $M_{\star} \geq 10^{9.5} M_{\odot}$. Similarly, T. Nanayakkara et al. (2025) select galaxies via UVJ colours but with $M_{\star} \gtrsim 10^{10.5} M_{\odot}$. Colour–colour selections have been reported to suffer from contamination of obscured star formation or strong emission lines (C. Schreiber et al. 2018; Y. Zhang et al. 2026) and can also miss significant numbers of quiescent galaxies that fall outside the traditional criteria (E. Merlin et al. 2018), motivating the development of alternative methods (e.g. A. S. Long et al. 2024). Finally, A. Weibel et al. (2025) and Y. Zhang et al. (2026) report galaxies with $\text{sSFR} < 10^{-10} \text{yr}^{-1}$. The former work for a single $M_{\star} = 10^{10.23} M_{\odot}$ galaxy (hence the large error) and at higher redshift, where our threshold $\text{sSFR} < 0.2/t_{\text{age}} \approx 3 \times 10^{-10}$ diverges more, biasing simulation results higher); the latter for $M_{\star} > 10^{10.3} M_{\odot}$ ($m_{\text{F444W}} < 24$ in their table 1, corresponding to a complete sample above that stellar mass).

A more detailed comparison, matching the exact observational selection criteria used to compute number densities, is left for future work. For reference, E. Chaikin et al. (2026b) present COLIBRE results with different $M_{\star}$ cuts ($> 10^{10} M_{\odot}$, $> 10^{10.5} M_{\odot}$, and $> 10^{11} M_{\odot}$), although they adopt an $\text{sSFR} < 10^{-10} \text{yr}^{-1}$ criterion for quiescence.

- *Photometric versus spectroscopic measurements:* Only two studies provide a fully robust spectroscopic sample (T. Nanayakkara et al. 2025; Y. Zhang et al. 2026), plus the A. Weibel et al. (2025) galaxy, which is spectroscopically confirmed as well. Most other works rely on photometric redshifts, which can misidentify MQGs due to dust obscuration, old stellar ages, AGN activity, or reduced star formation (B. Forrest et al. 2024; Y. Zhang et al. 2026). Some studies account for errors in the photometric (F. Valentino et al. 2023; S. Alberts et al. 2024) or spectroscopic redshifts (T. Nanayakkara et al. 2025; Y. Zhang et al. 2026), or apply contamination corrections (S. D. Stevenson et al. 2026), whereas others consider only Poisson errors.

- *Area coverage:* Sample size and coverage statistics also play a role; some data sets cover relatively small areas of the sky, potentially targeting overdense or underdense regions. This is particularly true for the photometric samples from A. C. Carnall et al. (2023), F. Valentino et al. (2023), S. Alberts et al. (2024; all in overdense regions, with at most dozens of objects), as well as the spectroscopic samples from A. Weibel et al. (2025; a single galaxy in a pronounced overdensity) and T. Nanayakkara et al. (2025; covering a smaller region). Some works account for cosmic variance in their error bars (W. M. Baker et al. 2025c; Y. Zhang et al. 2026), which explains the larger uncertainties.

- *Choice of SFR time-scale:* The SFR time-scale deduced from modelling of the SED can depend on the photometric bands or spectral features used to infer the galaxy’s SFR (R. C. Kennicutt & N. J. Evans 2012). Some photometric studies adopt a 100 Myr time-scale (e.g. S. Alberts et al. 2024; W. M. Baker et al. 2025c), while spectroscopic analyses use shorter time-scales of around 10 Myr (e.g. Y. Zhang et al. 2026). We tested the impact of varying these time-scales and found that the results are significantly affected at $z > 3$ only when using the 100 Myr averaged SFRs (see Appendix A). This indicates that MQG SFHs in COLIBRE can remain bursty over time-scales of 100 Myr. The dominant MQG population exhibiting multiple starburst episodes (Section 3.2) may therefore experience a final burst shortly before quenching,

⁵We homogenise the F. Valentino et al. (2023) results by combining $10^{9.5} \leq M_{\star}/M_{\odot} < 10^{10.6}$ and $M_{\star} > 10^{10.6} M_{\odot}$.

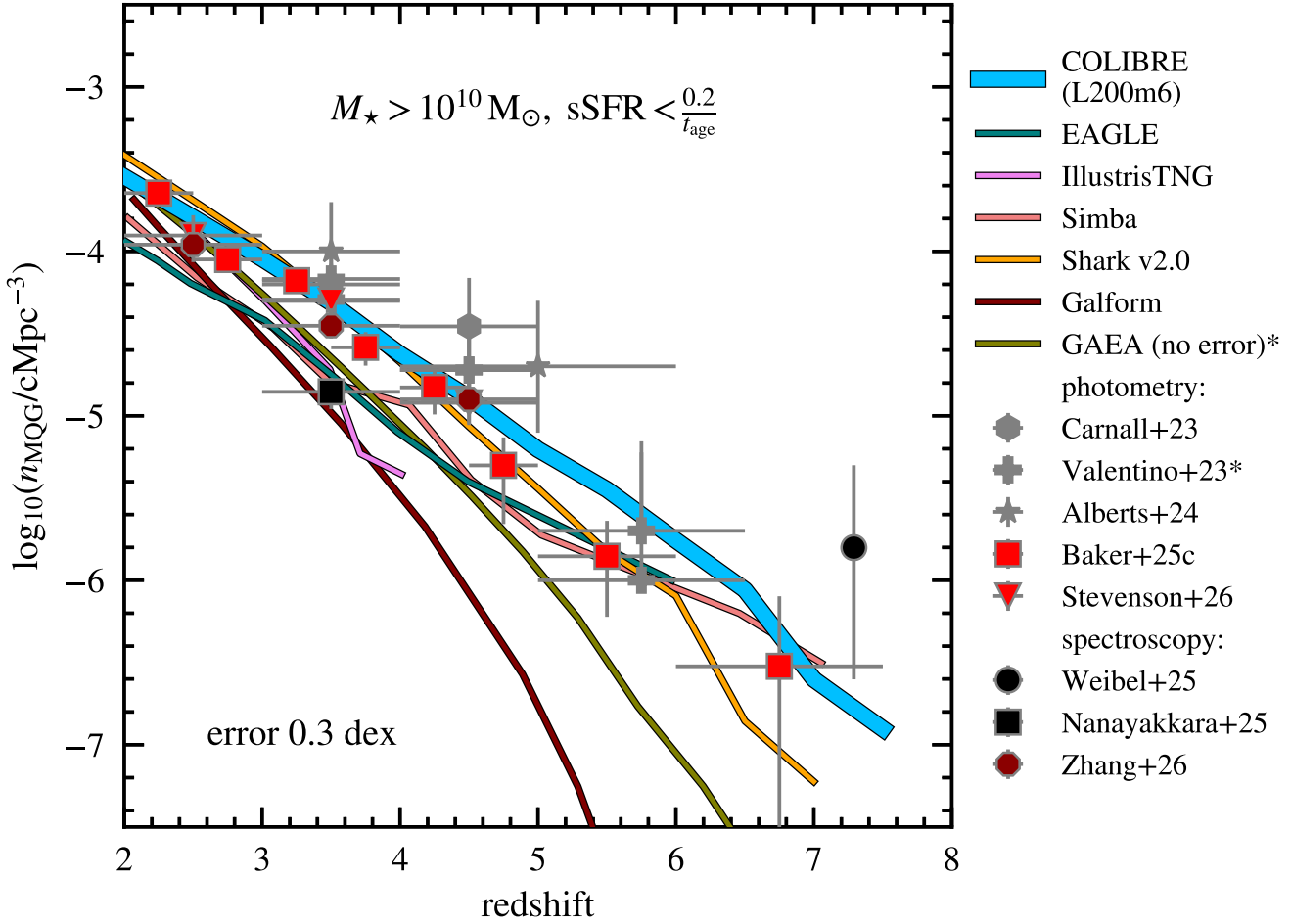


Figure 3. Comoving number density of MQGs, defined by $M_\star > 10^{10} M_\odot$ and $\text{sSFR} < 0.2/t_{\text{age}}$, as a function of redshift. Light-blue line shows predictions from our fiducial L200m6 COLIBRE simulation, with the selection at $2 \leq z \leq 8$, compared to results from other galaxy formation and evolution models in the literature (GAEA defines quenching using a fixed cut of $\text{sSFR} = 10^{-10} \text{yr}^{-1}$). Lines that terminate at $z < 8$ indicate that no galaxies are identified as MQGs beyond those redshifts. For all simulation results (except GAEA), $M_\star$ and SFR values in the simulations are convolved independently with a Gaussian distribution (mean 0, standard deviation 0.3 dex) representing a reasonable error budget for these quantities. These are compared with the latest *JWST* observational estimates: black (smaller area) and dark red (larger area) points show spectroscopic measurements, while grey (smaller area) and red (larger area) points correspond to photometric measurements. Observational data are taken from A. C. Carnall et al. (2023), F. Valentino et al. (2023), S. Alberts et al. (2024), W. M. Baker et al. (2025c), A. Weibel et al. (2025), T. Nanayakkara et al. (2025), S. D. Stevenson et al. (2026), and Y. Zhang et al. (2026).

strong enough to affect the time-averaged SFR. Observationally, MQGs at $3 < z < 5$ may be dominated by recently quenched systems within the last $\lesssim 150$ Myr (E. Merlin et al. 2025).

- **Wavelength coverage:** The wavelength range used in SED fitting is critical for mitigating dust contamination. For example, UV-near-infrared(NIR) photometry alone is insufficient to constrain AGN contributions (W. Chang et al. 2026a). The incorporation of the mid-infrared (MIR) data, such as *JWST*/MIRI observations (e.g. T. Wang et al. 2025b), has proven to provide stronger constraints. F. Valentino et al. (2023), A. Weibel et al. (2025), and W. M. Baker et al. (2025c) include them when available.

Taking these factors into account, larger, more robust samples provide more consistent and reliable results. In Fig. 3, these are some photometric data (e.g. W. M. Baker et al. 2025c; S. D. Stevenson et al. 2026) (light red) and spectroscopic data with incompleteness corrections (e.g. Y. Zhang et al. 2026) (dark red). These more robust data sets show better agreement with each other, and the simulations are no longer as far from the observed values,

reducing the tension highlighted in previous works (e.g. A. C. Carnall et al. 2023; F. Valentino et al. 2023). The observational landscape is evolving rapidly, especially with increasing sample sizes and a better understanding of the systematic effects associated with different selection criteria, as demonstrated by the recent works of T. Yang et al. (2026) and M. Shuntov et al. (2026).

We conclude that COLIBRE predictions are broadly consistent with the most recent and robust *JWST* measurements (red and dark red points), particularly after invoking an error budget of 0.3 dex in stellar masses and SFRs.

4.1.3 Comparison with other galaxy formation models

We also place our COLIBRE results in the context of other recent simulation predictions in Fig. 3. Here, we compare our fiducial run with hydrodynamical galaxy formation simulations: EAGLE (J. Schaye et al. 2015), ILLUSTRISTNG (A. Pillepich et al. 2018), and SIMBA (R. Davé et al. 2019); and semi-analytical models: SHARK v2.0 (C. d. P. Lagos et al. 2024), GALFORM (C. G. Lacey et

al. 2016), and GAEA (G. De Lucia et al. 2024). Except for GAEA, all models adopt the same quenching definition (with t_{age} in Section 3.1 computed using the corresponding cosmology of each simulation) and include Gaussian-distributed errors in their measurements, although the convolution is not repeated 100 times as for the COLIBRE results. As a result, the reported number densities may be affected by the specific random realization of the Gaussian errors, leading to values that are either higher or lower than the ensemble median. GAEA defines quenching using a fixed threshold of $\text{sSFR} = 10^{-10} \text{ yr}^{-1}$.

For EAGLE, we use the ‘L100N1504’ simulation with $L = 100 \text{ cMpc}$, $m_g \sim 10^6 M_\odot$ and $m_{\text{DM}} \sim 10^7 M_\odot$; for ILLUSTRISTNG, the ‘TNG100’ run with $L \approx 111 \text{ cMpc}$, $m_g \sim 10^6 M_\odot$ for the initial gas cell mass and $m_{\text{DM}} \sim 10^7 M_\odot$; while for SIMBA, the ‘m1000n1024’ run with $L \approx 147 \text{ cMpc}$, $m_g \sim 10^7 M_\odot$ per gas element mass and $m_{\text{DM}} \sim 10^8 M_\odot$. In the case of the SAMs, SHARK v2.0 has been run on a $L = 800 \text{ cMpc}$ box with $m_{\text{DM}} \sim 10^8 M_\odot$; GALFORM on a $L \approx 710 \text{ cMpc}$ box with $m_{\text{DM}} \sim 10^9 M_\odot$; while GALFORM on a $L \approx 685 \text{ cMpc}$ per side with $m_{\text{DM}} \sim 10^9 M_\odot$. The larger volumes of the SAMs provide better number statistics, reducing cosmic variance, probing lower number densities (as seen in Fig. 3) and capturing more extreme overdensities.

COLIBRE and SHARK v2.0 tend to predict higher number densities compared to the other models over the redshift range, with COLIBRE about 0.5 dex higher for $z > 5$. In COLIBRE, E. Chaikin et al. (2026c) show clearly that this arises from the allowance for BH accretion above the Eddington limit. The explicit modelling of the cold gas phase enables the resolution of higher gas densities, which in turn lead to higher BH accretion rates, as the accretion rate scales directly with the local gas density (see equation 2 of Paper II). This allows BHs to enter the super-Eddington regime, common at these high redshifts (F. Huško et al. 2025), thereby accelerating BH growth and triggering stronger AGN feedback and earlier quenching.

