



Co-evolution of Interstellar Polycyclic Aromatic Hydrocarbons

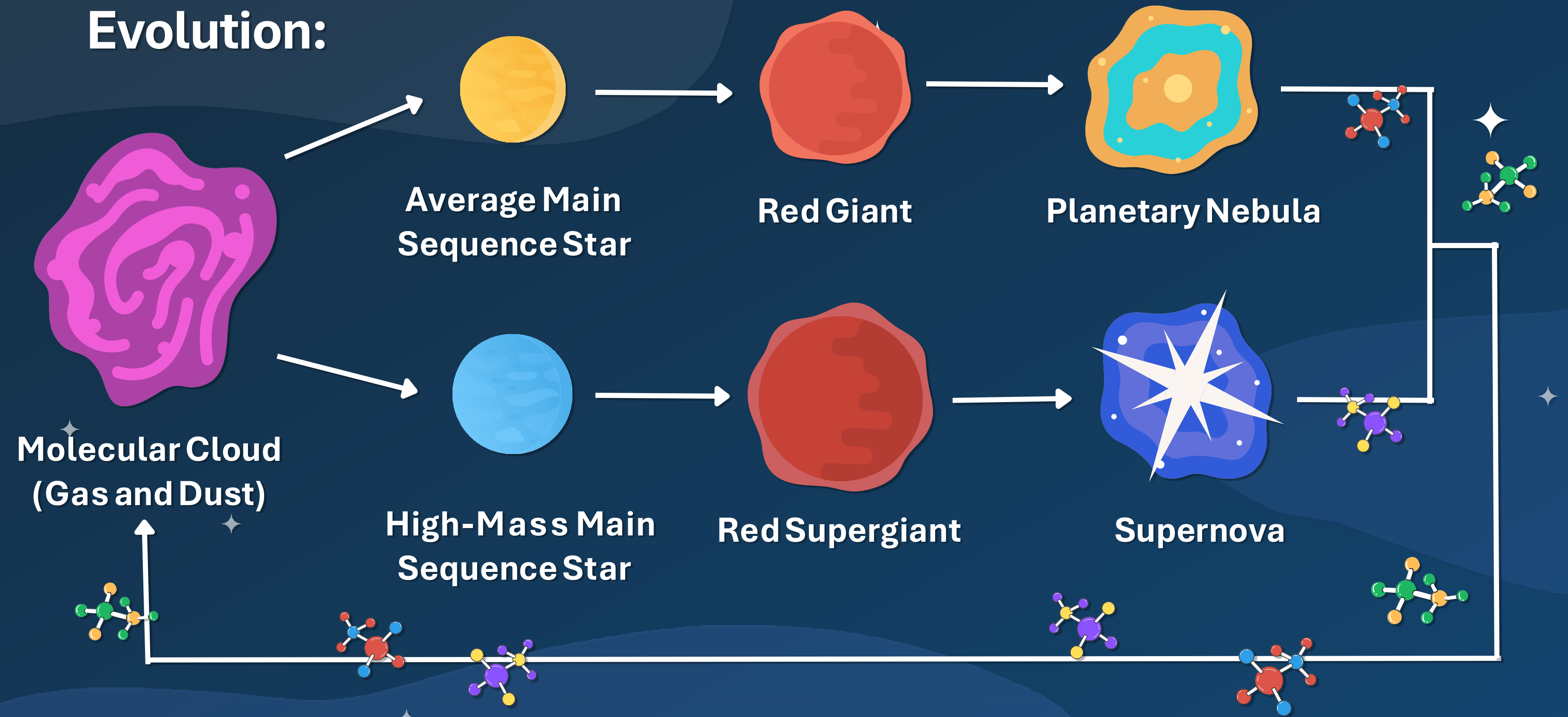
Congcong Zhang

Xiangtan University

