

## Molecular emission lines from simulations of AGN-driven molecular outflows

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#### Observations of fast molecular outflows

. . . . . . . 0.03 0.3 Flux [Jy] 0.02 [Jy] Flux 0.01 0.1 0 0 1000 -1000 -500 500 -1000 -500 500 1000 0 0 Velocity [Km/s] Velocity [Km/s]

#### CO 1-0 line in Mrk 231

Feruglio et al. (2010)



### Introduction

#### Acceleration of cold clouds



Scannapieco & Brüggen (2015)



## Introduction

#### In-situ molecule formation

#### An energy-driven AGN wind



### Simulations



- > 3D simulations of an isotropic AGN wind.
- > 1.6-5.0 kpc box, periodic boundary conditions.
- > Inject wind particles, initial  $v = 30,000 \text{ km s}^{-1}$ ,  $dP/dt = L_{AGN}/c$ .

### Simulations



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#### Chemistry

- > Evolve time-dependent chemistry of 157 species, including 20 molecules.
- > Most importantly:  $H_2$ , CO, OH and HCO<sup>+</sup>.
- ➤ We assume a Milky Way dust-to-metals ratio.

### Simulations



#### Parameters

$n_{\rm H}$ (cm <sup>-3</sup> )	L <sub>AGN</sub> (erg s <sup>-1</sup> )	Z / Z <sub>sol</sub>
10	$10^{46}$	1.0
1	$10^{46}$	1.0
10	$10^{45}$	1.0
10	$10^{46}$	0.1

### Simulations



#### nH10\_L45\_Z1



### Simulations





# Simulations $H_2$ outflow rates

















## Molecular Emission Lines



- ➤ We use the Monte Carlo radiative transfer code RADMC-3D (Dullemond et al. 2012).
- Interpolate particles from the simulations onto an AMR grid, with maximum spatial resolution of 0.07 pc.
- > Use non-equilibrium chemical abundances from the simulations.
- ➤ CO emission, warm (few hundred K) H<sub>2</sub> emission, and OH absorption.





## CO 1-0 line emission

#### nH10\_L45\_Z1

$${0 \over \log_{10} W_{
m CO}} {1 \over {
m (Jy \ km \ s^{-1} \ arcsec^{-2})}}$$





Richings & Faucher-Giguère (2018)

### Comparison with CObased observations





Richings & Faucher-Giguère (2018)

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	$\alpha_{\rm CO} = M_{\rm H2} / L_{\rm CO}^{*}$		
Simulation	(1-0)	(2-1)	(3-2)
nH10_L46_Z1	0.13	0.08	0.06
nH10_L45_Z1	0.15	0.09	0.07
nH10_L46_Z0.1	1.77	0.82	0.80

\*Units: M<sub>sol</sub> (K km s<sup>-1</sup> pc<sup>2</sup>)<sup>-1</sup>





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\*Units:  $M_{sol}$  (K km s<sup>-1</sup> pc<sup>2</sup>)<sup>-1</sup>

> Observations typically assume:  $\alpha_{CO(1-0)} = 0.8 M_{sol} (K \text{ km s}^{-1} \text{ pc}^2)^{-1}.$ 































### Warm H<sub>2</sub> Emission JWST Predictions





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Richings & Faucher-Giguère (in prep)

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### Warm H<sub>2</sub> Emission JWST Predictions





Summary



- ➤ Molecular outflow rates up to 140 M<sub>sol</sub> yr<sup>-1</sup> formed within the AGN wind after 1 Myr.
- > CO to H<sub>2</sub> conversion factor at solar metallicity:  $\alpha_{CO (1-0)} = 0.13 M_{sol} (K \text{ km s}^{-1} \text{ pc}^2)^{-1}.$
- > Strong warm H<sub>2</sub> emission, with  $T_{exc} \sim 400$  K at solar metallicity.
- ➤ Warm H<sub>2</sub> emission observable by JWST out to redshift 1.6 at an SNR of 3 (redshift 1.5 at an SNR of 10).