The other models underpredict the observations: EAGLE and SIMBA at $z \lesssim 5$, while GALFORM and GAEA at $z \gtrsim 3$. Although the GAEA number densities are not convolved with observational errors, we verified that its raw simulated number densities are still lower than those of COLIBRE in the $z \gtrsim 4$ regime. These discrepancies reflect differences in sub-grid physics, especially AGN feedback, which plays a central role in regulating the quenching of massive galaxies (C. d. P. Lagos et al. 2025). Other simulations, not included in Fig. 3, predict higher number densities without accounting for observational uncertainties: for example, MAGNETICUM (L. C. Kimmig et al. 2025) and THESAN (H. G. Chittenden et al. 2026). However, we note that MAGNETICUM has only been run down to $z \approx 2$, where it overpredicts the number densities (C. d. P. Lagos et al. 2025); while THESAN, which explores a regime of suppressed AGN feedback efficiency, focuses on $z \geq 5.5$ and has not been tested in the local Universe. ASTRID, also not included in the comparison, predicts significantly lower number densities than ILLUSTRISTNG (E. J. Weller et al. 2025).

4.2 Stellar mass functions of MQGs

The works of C. d. P. Lagos et al. (2025) and W. M. Baker et al. (2025c) show that the SMF is an important diagnostic of predictions of MQGs. While the number densities can compare reasonably well with observations, the SMF can reveal deficiencies and, in some cases, sharp tensions with the observations.

4.2.1 Results

We analyse the SMF of MQGs in Fig. 4. The left panel presents the SMF predicted by COLIBRE at different redshifts $2 \leq z \leq 7$ for the fiducial L200m6 simulation. The predictions show a clear increase in the number of MQGs with decreasing redshift, as expected: galaxies need time to assemble enough stellar mass to be classified as massive, and additional time for quenching mechanisms to suppress their star formation. Consequently, the population shifts towards higher stellar masses at lower redshifts. Interestingly, these galaxies exhibit a peak around $M_* \approx 10^{10.5} M_\odot$, where quenching is most efficient: galaxies are massive enough for the quenching mechanism to act strongly, yet extremely massive systems remain rare. Once quenched, they undergo little further stellar mass growth.

For comparison, in Fig. 4 we also show observational results from W. M. Baker et al. (2025c) and S. D. Stevenson et al. (2026). The COLIBRE results are broadly consistent with current observational constraints, which also show a similar peak (at around $M_* \approx 10^{10.6} M_\odot$ in W. M. Baker et al. 2025c). A comparable peak is also reported in M. Shuntov et al. (2026) using the larger COSMOS-Web survey, although that study has reduced filter coverage and depth. We further test the impact of excluding satellite galaxies from the MQG selection and find that the SMF still peaks at a similar stellar mass to the case where both centrals and satellites are included. Differences between the two selections emerge only at the low-mass end across $2 \leq z \leq 6$, with a small fraction of quenched satellites already present by $z = 5$, potentially consistent with recent observational discoveries of such systems in overdense regions (W. M. Baker et al. 2026).

While the observational data used here are robust in terms of large sample sizes and reliable selection of massive quenched systems, they are photometrically derived and thus may suffer from systematic uncertainties (B. Forrest et al. 2024). The lack of similarly large spectroscopic samples to measure SMFs highlights the need for future follow-up campaigns. Upcoming wide-area photometric surveys such as MINERVA (A. Muzzin et al. 2025), with extensive NIR and MIR coverage, will help reduce systematics and provide valuable targets for spectroscopic confirmation.

For completeness, we note that the SMF for the L400m7 simulation shows an excess of galaxies around $M_* \approx 10^{10.6} M_\odot$ at all redshifts, consistent with the overestimated number densities discussed in Section 4.1.1. In contrast, the L200m7h SMF at $z = 2$ predicts fewer galaxies at $M_* \lesssim 10^{10.4} M_\odot$ and more at the high-mass end ($M_* \gtrsim 10^{11.2} M_\odot$), while at $z > 2$ it yields lower SMF values across the full mass range.

4.2.2 Comparison with galaxy formation models

The right panel of Fig. 4 presents the SMF after convolving stellar masses and SFRs with a Gaussian-distributed error of width 0.3 dex (as was computed for the number densities) at $z = 3$ in COLIBRE (L200m6). These results are compared with similarly error-convolved predictions from other galaxy formation and evolution models for the $z = 3$ SMF with the same definition of ‘massive quenched’ (except for GAEA, for which the quenching definition at this redshift is effectively similar, since $0.2/t_{\text{age}} \approx 10^{-10} \text{ yr}^{-1}$, and where Gaussian-distributed errors are applied only to M_*). A general trend emerges: models either accurately reproduce the low-mass end of the SMF (EAGLE, GALFORM), the high-mass end (SHARK v2.0), or both ends but not the intermediate mass regime (SIMBA), but none match the full mass range simultane-

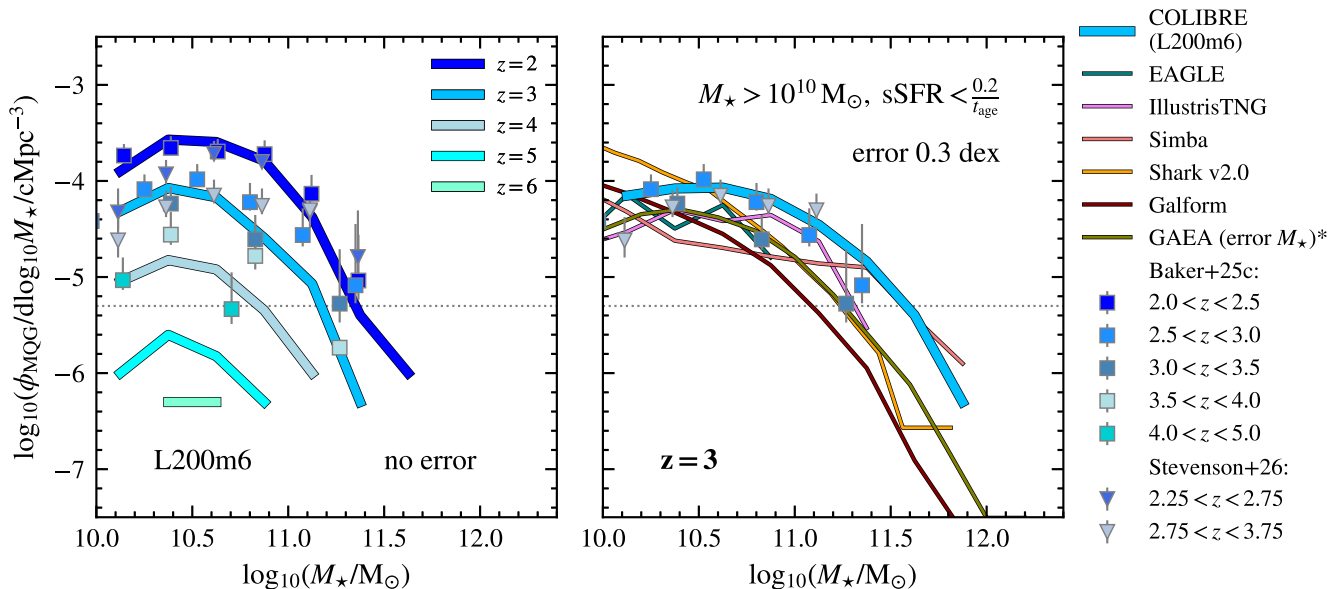


Figure 4. SMF of MQGs, defined by $M_* > 10^{10} M_\odot$ and $\text{sSFR} < 0.2/t_{\text{age}}$, from the fiducial L200m6 simulation. *Left panel:* predicted simulation values at different redshifts $2 \leq z \leq 6$ (colour-coded as labelled in the left panel), compared with observational estimates from W. M. Baker et al. (2025c) and S. D. Stevenson et al. (2026) within the same redshift range, as labelled. *Right panel:* the SMF at $z = 3$ from COLIBRE in light blue (fiducial L200m6) compared with results from other galaxy formation and evolution models, where M_* and SFR values in the simulations are convolved independently with a Gaussian distribution (mean 0, standard deviation 0.3 dex) representing a reasonable error budget for these quantities (GAEA defines quenching using a fixed cut of $\text{sSFR} = 10^{-10} \text{ yr}^{-1}$ and its results are convolved only in M_* with potential observational errors). The horizontal dotted line denotes the threshold of 10 galaxies for COLIBRE, below which the statistics become unreliable.

ously. This has been noted in C. d. P. Lagos et al. (2025) and W. M. Baker et al. (2025c) and linked to the different AGN feedback prescriptions. In contrast, COLIBRE performs well across the full stellar mass range. While GAEA and ILLUSTRISTNG may appear to match the full mass range, GAEA produces fewer galaxies above $M_* \sim 10^{10.5} M_\odot$. We verified that the different error convolution does not primarily drive this, since the raw SMF also remains below that of COLIBRE at the high-mass end. ILLUSTRISTNG suffers from small-number statistics at the high-mass end, with the number density of MQGs that declines rapidly beyond $z > 3$ (Fig. 3). Overall, the consistency of both SMFs and number densities in COLIBRE, once reasonable uncertainties in stellar masses and SFRs are considered, highlights its robust performance in reproducing MQG properties compared to other models. The SMF results derived with the error convolution across the full redshift range are shown in Appendix C.

4.3 Star formation histories of MQGs

SFHs provide key insights into how galaxies assemble their stellar mass (through a single intense starburst, multiple bursts, or an extended period of star formation) and how quenching occurs, either abruptly or gradually. Here, we reconstruct SFHs (Section 3.2) for the selected MQGs in COLIBRE and compare with observational data. Before we present our main results, it is important to note some caveats for the following subsections in Section 4 compared to observations:

- To select massive quenched systems, we use the predicted M_* and SFR of galaxies in COLIBRE, ignoring any potential uncertainties in these quantities.
- The observational samples considered here consist of spectroscopically confirmed galaxies. This is important, as photomet-

rically selected galaxies are less robust as explained earlier, particularly at high redshift (B. Forrest et al. 2024).

- The definition of ‘massive quenched’ varies across observational studies; this should be kept in mind when interpreting results.

In Fig. 5, we show the fiducial COLIBRE simulation predictions for SFH properties as a function of M_* , compared to recent *JWST* spectroscopic observations, displayed as individual data points colour-coded by spectroscopic redshift. Observationally, SFHs are derived from SED modelling. For the data from T. Nanayakkara et al. (2025), W. M. Baker et al. (2025a), we use the full SFH Markov chain Monte Carlo (MCMC) output provided by the SED-fitting code PROSPECTOR (B. D. Johnson et al. 2021), computing each galaxy’s properties as the median and the 16th and 84th percentile range of the MCMC. For T. Nanayakkara et al. (2025), we adopt an exponentially increasing continuity prior between SFH bins rather than the manuscript’s fiducial choice, which is broadly consistent with expectations from Λ CDM cosmology (A. Dekel et al. 2013), as it favours a gradual stellar mass build-up at high redshift and reduces biases toward older time-scales (C. Turner et al. 2025). For A. C. Carnall et al. (2024), we use the values reported directly in the paper.

4.3.1 Formation time-scale

In the top panel of Fig. 5, we show the formation time-scale for MQGs (the lookback time from the time of selection at which 50 per cent of the stellar mass without accounting for mass losses was formed; see Section 3.2) as a function of M_* . Each colour represents the median relation at a different selection redshift, with shaded areas indicating the corresponding 16th and 84th percentile range. Here, we focus on MQGs selected at $2 \leq z \leq 5$,

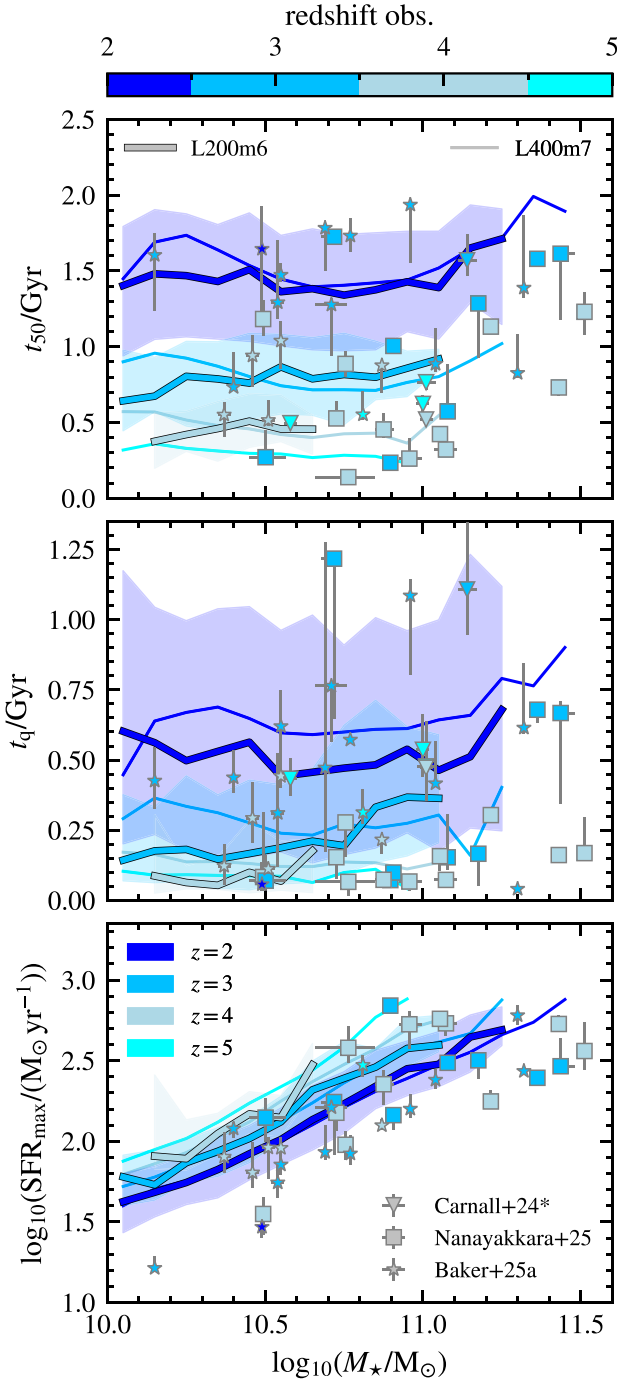


Figure 5. SFH properties of MQGs as a function of M_* . Thick solid lines show the median predictions from L200m6 at different redshifts $2 \leq z \leq 5$ (as labelled in the bottom panel), with shaded regions indicating the 16th and 84th percentile range. At $z = 5$, MQGs are too few to split into stellar mass bins (9 galaxies). Thin solid lines show the corresponding medians from L400m7. These are compared to recent *JWST* spectroscopic measurements (A. C. Carnall et al. 2024; T. Nanayakkara et al. 2025; W. M. Baker et al. 2025a), shown as symbols colour-coded by observed galaxy redshift, with the corresponding colourbar at the top. *Top panel:* formation times (t_{50}), defined in Section 3.2. *Middle panel:* quenching times (t_q), defined in Section 3.2 (for A. C. Carnall et al. 2024, defined as the earliest lookback time at which the galaxy first crosses $sSFR < 0.2/t_{age}$). *Bottom panel:* SFR peak (SFR_{max}) (no data from A. C. Carnall et al. 2024).

although there are too few galaxies at $z > 4$ for L200m6 to compute reliable medians per stellar mass bin. In L200m6, the simulated galaxies undergo a rapid mass assembly, forming the bulk of their mass early in cosmic time, with no significant dependence on stellar mass. This differs from a recent observational result (H.-H. Leung et al. 2026), which finds a steeper relation indicative of downsizing at these redshifts, with more massive MQGs forming earlier than their lower-mass counterparts.