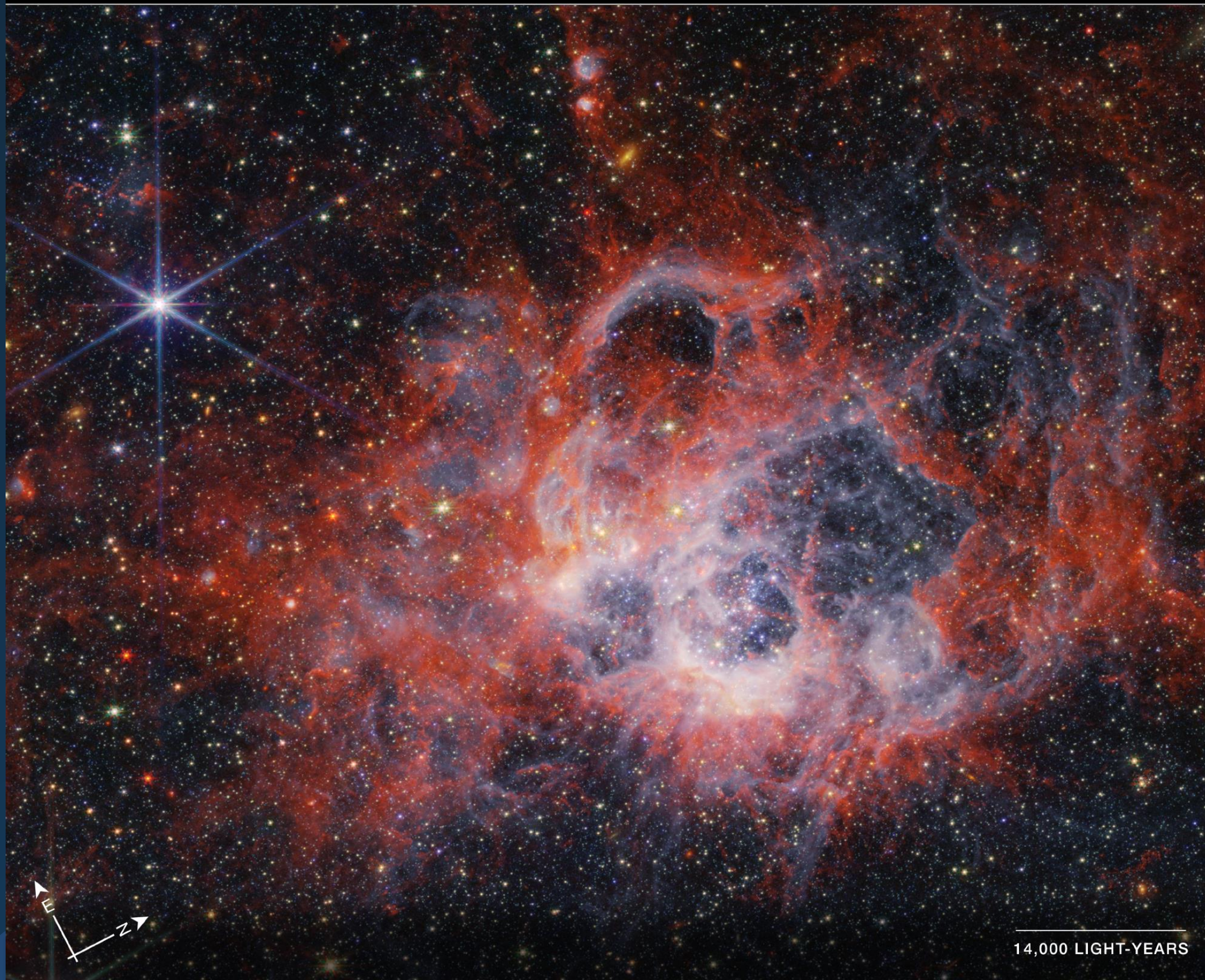
University of Science and Technology of China

University of Western Ontario, London, CA

A Note on Stellar Evolution:



