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Intertwined formation of H2 , dust, and stars in cosmological simulations

Molecular hydrogen (H2) plays a crucial role in the formation and evolution of galaxies, serving as the primary fuel reservoir

for star formation. In a metal-enriched Universe, H2 forms mostly through catalysis on interstellar dust grain surfaces. However, due

to the complexities of modelling this process, star formation in cosmological simulations often relies on empirical or theoretical

frameworks that have only been validated in the local Universe to estimate the abundance of H2.

We model the connection between the formation of stars, dust, and H2 formation processes in cosmological simulations. The model reproduces, reasonably well, the main statistical properties of the observed galaxy population for the stellar, dust, and H2 components. The molecular hydrogen cosmic density evolution in our simulated boxes peaks around redshift z = 1.5, consistent with observations. Following its peak, ρ H2 decreases by a factor of two towards z = 0, a milder evolution

than observed. Similarly, the evolution of the molecular hydrogen mass function since z = 2 displays a gentler evolution when compared to observations. Our model recovers the integrated molecular Kennicut-Schmidt (mKS) law between the surface star formation rate (Σ SFR) and surface H2 density (Σ H2) satisfactorily at z = 0. This relationship is already evident at z = 2, albeit with a higher normalization. We find hints of a broken power law with a steeper slope at higher Σ H2. We also study the H2-to-dust mass ratio in galaxies as a function of their gas metallicity and stellar mass, observing a decreasing trend with respect to both quantities. The H2-to-dust mass fraction for the global population of galaxies is higher at higher redshift. The analysis of the atomic-to-molecular transition on a particle-by-particle basis suggests that gas metallicity cannot reliably substitute the dust-to-gas ratio in models attempting to simulate dust-promoted H2.

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