Selections at higher redshift correspond to later t_{50} due to the limited cosmic time available, but also to earlier median z_{50} values: $z_{50} = 3.40$ at $z = 2$, $z_{50} = 4.47$ at $z = 3$, $z_{50} = 5.25$ at $z = 4$, $z_{50} = 6.08$ at $z = 5$, and $z_{50} = 7.28$ at $z = 6$ (for 2 galaxies), consistent with expectations. The scatter decreases with redshift, which may reflect smaller sample sizes at higher redshifts. In L400m7 (thin lines), t_{50} interestingly peaks at $M_* \approx 10^{10.2} M_\odot$ and increases again at higher masses.

Qualitatively, the simulation values in the top panel are consistent with the observational sample. The T. Nanayakkara et al. (2025) data show shorter formation time-scales around $M_* \approx 10^{11} M_\odot$, indicating later mass assembly and burstier SFHs than in COLIBRE, a trend also seen across the full mass range in W. M. Baker et al. (2025a). However, as discussed in Section 4.3.4, early-time SFHs are observationally uncertain because old stellar populations provide limited constraints. The same applies to the few longer time-scales inferred from $z \approx 3$ observations. Observed galaxies at the high-mass end ($M_* \gtrsim 10^{11.2} M_\odot$) are not well matched by the simulation medians either, although we require at least 5 galaxies per stellar mass bin to compute the medians, and thus galaxies of these masses may exist but with insufficient statistics. The A. C. Carnall et al. (2024) observations display a different behaviour compared to the other two studies. This is likely due to their distinct SFH parametrization using a double power-law in BAGPIPES (A. C. Carnall et al. 2018; parametric form as opposed to the non-parametric of the other two works, discussed in Section 4.3.4), which tends to produce SFHs resembling a single burst with minimal star formation outside that period.

4.3.2 Quenching time-scale

In the middle panel of Fig. 5, we examine the quenching time-scale (as defined in lookback time from the time of selection in Section 3.2). We find no strong trend with M_* for L200m6. Higher-redshift systems exhibit lower t_q values, although this trend is less pronounced than for the formation times. Galaxies at earlier times quenched more recently relative to their selection redshift, as expected, since the available cosmic time is shorter. The median values are $z_q = 2.36$ for selection at $z = 2$; $z_q = 3.26$ at $z = 3$; $z_q = 4.20$ at $z = 4$; $z_q = 5.27$ at $z = 5$; and $z_q = 6.14$ at $z = 6$ (for 2 galaxies).

The L400m7 simulation (thin lines) exhibits the same peak in t_q as in t_{50} , around $M_* \approx 10^{10.2} M_\odot$. Although not shown, the scatter at $z = 2$ is comparable to that in L200m6, despite the larger number of galaxies. L200m7h shows significantly shorter quenching time-scales ($t_q \lesssim 0.4$ Gyr) at $z = 2$ for low-mass systems ($M_* < 10^{10.5} M_\odot$), producing a non-flat positive correlation between quenching time and stellar mass, where more massive galaxies quench earlier. This may hint at the observational trend that more massive systems at $z \gtrsim 3$ tend to have longer quenching time-scales (E. Merlin et al. 2025), a trend that is also weakly present in L200m6.

COLIBRE predictions broadly agree with observations, indicative of recent quenching $t_q \lesssim 0.6$ Gyr. The simulated data recover the W. M. Baker et al. (2025a) data well. The T. Nanayakkara et al. (2025) data show shorter quenching time-scales around $M_* \approx 10^{11} M_\odot$, consistent with the later formation time-scales found previously due to burstier SFHs. The high-mass end is not well reproduced either, as the simulations lack a statistically significant population of systems in that regime. A. C. Carnall et al. (2024) use a different definition for t_q (the earliest lookback time at which the galaxy first crosses $sSFR < 0.2/t_{\text{age}}$) yielding longer values, although they follow the same overall trend as $sSFR < 0.2/t_{\text{age}}$ because of the double power-law SFH parametrization (parametric form).

4.3.3 Peak of SFR

Finally, we show the SFR peak, SFR_{max} , in the bottom panel of Fig. 5. The lookback time of the SFR peak, $t_{SFR_{\text{max}}}$, follows a similar trend to that of t_{50} (as shown in Fig. 1). SFR_{max} increases with galaxy mass, reflecting the stronger SF episodes required to assemble more stellar mass. The peak also decreases toward lower redshift, indicating that stellar mass can be built up more gradually over time, rather than through a single intense starburst as seen for MQGs selected at $z = 4$. Observational results exhibit considerable scatter but generally follow a similar trend with selection redshift. Values in T. Nanayakkara et al. (2025) and W. M. Baker et al. (2025a) are quantitatively reproduced, although the simulated values are systematically higher than the observational estimates. This difference is driven by the broader lookback-time bins used in observational reconstructions based on non-parametric SED fitting (see Fig. D1). We verify that adopting coarser time bins of 100 Myr (comparable to observational constraints) reduces the inferred SFR_{max} values. In addition, a fraction of galaxies experience very strong starbursts in L200m6 ($SFR_{\text{max}} > 300 M_\odot \text{ yr}^{-1}$): 10 per cent at $z = 2$, 14 per cent at $z = 3$, 23 per cent at $z = 4$, 27 per cent at $z = 5$ (3 galaxies), and 50 per cent at $z = 6$ (1 galaxy). This may point to an evolutionary link with highly star-forming galaxies.

4.3.4 Discussion

The level of agreement between simulations and observations is highly sensitive to sample selection and the assumptions made during SED fitting, even when spectroscopic data are available. Choices made during SED fitting can introduce systematic biases that affect the inferred galaxy properties. In particular, the complex SFHs involving multiple bursts, described in Section 3.2, are challenging to recover via SED fitting (K. A. Suess et al. 2022; B. Wang et al. 2025a).

For example, T. Nanayakkara et al. (2025) compare two different codes: PROSPECTOR and FAST++ (M. Kriek et al. 2009). While both produce qualitatively consistent average SFHs for large samples, individual SFHs differ due to distinct assumptions regarding metallicity, SFHs, SSPs, and other parameters. In particular, the parametric nature of FAST++ (the BAGPIPES results from A. C. Carnall et al. 2024) favours less gradual mass build-up and narrower bursts than the more flexible SFH parametrization of PROSPECTOR; this results in stronger early-time enhancement (fig. 11 in T. Nanayakkara et al. 2025). Some scatter in derived properties such as stellar masses is therefore expected (J. Leja et

al. 2019b), and according to T. Nanayakkara et al. (2025) could be up to ≈ 0.4 dex.

Even within PROSPECTOR, choices such as the selection of SSP models and the priors used in non-parametric SFH reconstructions can influence the inferred properties of individual galaxies. These effects are typically minor, but they become more pronounced during the first ≈ 250 Myr of cosmic history, when old stellar populations dominate the observed spectrum and time resolution is inherently limited, likely contributing to the shorter observational time-scales. Incorporating rest-frame NIR data helps mitigate these uncertainties. In this work, we compare to the results of T. Nanayakkara et al. (2025), who use an exponentially increasing continuity prior between SFH bins, motivated by the average halo mass accretion rate over cosmic time (A. Dekel et al. 2013), which is consistent with expectations from a Λ CDM framework. By contrast, W. M. Baker et al. (2025a) also employ PROSPECTOR with a non-parametric SFH, but adopt a flat continuity prior (J. Leja et al. 2019a), use different lookback time binning, and rely on distinct SSP models: C3K (C. Conroy et al. 2009) in T. Nanayakkara et al. (2025) versus MILES (J. Falc3n-Barroso et al. 2011) in W. M. Baker et al. (2025a); among other methodological differences. Appendix D illustrates how these choices affect the recovered median SFH shapes of observed galaxies.

We emphasize that, although observational estimates of these SFH properties carry significant uncertainties, and we have not applied the 0.3 dex convolution error for M_* and SFR when selecting our sample for this analysis, there is still overall broad agreement between our COLIBRE predictions and the observational estimates across all measured properties. Performing SED-fitting of COLIBRE MQGs is left for future work and will help clarify these comparisons.

4.4 Dust and molecular hydrogen fractions of MQGs

Dust and molecular gas are fundamental components in quenched galaxies, closely tied to their SFH. Molecular gas, the primary fuel for star formation, is expected to be depleted in MQGs due to quenching mechanisms such as gas ejection or thermal heating, resulting in low gas reservoirs. Dust exhibits a similar decline: it originates from star formation processes, grows within the ISM, and can be destroyed or expelled by feedback. Importantly, dust grains facilitate the formation of molecular hydrogen, and their emission is commonly used as a proxy for molecular gas content (L. J. Tacconi, R. Genzel & A. Sternberg 2020). As such, molecular gas, dust, and star formation are intimately connected, and their co-evolution provides key insights into the quenching process.

Observations at lower redshift indicate that the dust (R. Gobat et al. 2018; G. E. Magdis et al. 2021) and molecular gas (J. Spilker et al. 2018) content of MQGs can evolve significantly. However, constraints for high-redshift quiescent galaxies remain limited: their emission is intrinsically faint, and until recently, telescopes lacked the sensitivity to detect them. Consequently, most available measurements are either upper limits from non-detections or are biased toward quiescent systems that are unusually gas- and dust-rich. Upcoming observations with instruments such as JWST MIRI and NIRSpec, deep ALMA surveys, and the future PRIMA space-based observatory (A. L. Faisst et al. 2025, covering the wavelength gap between the previous two) are expected to improve these measurements substantially, making theoretical predictions from simulations particularly valuable. COLIBRE provides an ideal testbed for such predictions, as it models dust

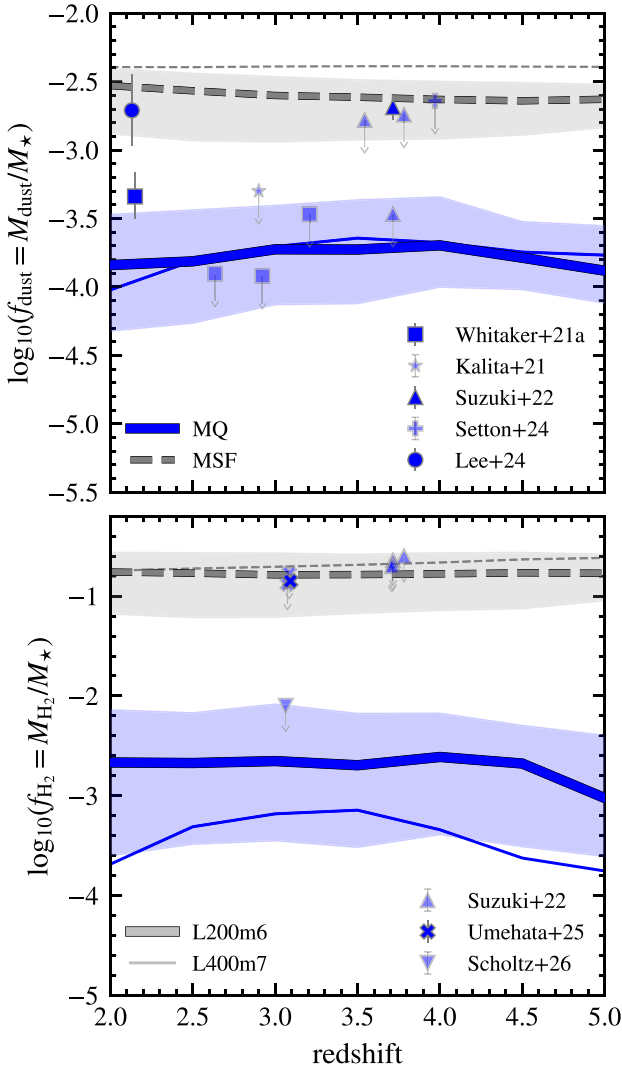


Figure 6. Dust fraction, $f_{\text{dust}} = M_{\text{dust}}/M_{\star}$, (top panel) and molecular hydrogen fraction, $f_{\text{H}_2} = M_{\text{H}_2}/M_{\star}$, (bottom panel) as a function of redshift at $2 \leq z \leq 5$ for L200m6. Median values for the MQGs (thick solid blue) and MSFGs (thick dashed grey) with the corresponding 16th and 84th percentile range at each selection redshift. At $z = 6$, MQGs are too few to define a median (2 galaxies), since we consider here all galaxies together rather than splitting by stellar mass bins. Thin lines show the corresponding median from L400m7. Observational data of MQGs are taken from the literature: for dust fractions from K. E. Whitaker et al. (2021a), B. S. Kalita et al. (2021), T. L. Suzuki et al. (2022), D. J. Setton et al. (2024), M. M. Lee et al. (2024), and for molecular hydrogen fractions from T. L. Suzuki et al. (2022), H. Umehata, M. Kubo & K. Nakanishi (2025), J. Scholtz et al. (2026). Arrows indicate upper limits from non-detections (also shown with a more faded colour).

self-consistently and captures a cold gas phase, with temperatures as low as ~ 10 K (Section 2). This enables a relatively realistic treatment of both components and a direct investigation of their content.