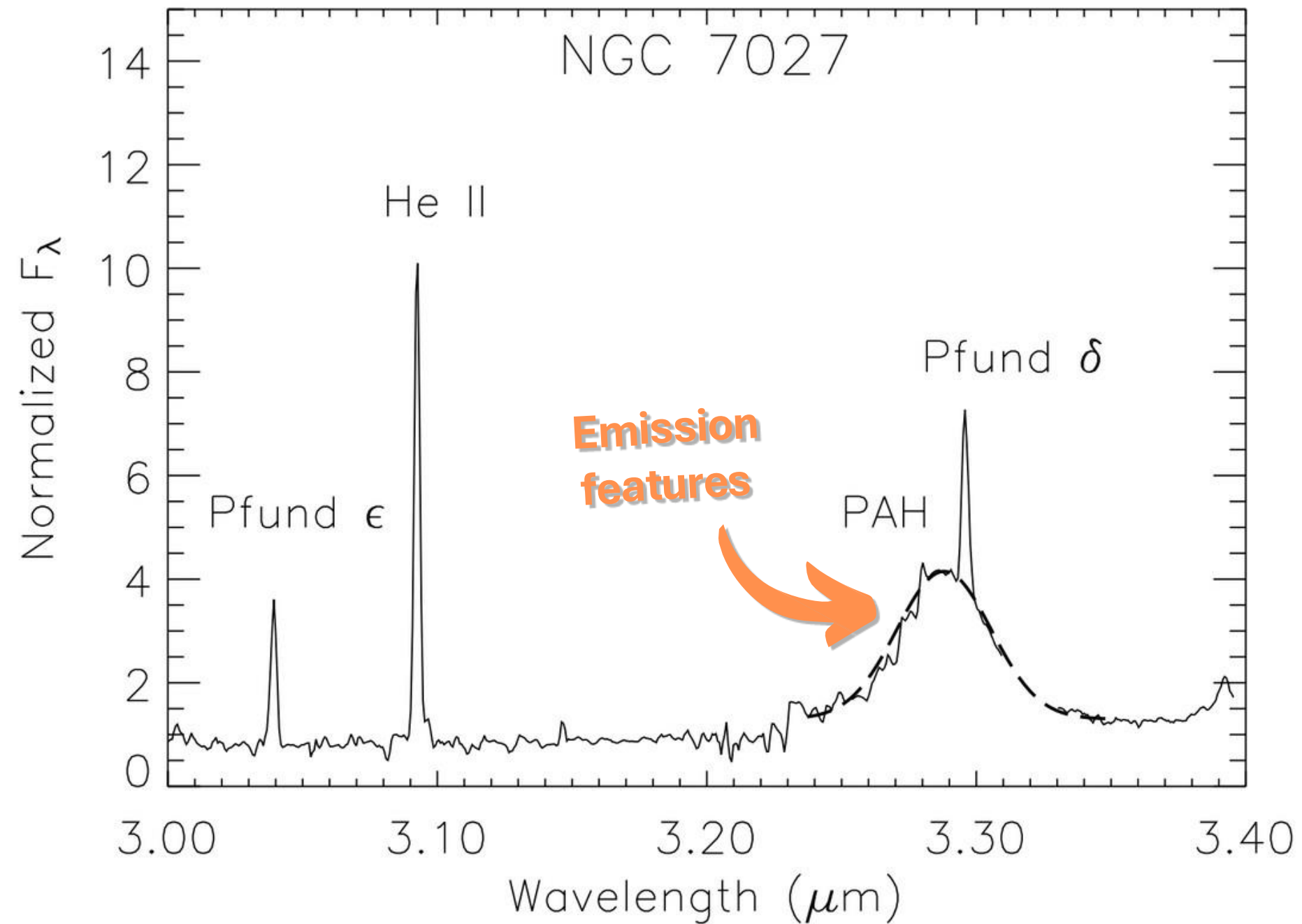
Need dying stars to release heavy elements!