4.4.1 Dust fraction evolution

Fig. 6 shows the evolution of the dust fraction, $f_{\text{dust}} = M_{\text{dust}}/M_{\star}$, for MQGs as a function of selection redshift. The blue line in-

dicates the median value, with shaded regions representing the 16th and 84th percentile range. We find that the dust fraction remains roughly constant at $f_{\text{dust}} \sim 10^{-4}$ across $2 \leq z \leq 6$ for both L200m6 (thick) and L400m7 (thin lines) (beyond $z > 5$ there are only 2 MQGs for L200m6). For comparison, the dust fractions of massive star-forming galaxies (MSFGs; selected using the same stellar mass cut and sSFR threshold as in Section 3) are shown (dashed grey line). MSFGs exhibit dust fractions at least two orders of magnitude higher than MQGs, consistent with the expectation that ISM material in passive systems is removed by the feedback processes responsible for quenching, even at high redshift and over short time-scales (A. Leńiewska, J. Hjorth & C. Gall 2025).

Observational constraints on dust content are typically obtained from far-infrared/sub-mm continuum data by fitting a modified blackbody spectrum to the SED, assuming a fixed dust temperature and emissivity. These assumptions, however, introduce significant uncertainties, especially at high redshift (L. Sommovigo & H. Algera 2025). The top panel of Fig. 6 compiles current dust measurements and upper limits for spectroscopically confirmed quenched galaxies.⁶ M. M. Lee et al. (2024) report a single source with unusually high dust content, clearly at odds with the MQGs in our simulations and likely representing a rare dust-rich quenched system, same as one galaxy in T. L. Suzuki et al. (2022), and another one in K. E. Whitaker et al. (2021a) (although the dust fraction is slightly lower). These systems are rare in COLIBRE (Fig. 7), but there is overlap with the K. E. Whitaker et al. (2021a) system. Other observations shown with arrows and a more faded colour (B. S. Kalita et al. 2021; K. E. Whitaker et al. 2021a; T. L. Suzuki et al. 2022; D. J. Setton et al. 2024) are upper limits, which are consistent with our predictions. Additional measurements from J. C. Siegel et al. (2025) and W. Chang et al. (2026b) are not included in the figure. Most correspond to non-detections, except for one (likely dust-rich) system reported by W. Chang et al. (2026b), with $f_{\text{dust}} \approx 10^{-3}$ at $z \approx 3.5$, which also lies above the median trend predicted by COLIBRE.

4.4.2 Molecular hydrogen fraction evolution

Molecular gas observations are less reliable due to the absence of strong emission lines or direct H_2 detections. Molecular gas masses are therefore typically inferred either from dust continuum measurements, assuming a dust-to-gas ratio (DGR; e.g. K. E. Whitaker et al. 2021b; W. Chang et al. 2026a), or from emission of tracers such as CO, $[\text{C II}]$, or $[\text{C I}]$ (e.g. T. L. Suzuki et al. 2022), which rely on uncertain conversion factors. The bottom panel of Fig. 6 shows the median molecular gas fraction, here referring exclusively to H_2 , and its scatter in these systems. For L200m6, the molecular hydrogen fraction remains roughly constant over time and is about two orders of magnitude lower in MQGs than in star-forming counterparts, consistent with H_2 photodissociation driven by feedback processes. In L400m7, the molecular hydrogen fraction is about 1 dex lower. Visual inspection of individual evolutionary histories suggests a more efficient destruction of molecular gas by a more bursty feedback while the dust content

⁶M. M. Lee et al. (2024) and T. L. Suzuki et al. (2022) only account for photometric errors (the latter one not including $M_{\star}$ uncertainties); while K. E. Whitaker et al. (2021a) consider uncertainties additionally when varying the dust temperature.

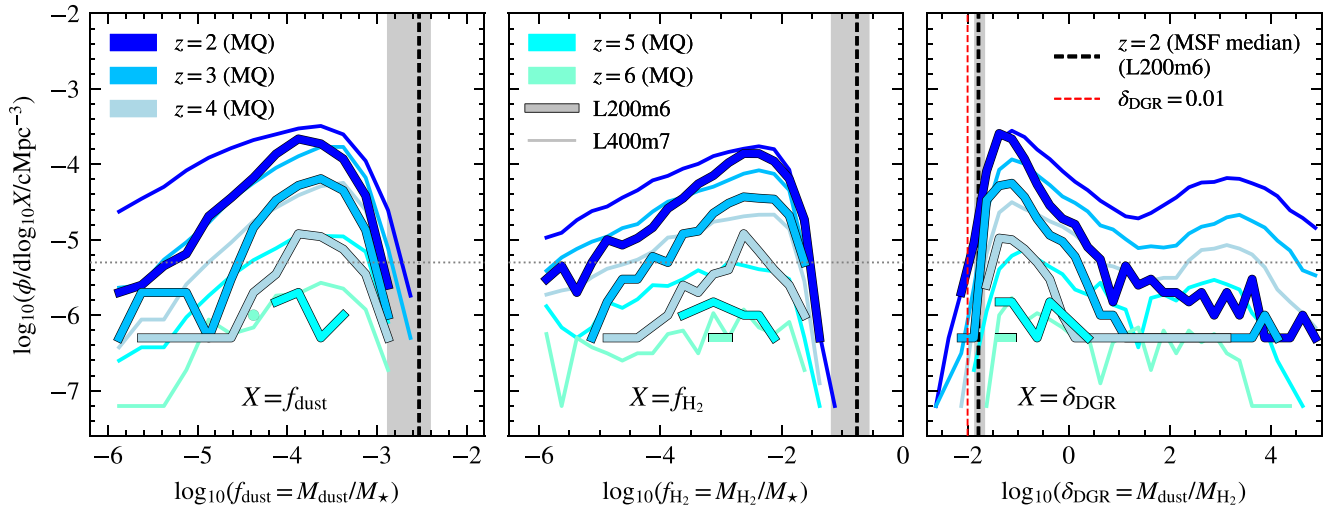


Figure 7. Distribution functions of dust fraction, $f_{\text{dust}} = M_{\text{dust}}/M_{\star}$ (left panel), molecular gas fraction, $f_{\text{H}_2} = M_{\text{H}_2}/M_{\star}$ (middle panel), and dust-to-gas ratio, $\delta_{\text{DGR}} = M_{\text{dust}}/M_{\text{H}_2}$ (right panel) for L200m6. Solid lines show the distributions for MQGs, colour-coded by selection redshift ($2 \leq z \leq 6$). Vertical dashed lines indicate the median values for MSFGs at $z = 2$, with shaded regions marking the corresponding 16th and 84th percentile range. Thin lines show the corresponding medians for MQGs from L400m7. In the right panel, the red vertical dashed line marks the canonical value $\delta_{\text{DGR}} = 0.01$. The horizontal dotted line denotes the threshold of 10 galaxies for L200m6, below which the statistics become unreliable.

remains comparable. A detailed investigation of this difference is beyond the scope of this paper.

Observational estimates not derived from the dust continuum, and thus not requiring corrections, as they trace H_2 alone, are included: most of them are upper limits either from [C I] (T. L. Suzuki et al. 2022) or CO (H. Umehata et al. 2025; Scholtz et al. 2026), illustrating the difficulty of measuring molecular gas in these systems due to their low reservoirs. An exception is one of the galaxies in H. Umehata et al. (2025), which represents the first CO detection of an early MQG. The system in J. Scholtz et al. (2026) hosts a neutral outflow that efficiently removed gas, indicative of ejective AGN feedback. An additional non-detection for a $z \approx 3.25$ MQG was reported by W. Wang et al. (2026), with $f_{\text{H}_2} \lesssim 10^{-1}$. The COLIBRE predictions are consistent with all the observational upper limits, although they do not reproduce the CO-detected system from H. Umehata et al. (2025), which likely corresponds to a gas-rich MQG. However, this interpretation depends on the adopted conversion factor between CO and H_2 , which itself carries substantial uncertainties (A. D. Bolatto, M. Wolfire & A. K. Leroy 2013). The inferred gas masses also depend on the tracer used. C. D’Eugenio et al. (2026) analysed the same sample from H. Umehata et al. (2025), together with an extra non-detected system, using [C II] observations and found a difference of up to ~ 0.4 dex for the CO-detected galaxy.

4.4.3 Distribution functions

In Fig. 7, we show (from left to right) the distributions of the dust fraction, f_{dust} ; molecular hydrogen fraction, f_{H_2} ; and dust-to-gas ratio (DGR), $\delta_{\text{DGR}} = M_{\text{dust}}/M_{\text{H}_2}$ for L200m6 (thick) and L200m7 (thin lines). Each coloured line represents the distribution at a different redshift, while vertical dashed lines indicate the median values for MSFGs of the same stellar mass.

Focusing on f_{dust} (left panel), for L200m6 we see that typical values cluster around $f_{\text{dust}} \sim 10^{-4}$ but the distribution has extended tails. Some galaxies reach $f_{\text{dust}} \sim 10^{-3}$, comparable to values found in MSFGs. These likely represent galaxies that have not

yet removed their dust, consistent with the fact that systems with $f_{\text{dust}} > 10^{-4}$ show shorter median quenching times ($t_{\text{q}} \sim 0.4$ Gyr) than those with $f_{\text{dust}} \leq 10^{-4}$ ($t_{\text{q}} \sim 0.7$ Gyr) at $z = 2$. Appendix F shows that this correlation is shallow and exhibits substantial scatter, though, likely reflecting a mixture of systems that are still quenching and others that have begun to reform their dust content. This behaviour is visible in the individual galaxy evolutionary histories and gas/dust images in appendix B of Paper II.

The L400m7 simulation exhibits a higher distribution, as was seen for the number densities. Interestingly, it also shows an increased number of galaxies with extremely low dust fractions ($f_{\text{dust}} < 10^{-4}$), particularly at $z = 2$; a distinct feature confirmed by normalising the distribution by the total number of galaxies at each redshift. This may suggest that a more bursty feedback implementation can reduce dust content more dramatically. A similar broadening at the low-dust end is observed in L200m7h. This may occur because jets affect dust more strongly. In SIMBA, the combination of AGN feedback and fast/slow quenching determines the future fate of dust: the jet mode removes dust over short (slow quenchers) or long (fast quenchers) time-scales, while radiative-mode systems allow dust regrowth in the ISM (G. Lorenzon et al. 2025). Prospective work could explore whether similar correlations exist in COLIBRE.

Dust may regrow in the ISM or through external processes after quenching, potentially linked to AGN feedback. Both scenarios have been proposed in both observations (e.g. D. Donevski et al. 2023; T. Kakimoto et al. 2024) and other simulations, including SIMBA (G. Lorenzon et al. 2025). SIMBA, like COLIBRE, includes explicit ISM dust growth, but following R. McKinnon et al. (2017). Unlike COLIBRE, however, SIMBA’s dust budget is dominated by direct stellar production, driven by the order-of-magnitude larger stellar dust yields adopted from E. Dwek (1998) (see fig. 1 in J. W. Trayford et al. 2026), and it does not model the cold ISM.

Focusing on the molecular hydrogen fraction (middle panel), we see that the peak values for the quenched population are more than an order of magnitude lower than those of star-forming galaxies for L200m6, consistent with gas depletion

due to quenching. Nevertheless, a fraction of galaxies retain significant molecular gas reservoirs, with $f_{\text{H}_2} > 10^{-2}$. These are relatively high-dust content galaxies (see the correlation between f_{dust} and f_{H_2} in Appendix F) that quench at later times.

L400m7 again shows a larger number of galaxies with extremely low molecular gas fractions ($f_{\text{H}_2} < 10^{-4}$), across the entire redshift range analysed, a trend confirmed by normalizing the histogram by the number of galaxies at each redshift. This supports the idea that burstier feedback removes molecular gas more efficiently (at least at $z > 2$). In contrast, L200m7h produces results similar to L200m6 for f_{H_2} .

The DGR distribution (right panel) reveals that passive galaxies exhibit a wide scatter in this quantity, with median values intriguingly higher ($\delta_{\text{DGR}} \sim 0.1$) than those of star-forming galaxies. Gas metallicity (measured within the 50 kpc fiducial aperture as the gas-mass-weighted linear sum of the diffuse oxygen-to-hydrogen ratio, excluding metals locked into dust) for MQGs is lower and yet, they have a higher DGR (e.g. the median values for $12 + \log_{10}(\text{O}/\text{H})$ at $z = 2$ are ≈ 8.14 for MQGs and ≈ 8.49 for MSFGs). This suggests that molecular gas is destroyed more rapidly than dust. L400m7 (and similarly L200m7h) predicts a pronounced local peak in DGR around $\delta_{\text{DGR}} \sim 10^3$, corresponding to galaxies that retain significant dust, potentially linked to the more efficient feedback and destruction of H_2 in these simulations.

Here, we omit galaxies with $M_{\text{H}_2} = 0$. In L200m6, only ≈ 2 per cent of MQGs at $z = 2$ fall into this category (and 90 per cent of those also have $M_{\text{dust}} = 0$), with the fraction decreasing toward higher redshifts. The $z = 2$ median value for MSFGs is computed including the $M_{\text{H}_2} = 0$ cases, although in practice none occur.

The DGR results support the idea that dust content may more closely reflect the nature of the quenching feedback (e.g. AGN-driven), with molecular gas and dust evolving on different time-scales. This behaviour has been reported using SIMBA (G. Lorenzon et al. 2025). However, in SIMBA the H_2 content is computed using the M. R. Krumholz & N. Y. Gnedin (2011) prescription rather than by resolving the cold ISM, and its DGRs are systematically lower than in COLIBRE. The latter difference arises from the contrasting dust models: in SIMBA, stellar yields play the dominant role, while ISM dust growth is insufficient to offset them, resulting in systematically lower dust masses and DGRs. In contrast, J. W. Trayford et al. (2026) show that dust growth via accretion in the cold, dense ISM (along with grain size transfer processes) dominates in COLIBRE. Removing this channel reduces the cosmic dust density by more than 0.5 dex relative to the fiducial model (see their section 4.2).

Moreover, the common observational assumption of a constant DGR of ~ 0.01 (red vertical dashed line) for the total ISM gas content (not only for the dense, cold H_2 ; see e.g. K. E. Whitaker et al. 2021a; D. J. Setton et al. 2024) may be an oversimplification, as even when computing the ratio as $M_{\text{dust}}/(M_{\text{HI}} + M_{\text{H}_2})$ including neutral hydrogen, the model predicts substantially lower DGRs, with median values of ~ 0.001 for MQGs.

More observational data are needed to robustly test these predictions. While recent programs are beginning to address this, current samples remain small. Future surveys will increase the number of detected objects and may enable stacking analyses for dust and molecular gas measurements, including non-detections, following the approach of S. Adscheid et al. (2025), but for spectroscopic samples. This will be crucial since, as noted earlier, existing observations are biased toward dust- and gas-rich systems.

4.5 Sizes of MQGs

Quenched galaxies are known to evolve in size, with trends differing from those of their star-forming counterparts at $z \lesssim 3$. A. van der Wel et al. (2014) find that quenched systems are more compact than star-forming galaxies and exhibit a more dramatic evolution, reaching much smaller sizes near $z = 3$ than their descendants at $z \approx 0$ (F. Buitrago et al. 2008; P. G. van Dokkum et al. 2008; S. E. Cutler et al. 2022). Thanks to the high resolution of *JWST*, direct measurements of rest-frame NIR and optical sizes are now possible up to $z \approx 5$. Observations reveal that high- z MQGs are very compact, with typical effective radii below 1 kpc (C. C. Williams et al. 2024; K. Ito et al. 2024; L. Wright et al. 2024; L. Kawinwanichakij et al. 2026). These studies also report negative colour gradients (K. Ito et al. 2024; L. Wright et al. 2024), indicative of older stellar populations in the centre, which supports an inside-out growth scenario.

In simulations, reproducing such compact sizes can be challenging because of resolution limitations (R.-S. Remus & L. C. Kimmig 2025). It is therefore interesting to examine the sizes of MQGs in COLIBRE.

4.5.1 Results and discussion

The top panel of Fig. 8 shows the galaxy mass–size relation for MQGs from the fiducial L200m6 simulation, where sizes are defined by the stellar half-mass radius averaged over three random projections (r_* ; see Section 3). These are shown as solid coloured lines for $2 \leq z \leq 4$ for the fiducial simulation. Dashed lines indicate the corresponding relation for MSFGs at the same redshifts. Overall, we find no significant differences between the two populations, although MQGs appear slightly more compact at the low-mass end ($M_* \lesssim 10^{10.5} M_\odot$) at $z = 2$. This result is consistent with K. Ormerod et al. (2024), who report no distinction between both populations at $z > 3$; but contrasts with A. van der Wel et al. (2014), who find that quenched systems are more compact even at $z \approx 2 - 3$, as well as L. Yang et al. (2025), where this trend is extended to $z \approx 4$.

Blue arrows indicate the gravitational softening length, ϵ_{prop} , at different redshifts (see Table 1). Gravity is softened below $3\epsilon_{\text{prop}}$. The flattening of the median sizes of low-mass galaxies occurs on scales of order ϵ_{prop} , suggesting that caution is needed when interpreting predictions on these scales. However, the flattening at our low-mass end (when including all systems, MQGs, and MSFGs) is also present in L400m7 (see Appendix E), which has a larger softening length, as well as in L025m5 and L050m5, which have a smaller softening length (fig. 10 in A. D. Ludlow et al. 2026). This suggests that the shape of the size–mass relation is not dictated by softening. A. D. Ludlow et al. (2023) reported a similar result for EAGLE (see their fig. 8), where median sizes flatten at low masses on a scale comparable to the softening length, a result they attributed to poor DM mass resolution. Given that the size–mass relations in COLIBRE converge well with respect to both $3\epsilon_{\text{prop}}$ and m_{DM} , their shapes appear robust to numerical effects. Furthermore, A. D. Ludlow et al. (2026) found that the median stellar surface density profiles in COLIBRE are independent of resolution down to radii substantially smaller than ϵ_{prop} , again suggesting that softening length itself does not limit our ability to resolve galaxy structure.

We find that galaxies become larger with decreasing redshift, highlighting their size evolution. The most massive systems are also more extended, and the slope of the mass–size relation ap-

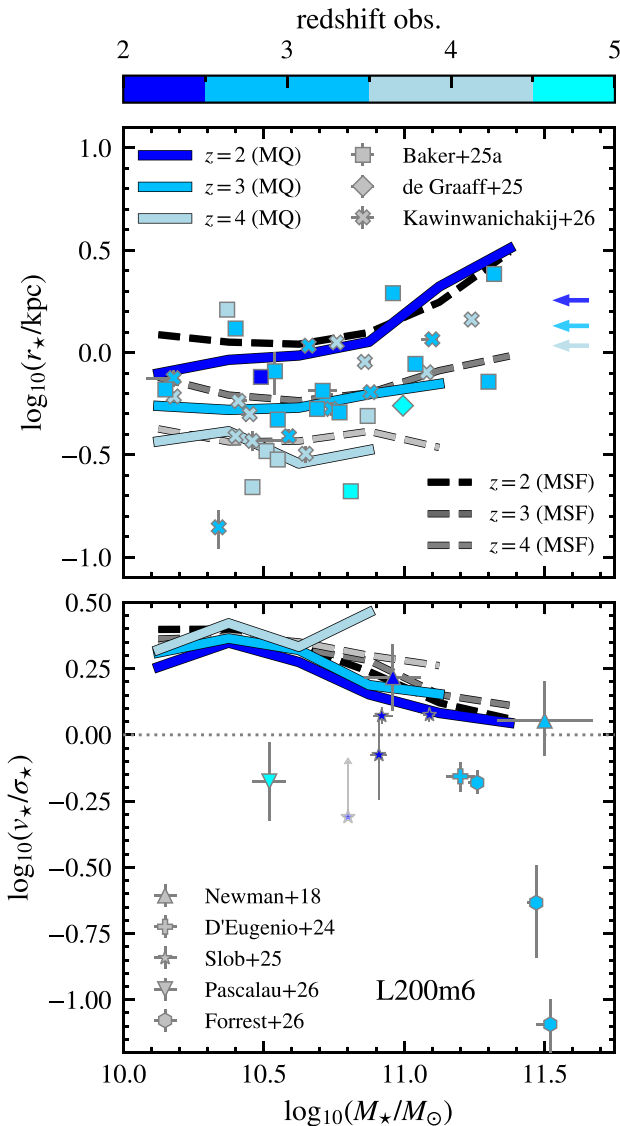


Figure 8. Stellar size–mass relation, with r_* defined as the half-mass radius (*top panel*); and v_*/σ_* versus stellar mass relation (*bottom panel*) for L200m6. Solid blue-palette lines show the median predictions for MQGs, and dashed grey-palette lines for MSFGs at different selection redshifts, $2 \leq z \leq 4$. At $z > 4$, the number of massive quenched systems is too small to define a median split in stellar mass bins (9 galaxies at $z = 5$ and 2 at $z = 6$). Observational data of MQGs are from W. M. Baker et al. (2025a), A. de Graaff et al. (2025), and L. Kawinwanichakij et al. (2026) for the size–mass relation (defined as half-light radius), and A. B. Newman et al. (2018), F. D’Eugenio et al. (2024), M. Slob et al. (2025), R. G. Pascalau et al. (2026), and B. Forrest et al. (2026) for the v_*/σ_* –mass relation. Arrows in the error bars indicate lower limits for galaxies where rotational velocity could not be constrained (also shown with a more faded colour). Blue arrows in the size–mass relation mark the gravitational softening length, ϵ_{prop} , at each redshift.

pears to change around $M_* \sim 10^{10.8} M_\odot$, at least in the $z = 2$ results. This trend is consistent with Z. Ji et al. (2026), who identify a similar transitional mass scale for MQGs, where more massive objects evolve more rapidly with likely higher *ex situ* stellar mass contributions. We also find that the most compact galaxies tend to have later formation times (with median $t_{50} \approx 1.3$ Gyr for $r_* \leq$

1 kpc, while $t_{50} \approx 1.5$ Gyr for $r_* > 1$ kpc at $z = 2$, and similar at other redshifts as shown in Appendix F) in agreement with observational results (see fig. 11 in L. Kawinwanichakij et al. 2026).

The galaxy sizes in our analysis are defined as the stellar half-mass radius. Observational studies, however, typically use half-light radii, and are influenced by projection effects (although in our case, averaging over three random projections helps to minimize these). Observationally, galaxy sizes are typically measured by fitting a J. L. Sérsic (1968) profile to the surface brightness distribution (including point spread function (PSF) convolution) and deriving the half-light effective radius. The inferred sizes depend not only on the fitting algorithm used (B. Häussler et al. 2007) but also on the wavelength probed (K. A. Suess et al. 2019), with NIR measurements offering the most reliable tracer of stellar mass (E. F. Bell & R. S. de Jong 2001). For this reason, we introduce NIR-based observations in Fig. 8, despite the methodological and sample selection differences with simulations. Taking these caveats into account, the agreement with A. de Graaff et al. (2025), L. Kawinwanichakij et al. (2026), W. M. Baker et al. (2025a) appears to be of a qualitatively good nature.

4.6 Kinematics of MQGs

We also examine the kinematics of MQGs, characterized by the stellar rotation-to-dispersion velocity ratio, v_*/σ_* . At $z \approx 0$, MQGs are primarily dispersion-dominated, but their rotational support increases at higher redshift (P. G. van Dokkum et al. 2008; A. van der Wel et al. 2011; S. Belli, A. B. Newman & R. S. Ellis 2017). Measuring stellar kinematics in these compact systems is challenging and, before *JWST*, was only feasible in strongly lensed cases (A. B. Newman et al. 2018). Observationally, v_*/σ_* is derived from spectral absorption features via line fitting, which requires very high signal-to-noise ratios and is particularly demanding at high redshift. Additional systematics arise from wavelength coverage, fitting codes, and modelling assumptions (S. Belli et al. 2017). *JWST* has now opened a new window: with NIRSpec/IFU and NIRSpec/MSA, spatially resolved kinematics can be obtained even for faint, compact galaxies, complemented by forward kinematic modelling (M. Slob et al. 2025; R. G. Pascalau et al. 2026). These advances highlight the importance of simulation-based predictions for interpreting observations.

4.6.1 Results and discussion

The bottom panel of Fig. 8 shows COLIBRE predictions for v_*/σ_* (computed as in Section 3.3) as a function of stellar mass in the range $2 \leq z \leq 4$ for L200m6. Solid blue-palette lines indicate the median values for MQGs, while dashed grey-palette lines show MSFGs. Observational results from lensed systems (A. B. Newman et al. 2018) and *JWST* (F. D’Eugenio et al. 2024; M. Slob et al. 2025; R. G. Pascalau et al. 2026; B. Forrest et al. 2026) are included for comparison.

The horizontal dotted line ($v_*/\sigma_* = 1$) serves as a reference. There is a clear offset between the simulation predictions and the observations: most COLIBRE MQGs lie above this threshold, appearing more rotationally supported than the observed galaxies. However, it is important to recall that the simulation values represent upper limits relative to the observations, due to differences in definitions and the caveats (Section 3.3). In addition, some observational values (e.g. B. Forrest et al. 2026) are reported using the spin parameter λ_* and have been converted to v_*/σ_* using the

relation in M. Cappellari (2016); apart from differences in sample selection. A more detailed comparison that closely mimics the observational analysis is left for future work.

Current observations suggest MQGs are commonly fast rotators at high redshift (R. G. Pescalau et al. 2026). One exception is the slow rotator reported by B. Forrest et al. (2026, the lowest data point), likely the result of a major merger or isotropic gas infall (values around $v_*/\sigma_* = 0.4$ are generally taken to indicate dispersion-dominated systems; M. Cappellari 2016). In COLIBRE, individual $z = 2$ MQGs show values as low as $v_*/\sigma_* \approx 0.6$ in the bottom right panel of Fig. F1. This would not correspond to slow rotators under the observational definition. However, we cannot draw this conclusion because the observational and simulation quantities are defined differently.

Both MQGs and MSFGs in COLIBRE become more dispersion-supported towards lower redshift, with the most massive systems showing the strongest bulge dominance by $z \lesssim 3$. At $z = 4$, there is a tentative increase in the rotational support of the most massive MQGs. Although this trend is based on a small number of objects, it may indicate that strongly rotationally supported discs are required to assemble such massive systems at very early cosmic times. At $z \gtrsim 2$, however, MQGs and MSFGs exhibit similar kinematics, implying that quenching preserves discs and precedes morphological transformation. This is consistent with the findings of L. C. Kimmig et al. (2025), who also report that the majority of systems are fast rotators, with a much smaller population of slow rotators formed by $z > 4$. Predictions for L400m7 are provided in Appendix E, where the trend reverses, with morphological transformation occurring before quenching. This is likely a consequence of its larger softening length, limiting the ability to resolve the internal structure of galaxies.

In the EAGLE simulations, C. d. P. Lagos et al. (2022) showed this behaviour with galaxies quenching first, and only later (≈ 2 Gyr) evolving into slow rotators through mergers (particularly dry mergers) that increase masses, sizes, and erode rotational support (see also C. d. P. Lagos et al. 2018). Feedback mechanisms do not appear to affect kinematics directly, as seen in F. D'Eugenio et al. (2024), where a rotation-supported system showed clear evidence of ejective feedback. The absence of star-forming gas in quenched galaxies likely makes mergers (particularly dry mergers) more effective at disrupting rotational support. This may explain why MQGs in COLIBRE show slightly lower v_*/σ_* than coeval MSFGs by $z \approx 2$, in agreement with R. G. Pescalau et al. (2026). However, this contrasts with the findings of M. Shuntov et al. (2026), who report that most high- z MQGs are bulge-dominated, implying that a morphological transformation occurred before quenching.

This emerging population of slow rotators is found primarily in dense environments or recently quenched systems, consistent with our finding of a correlation between dispersion and environment (Appendix F). More extended objects are also more dispersion-supported (lower left panel of Fig. F1), supporting the merger-driven scenario, since mergers increase size.

5 CONCLUSIONS

We have analysed predictions from the new COLIBRE hydrodynamical simulations in their multiple volumes, resolutions, and AGN feedback models for the population of MQGs; defined as galaxies with $M_* > 10^{10} M_\odot$ and $sSFR < 0.2/t_{\text{age}}$ at high-redshift ($z \geq 2$). Recent *JWST* surveys have suggested that MQGs are more abundant than previously observed. Given the poorly un-

derstood nature of these MQGs and current observational limitations, we investigated what the state-of-the-art COLIBRE galaxy formation model predicts for a wide range of their properties. Our main findings are as follows:

(i) **Number densities:** We studied how MQG number densities change across the COLIBRE simulations (Section 4.1.1). We find a clear resolution effect: higher-resolution runs produce less quenching, while the hybrid AGN feedback model yields even fewer quenched systems, underpredicting the observational estimates. The fiducial L200m6 simulation yields results broadly consistent with the most recent and robust observational estimates (those covering larger areas or larger spectroscopic samples), especially after we include uncertainties to the simulation values that exemplify observational uncertainties. Compared to most galaxy formation models that also reproduce observations at $z = 0$, COLIBRE predicts higher number densities (Fig. 3), driven directly by the importance of super-Eddington accretion at high redshift (E. Chaikin et al. 2026c) and indirectly thanks to the explicit modelling of the cold gas phase.

(ii) **Stellar mass functions:** MQG stellar mass functions in COLIBRE agree with the latest observations when uncertainties are considered, and outperform other models (Fig. 4).

(iii) **Star formation histories:** MQGs show good qualitative agreement with observationally inferred SFHs (Section 4.3), with extended formation times (median $t_{50} \approx 0.5\text{--}1.5$ Gyr), rapid quenching (median $t_q \lesssim 0.6$ Gyr), and evidence of strong starbursts.

(iv) **Dust and molecular hydrogen:** With its explicit modelling of dust and a cold ISM phase, COLIBRE predicts that MQGs have much lower dust and molecular hydrogen fractions (medians $f_{\text{dust}} \sim 10^{-4}$ and $f_{\text{H}_2} \sim 10^{-2.5}$) than massive star-forming counterparts, with potential evidence for dust regrowth (Section 4.4). Although current observations are limited in sample size and biased toward dust- and gas-rich systems, they generally agree with these predictions, with only a few cases showing very high dust and gas fractions (Fig. 6).

(v) **Stellar sizes and kinematics:** MQG sizes (in terms of the half-mass radius) and kinematics are broadly similar to those of coeval MSFGs (Fig. 8), suggesting a decoupling between quenching and morphological transformation at $z \gtrsim 2$, with the latter likely driven by subsequent mergers given the subtle signs of increased dispersion support by $z \approx 2$.

Taken together, the comparison between COLIBRE and current observations shows encouraging qualitative and often quantitative agreement across a wide range of properties. Although systematic differences remain, likely in some part attributable to observational uncertainties, sample selection, and measurement techniques, the level of tension previously reported between models and observations has decreased. We conclude that this convergence reflects progress in both simulations and observations. This also highlights the need for more accurate modelling of the physical processes that shape MQGs, as well as larger, deeper spectroscopic samples to further reduce systematics. We note that this observational field is rapidly evolving, so measurements may continue to change. Closing this gap will be key to advancing our understanding of the earliest quenched galaxies and their role in galaxy evolution.

Several caveats must be considered. From the simulation side, galaxy formation models are calibrated in the local Universe, and results at high- z remain sensitive to choices in e.g. AGN feedback modelling and uncertain parameters tied to BH physics,

relevant for MQGs (C. d. P. Lagos et al. 2025; F. Huško et al. 2026), as we further discuss in Paper II. From the observational side, caveats related to sample selection, wavelength coverage, and measurement techniques (discussed throughout this paper) must be borne in mind when interpreting results. Nevertheless, when these factors are accounted for, this work, together with Paper II, provides robust predictions within the COLIBRE model for the population of MQGs, offering insights into the physical mechanisms that shape their origin and evolution, and in the process easing the tension between observations and simulations. Its predictions also offer guidance for upcoming surveys, given current observational limitations.

ACKNOWLEDGEMENTS

We thank the anonymous referee for their constructive feedback. ACG acknowledges Research Training Program and ICRAR scholarships. ACG acknowledges support for this project by the University of Western Australia via a Research Collaboration Award. This work used the DiRAC@Durham facility managed by the Institute for Computational Cosmology on behalf of the STFC DiRAC HPC Facility (www.dirac.ac.uk). The equipment was funded by BEIS capital funding via STFC capital grants ST/K00042X/1, ST/P002293/1, ST/R002371/1, and ST/S002502/1, Durham University and STFC operations grant ST/R000832/1. DiRAC is part of the National e-Infrastructure. This project has received funding from the Netherlands Organization for Scientific Research (NWO) through research programme Athena 184.034.002. WMB would like to acknowledge support from DARK via the DARK Fellowship. This work was supported by a research grant (VIL54489) from VILLUM FONDEN. ABL acknowledges support from the Italian Ministry for Universities (MUR) program ‘Dipartimenti di Eccellenza 2023-2027’ within the Centro Bicocca di Cosmologia Quantitativa (BiCoQ), and support by UNIMIB’s Fondo Di Ateneo Quota Competitiva (project 2024-ATEQC-0050). EC acknowledges support from STFC consolidated grant ST/X001075/1. SP acknowledges support from the Austrian Science Fund (FWF) through grant-DOI: 10.55776/V982. JT acknowledges support from an STFC Early Stage Research and Development grant (ST/X004651/1). Minor typos, grammar, and spelling mistakes were identified with the assistance of ChatGPT-4o⁷ when preparing this document. No passages of text or structural outlines for this paper were created with the help of any large language models.

DATA AVAILABILITY

The data underlying this article will be provided upon reasonable request to the corresponding author.

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APPENDIX A: SELECTION CRITERIA OF MQGS

We analyse how different selection criteria for MQGs may affect our results, focusing on the evolution of number densities in our fiducial L200m6 simulation (Fig. A1).

First, we test the impact of the aperture used by SOAP to compute M_* and SFR (see Section 3). In the left panel, we compare our fiducial 50 pkpc spherical aperture with 1 pkpc (similar to the observational aperture to measure *JWST* colours) and 10 pkpc. The results show minor differences for the 10 pkpc aperture, while the number densities increase slightly for the smallest aperture. This is likely because some star-forming galaxies are misclassified as quiescent when outer, star-forming regions are excluded, leading

to better agreement with the observational data. This behaviour is consistent with the compact nature of MQGs (Section 4.5).

Second, we examine how the definition of SFR might bias the selection. Observations typically measure SFRs averaged over different time-scales depending on wavelength coverage and band availability (R. C. Jr Kennicutt 1998). While our fiducial choice is the instantaneous SFR, the middle panel shows results using 10 Myr and 100 Myr averages, representative of observational tracers. The number densities remain essentially unchanged for the 10 Myr average, indicating that these galaxies have been quiescent on average over such time-scales. This is consistent with spectroscopic observations tracing star formation over similar time-scales (Y. Zhang et al. 2026). In contrast, the 100 Myr average produces significantly lower number densities, particularly at $z > 3$. This suggests that the simulated SFHs remain bursty over ~ 100 Myr time-scales, causing some systems to move out of the quiescent category when averaged. These galaxies therefore appear to have quenched only recently, consistent with the discussion in Section 4.3.2 and with observational results from E. Merlin et al. (2025). On the other hand, some observations still recover high number densities even when using 100 Myr-averaged SFRs (W. M. Baker et al. 2025c), reflecting a smoother decline in star formation and a more gradual stellar mass build-up, as also seen in Appendix D. The impact of the adopted SFR time-scale on observed MQG number densities remains open.

Finally, in the right panel, we explore alternative definitions of ‘massive’ and ‘quenched’. Excluding satellites (blue–black bi-coloured solid line), identified by HBT-HERONS, does not have a great impact, particularly at $z \gtrsim 3$. These satellite galaxies are quenched by AGN feedback, as evidenced by their more massive BHs (fig. 5 of Paper II). In contrast, quenching due to environmental processes is not yet dominant at such high- z . The central-satellite hierarchy is determined with HBT-HERONS: in FoF groups with multiple substructures, the central subhalo is identified by retained mass and orbital kinetic energy in the group’s centre-of-mass frame. At the high- z we are interested in, the number fraction of MQG satellites relative to centrals is

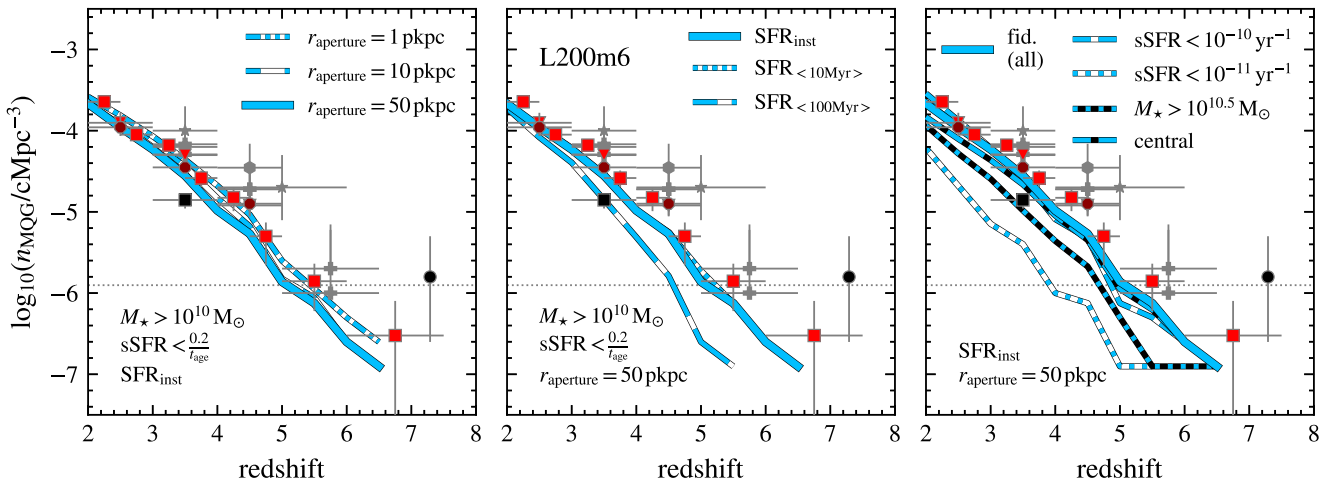


Figure A1. Comoving number density of MQGs as a function of redshift for different selection criteria. The panels show variations in aperture size for galaxy properties (*left*), instantaneous versus time-averaged SFR definitions (*middle*), and alternative ‘massive’ and ‘quenched’ thresholds (*right*), applied to the fiducial L200m6 simulation. Blue solid lines indicate the fiducial MQG selection described in Section 3.1: $r_{\text{aperture}} = 50$ pkpc, $\text{SFR}_{\text{inst}} M_* > 10^{10} M_\odot$, and $\text{sSFR} < 0.2/t_{\text{age}}$. Observational data are the same as in Fig. 2. The horizontal dotted line denotes the threshold of 10 galaxies, below which the statistics become unreliable.

≈ 0.31 at $z = 2$, ≈ 0.26 at $z = 3$, ≈ 0.13 at $z = 4$, ≈ 0.18 at $z = 5$, and 0.00 at $z = 6$ for L200m6.

For quenching, adopting a constant threshold of $\text{sSFR} < 10^{-10} \text{ yr}^{-1}$, as often in the literature (e.g. A. Weibel et al. 2025; Y. Zhang et al. 2026), yields results similar to our redshift-dependent definition, with differences emerging mainly at $z \gtrsim 5$ where both definitions diverge more. A stricter cut of $\text{sSFR} < 10^{-11} \text{ yr}^{-1}$ produces much lower number densities, showing that most of the MQGs in COLIBRE retain some residual star formation. This threshold has frequently been used to identify quiescent galaxies at high redshift in pre-*JWST* studies (e.g. M. Stefanon et al. 2013), although some *JWST* sources also satisfy this criterion (e.g. some galaxies in T. Nanayakkara et al. 2025). Increasing the mass threshold to $M_* > 10^{10.5} M_\odot$ reduces number densities slightly, indicating that MQGs are massive but not extreme outliers.

APPENDIX B: THE EFFECT OF ERROR CONVOLUTION ON THE NUMBER DENSITIES OF MQGS

In Fig. B1, we illustrate the impact of adopting different values for the width of the Gaussian-distributed convolution applied to the simulation properties independently (M_* and SFR), intended to represent a reasonable error budget for these quantities. The top panel shows the effect of increasing the common standard deviation applied to both M_* and SFR. The bottom panel presents a similar analysis but fixing the width of the M_* convolution to 0.1 dex, while varying the width applied to the SFR in the range 0.1 – 0.4 dex. This choice is motivated by the fact that stellar mass estimates are generally better constrained than SFRs. In both panels, we find that increasing the convolution scatter leads to higher inferred number densities, as expected. Even when adopting a relatively small error budget for stellar masses (bottom panel), the resulting number densities increase sufficiently due to the SFR error to more consistently reproduce the latest observational data (in red and dark red).

E. Chaikin et al. (2026b) report a similar effect, showing that adding only scatter to simulated M_* values (comparable to the uncertainties introduced in Section 4.1.1) has a significant impact on MQG number densities. Specifically, they find that increasing the scatter raises the number densities at higher redshifts and in higher stellar-mass bins. The dependence on scatter amplitude is explored in their fig. D3, albeit using a slightly different sample selection and including Poisson uncertainties. In general, a larger scatter produces a stronger increase in the number densities at fixed redshift and stellar mass.

Fig. B1 further shows that uncertainties in stellar mass have the largest impact for these systems, as the effect is much weaker when perturbing SFRs alone (lower panel). Although not shown explicitly, we verified this by varying σ_{M_*} while keeping $\sigma_{\text{SFR}} = 0.1$ dex fixed, finding a substantially stronger impact. This arises because (i) M_* enters both the ‘massive’ and ‘quenched’ selection criteria, and (ii) galaxies extend significantly into the quenched region in the SFR– M_* plane at intermediate masses ($10^9 M_\odot < M_* < 10^{10} M_\odot$), allowing them to scatter into the MQG selection, particularly at high redshift ($z \approx 6$). In contrast, the L400m7 simulation is largely unaffected by the error convolution in the lower panel of Fig. 2. This is partly because more efficient AGN feedback in L400m7 drives a larger quenched population in the SFR– M_* plane, so that the applied scatter moves galaxies into and out of the MQG selection more symmetrically, without introducing a strong net bias. By comparison, in L200m6 quenching is less

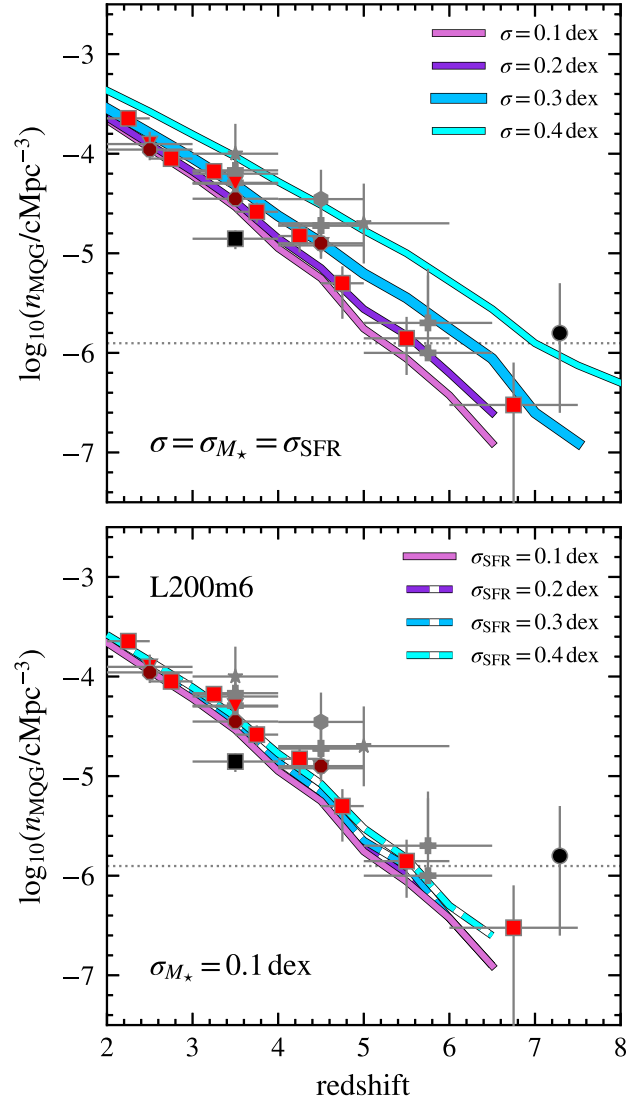


Figure B1. Comoving number density of MQGs as a function of redshift for different values of the Gaussian-distributed width applied independently to M_* and SFR when convolving these quantities with potential observational uncertainties. The panels show variations in the convolution width applied to both M_* and SFR when the two are assigned the same value (top), and variations in the SFR convolution width while fixing the M_* scatter to 0.1 dex (bottom); applied to the fiducial L200m6 simulation. The blue solid line indicates the fiducial error budget used in Sections 4.1 and 4.2: 0.3 dex in both M_* and SFR. Observational data are the same as in Fig. 2. The horizontal dotted line denotes the threshold of 10 galaxies, below which the statistics become unreliable.

efficient and galaxies retain higher residual SFRs. As a result, the quenched population is rarer, making the MQG selection more sensitive to perturbations introduced by the observational error convolution.

The exact impact of the different sources of errors in the derived stellar masses and SFRs has been subject to extensive discussion in the literature (e.g. A. S. G. Robotham et al. 2020; C. Pacifici et al. 2023; S. Bellstedt & A. S. G. Robotham 2025). For the population of high- z MQGs, T. Nanayakkara et al. (2025) show that random errors in stellar masses have

a magnitude ≈ 0.09 dex, but that systematic errors can shift the derived values by as much as ≈ 0.4 dex. Our purpose is not to isolate the magnitude of different errors, but to demonstrate the effect an error budget of $\approx 0.1 - 0.4$ dex can have on the derived number densities of MQGs. A more realistic calibration of these observational systematics will require forward modelling of simulated COLIBRE MQGs to generate mock photometric and spectroscopic observations, followed by analysis with modern SED-fitting tools (Nanayakkara et al., in preparation).

APPENDIX C: ERROR CONVOLUTION ON THE STELLAR MASS FUNCTIONS OF MQGS

In this appendix, we examine the impact of applying a Gaussian-distributed convolution, centred at 0 with a width of $\sigma = 0.3$ dex, to the simulated stellar masses and SFRs independently when computing the SMF of MQGs in the fiducial L200m6 simulation. The error-convolved SMF at $z=3$ is shown in Fig. 4 and compared with predictions from other galaxy formation and evolution models; here, we extend this analysis to the full redshift range $2 \leq z \leq 7$ in Fig. C1. In Fig. 4, we found that, relative to the latest *JWST* observations, the highest-mass end of the SMF and the predictions at $z \gtrsim 5$ lie towards the lower end of the observationally inferred range. When the same error convolution is applied across all redshifts, we find that it increases the number of systems in both regimes, thereby alleviating these discrepancies once potential uncertainties in the derivation of stellar masses and SFRs are taken into account.

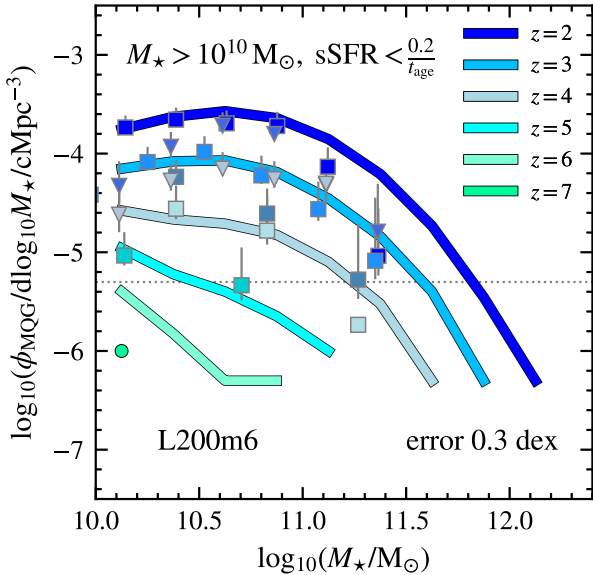


Figure C1. SMF of MQGs at different redshifts $2 \leq z \leq 7$ for the fiducial L200m6 simulation, where M_* and SFR values in the simulations are convolved independently with a Gaussian distribution (mean 0, standard deviation 0.3 dex) representing a reasonable error budget for these quantities. Observational data are the same as in Fig. 4. The horizontal dotted line denotes the threshold of 10 galaxies, below which the statistics become unreliable.

APPENDIX D: STAR FORMATION HISTORIES OF MQGS

We present in this appendix a comparison between the SFH shapes of MQGs selected from our fiducial L200m6 simulation and those derived observationally via SED fitting. These SFHs are used to obtain the time-scales described in Section 3.2 and analysed in Section 4.3.

Fig. D1 shows the median SFHs from COLIBRE (blue-palette solid lines) for different redshifts, $2 \leq z \leq 4$, compared with observational SFHs from T. Nanayakkara et al. (2025) in dark grey and W. M. Baker et al. (2025a) in red. Each panel corresponds to a stellar mass bin: the top panel shows low-mass MQGs and the bottom panel high-mass MQGs. In the simulations, higher selection redshifts correspond to more bursty SFHs. With less cosmic time available, galaxies must assemble through more in-

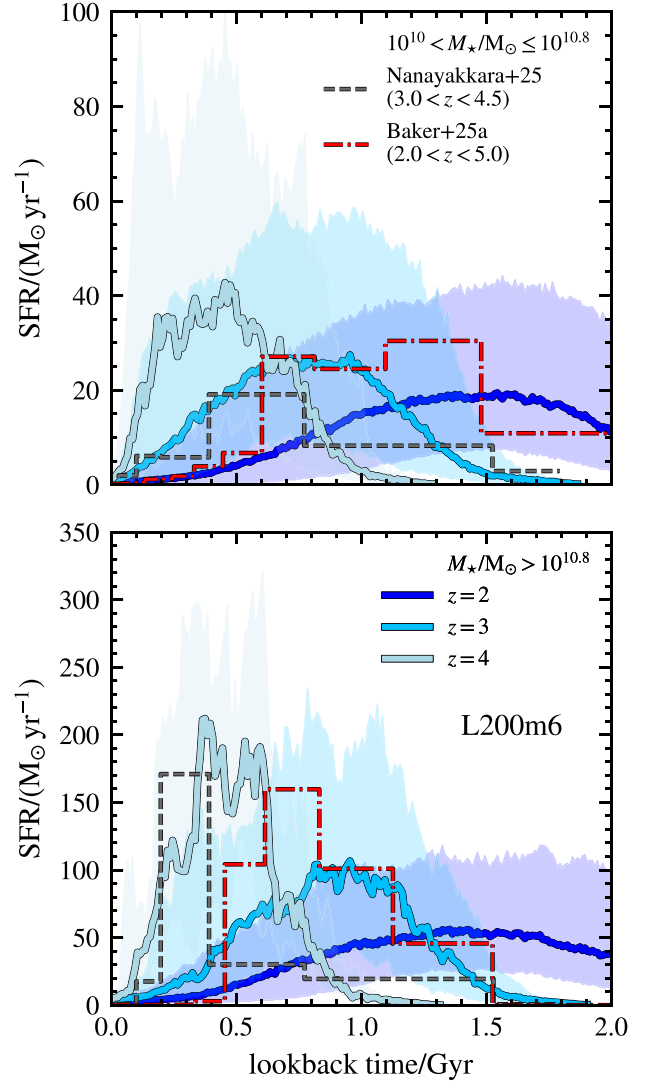


Figure D1. SFHs of MQGs. Solid lines show the median predictions from the L200m6 COLIBRE simulation at redshifts $2 \leq z \leq 4$, with different colours indicating selection redshift and shaded regions showing the 16th and 84th percentile range. These are compared to *JWST* spectroscopic measurements: dashed lines indicate the medians from T. Nanayakkara et al. (2025) and W. M. Baker et al. (2025a). *Top*: MQGs with $10^{10} < M_*/M_⊙ \leq 10^{10.8}$. *Bottom*: MQGs with $M_* > 10^{10.8} M_⊙$.

tense starbursts, leading to higher peaks and distributions skewed towards later times, consistent with the discussion in Section 4.3. As expected, the less massive MQGs (top panel) require less extreme bursts, reflected in their lower SFR values. The observations show similar behaviour: less bursty and more extended SFHs in the low-mass bin. However, the SFH peaks are lower in the observational data. This is because observational reconstructions use broader lookback-time bins. When we increase the bin size to 100 Myr in the simulations, the peaks from the SFHs derived from COLIBRE become less pronounced, bringing the results into better agreement with observations.

Interestingly, the W. M. Baker et al. (2025a) SFHs tend to assemble mass earlier than those of T. Nanayakkara et al. (2025). This is partly because the W. M. Baker et al. (2025a) sample is more skewed towards lower redshifts, but methodological differences in the SED fitting also contribute. Both studies use PROSPECTOR, but their assumptions differ in several ways. They do not cover the same spectral range: T. Nanayakkara et al. (2025) include the observed-frame NIR ($\lambda = 1 - 5 \mu\text{m}$), while W. M. Baker et al. (2025a) use rest-frame $\lambda > 0.35 \mu\text{m}$ for the spectrum to avoid the less well-understood rest-frame UV (while the entire SED for the photometry). Both adopt non-parametric SFHs, but one uses a flat continuity prior (J. Leja et al. 2019a) and the other an exponentially increasing prior in lookback time. They also use different lookback time intervals and different SSP models: C3K (C. Conroy et al. 2009) for T. Nanayakkara et al. (2025) versus MILES (J. Falcón-Barroso et al. 2011) for W. M. Baker et al. (2025a). On the other hand, both employ MIST isochrones (B. Paxton et al. 2015; which assume fixed solar abundances), a G. Chabrier (2003) IMF, and the D. Calzetti et al. (2000) dust attenuation law and uniform metallicity priors.

These methodological differences explain the behaviours seen in Fig. 5. Overall, despite observational biases, the simulation results reproduce the qualitative features of the observed SFHs.

APPENDIX E: SIZES AND KINEMATICS OF MQGS FOR THE L400M7 SIMULATION

We show results analogous to those in Sections 4.5 and 4.6 for the fiducial L200m6 simulation, but now for L400m7 in Fig. E1. We also comment on the L200m7h run where it differs. These results should be interpreted with caution because the larger gravitational softening lengths in these simulations (Table 1) shift the non-reliable regime to less compact systems.

In the top panel, we show the galaxy size–mass relation, which extends up to $z = 5$ owing to the larger volume of the L400m7 box. The blue arrows on the left-hand side indicate the corresponding softening length. Relative to L200m6, L400m7 displays a break in the power-law relation at slightly lower stellar masses ($M_\star \sim 10^{10.6} M_\odot$). L200m7h, in contrast, shows a shallower decrease in size with stellar mass beyond this break. The flattening at the low-mass end persists, suggesting it is not a direct consequence of the softening length, consistent with the behaviour seen across all resolutions at similarly high redshifts (see fig. 10 in A. D. Ludlow et al. 2026).

For the bottom panel, which presents the stellar kinematics via $v_\star/\sigma_\star$ versus stellar mass, the contrast between MQGs and MSFGs in L400m7 is even more pronounced than in L200m6. MSFGs display substantially higher rotational support at the low-mass end, whereas MQGs are more dispersion-dominated, effectively reversing the trend found in L200m6 and suggesting that morphological transformation may precede quenching, despite the

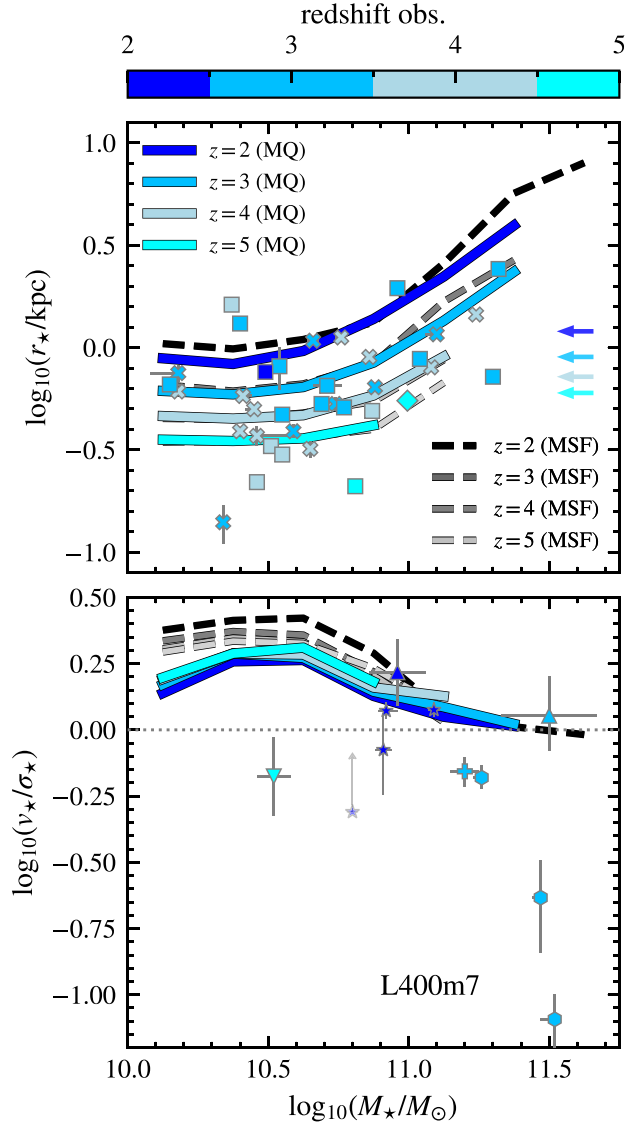


Figure E1. Stellar size–mass relation, with $r_\star$ defined as the half-mass radius (top panel); and $v_\star/\sigma_\star$ versus stellar mass relation (bottom panel) for L400m7. Solid blue-palette lines show the median predictions for MQGs, and dashed grey-palette lines for MSFGs at different selection redshifts, $2 \leq z \leq 5$. Observational data of MQGs are the same as in Fig. 8. Arrows in the error bars indicate lower limits for galaxies where rotational velocity could not be constrained (also shown with a more faded colour). Blue arrows in the size–mass relation mark the gravitational softening length, ϵ_{prop} , at each redshift.

two populations exhibiting similar sizes. This behaviour may result from the lower resolution and/or the burstier stellar feedback in L400m7, which could more easily perturb the shallower gravitational potentials of low-mass galaxies, affecting their stellar kinematics without significantly altering their sizes. However, a detailed investigation of the origin of this behaviour is beyond the scope of this paper. Although not shown, in L200m7h, the difference between MQGs and MSFGs extends across the entire stellar mass range, suggesting that jet feedback may further enhance the dispersion support of MQGs. However, these differences should be interpreted cautiously, as the larger softening lengths in these runs likely affect the reliability of the kinematic measurements.

APPENDIX F: CORRELATIONS FOR MQGS

We present correlations for MQGs predicted by the COLIBRE model in Fig. F1, with median values of Y versus X properties indicated in different colours for different selection redshifts ($2 \leq z \leq 4$) in the L200m6 simulation. Scatter points in the background represent individual galaxies selected at $z = 2$, colour-coded by a third Z property. Satellite MQGs are highlighted with red scatter points.

In the upper left panel, we plot dust fraction versus quenching time-scale, showing that galaxies that quenched earlier have lower dust content relative to their stellar mass. This relation becomes steeper at higher redshifts, indicating that dust is depleted after quenching. However, the large scatter is potentially driven by dust regrowth (together with renewed H_2 formation), as suggested in the evolutionary histories and the corresponding gas/dust images for these systems in appendix B of Paper II, where some individual systems clearly exhibit this behaviour, with dust even present in the galactic outskirts. The dust removal seems to be quicker the higher the redshift, as recently reported observationally with AGN as the main responsible mechanism (A. Leśniewska et al. 2025). The scatter points further show that dust fraction and quenching times correlate with sSFR: galaxies with lower sSFR have lower dust content, suggesting that dust directly traces star formation.

The upper right panel further finds a correlation between dust fraction and H_2 fraction for MQGs, indicating that molecular hydrogen and dust are removed consistently in these systems. The points are colour-coded in this case by gas metallicity (mea-

sured within the 50 pkpc fiducial aperture as the linear sum of the diffuse oxygen over hydrogen ratio of gas, multiplied by the gas mass), showing that, as expected, more metal-rich systems have higher dust fractions. A tail of systems with relatively high metallicity but low dust fraction ($f_{\text{dust}} \lesssim 10^{-4}$) corresponds to satellite galaxies (in red).

The lower left panel presents galaxy size versus formation time-scale, indicating that earlier-formed galaxies are more extended, having had more time to grow. This trend reflects hierarchical structure formation, where objects start smaller and grow over time. Colour-coding by quenching time-scales further demonstrates that formation and quenching times are correlated. In the lower right panel, more rotation-supported systems tend to reside in lower-mass haloes (where M_{halo} is the total mass of the 3D FoF group to which the galaxy belongs). This is in agreement with the observational results in L. Kawinwanichakij et al. (2026), where more dispersion-supported systems live in denser environments, highlighting the role of environment in shaping morphology at such early times. Further details on the role of the environment for these systems in Paper II. Colour-coding by galaxy size in the lower right panel indicates that rotation-supported systems are more compact than dispersion-supported systems, a direct consequence of their later formation times (bottom left panel of Fig. F1). Although not shown, we also identify a shallower trend in which earlier-formed galaxies inhabit more massive haloes, a direct link between DM haloes and galaxies (S. D. M. White & C. S. Frenk 1991).

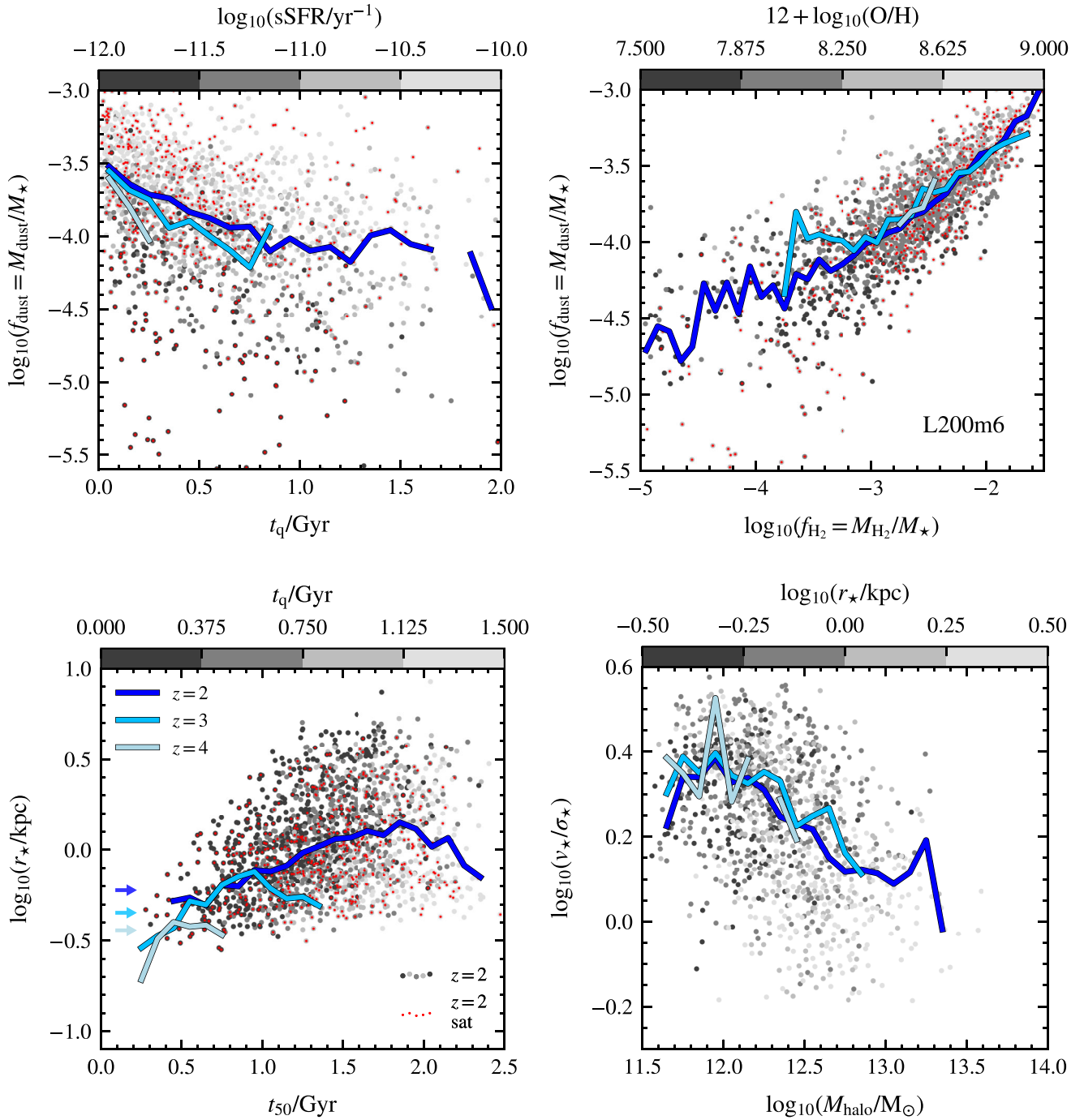


Figure F1. Dust fraction ($f_{\text{dust}} = M_{\text{dust}}/M_{\star}$) versus quenching time, colour-coded by sSFR (*upper left panel*); dust fraction ($f_{\text{dust}} = M_{\text{dust}}/M_{\star}$) versus molecular hydrogen fraction ($f_{\text{H}_2} = M_{\text{H}_2}/M_{\star}$), colour-coded by gas metallicity ($12 + \log_{10}(\text{O}/\text{H})$) (*upper right panel*); half-mass radius versus formation time-scale, colour-coded by quenching time (*lower left panel*); and $v_{\star}/\sigma_{\star}$ versus halo mass only for central galaxies, colour-coded by half-mass radius (*lower right panel*) for MQGs in L200m6. Solid lines show the median values at different redshifts ($z = 2, 3, 4$), while (red) scatter points represent individual (satellite) $z = 2$ MQGs, colour-coded by the properties indicated above. Blue arrows in the galaxy sizes mark the gravitational softening length, ϵ_{prop} , at each redshift.

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