JWST NIRCam NGC 604

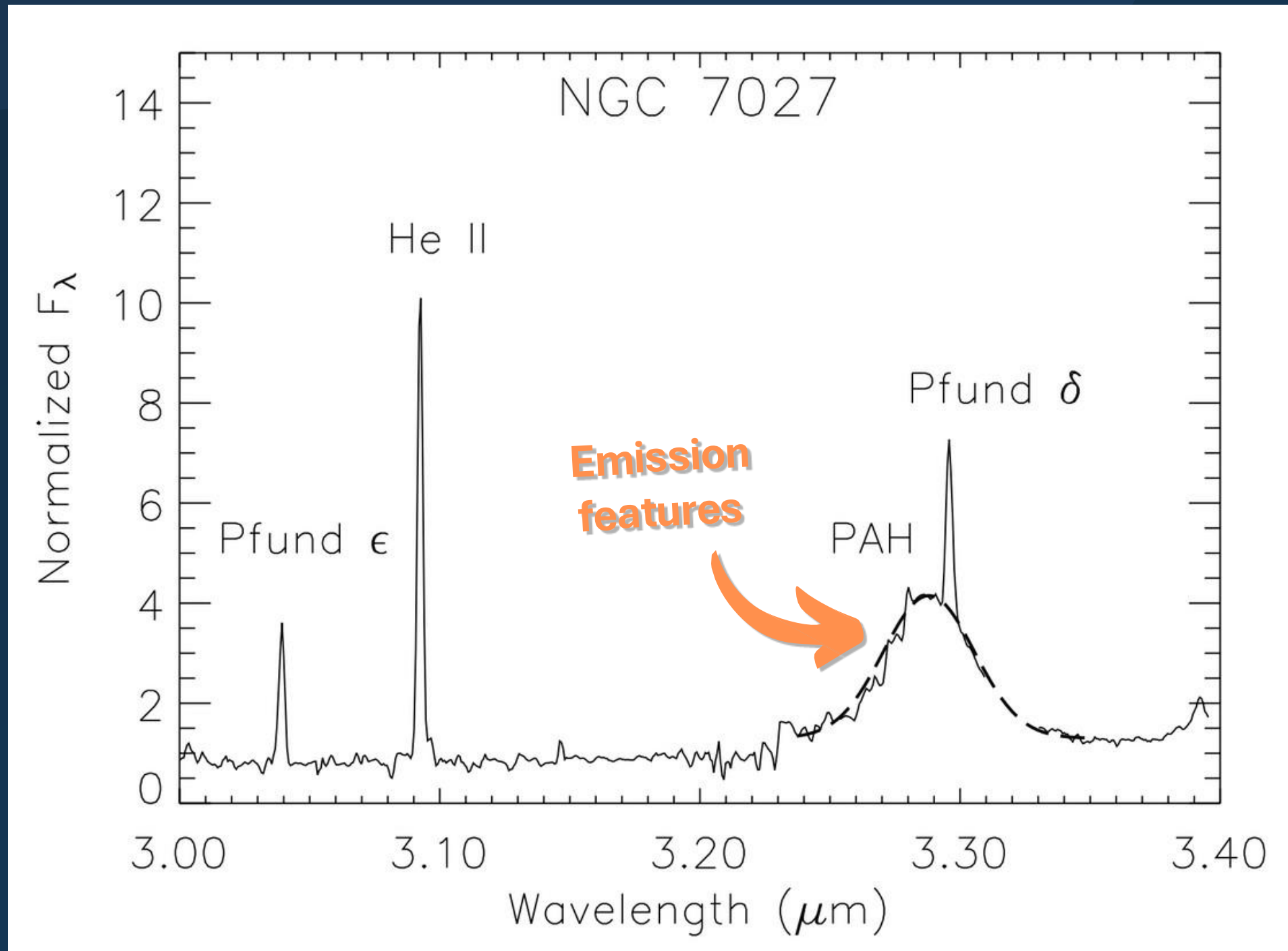
- ◆ Stellar winds from bright, hot young stars carve out cavities in surrounding gas and dust;
- ◆ The bright orange signify polycyclic aromatic hydrocarbons (PAHs);
- ◆ The deeper red signifies molecular hydrogen.

Emission Features



Smith, E.C.D., & McLean, I.S. 2008, *ApJ*, 676:408-415.

Emission Features



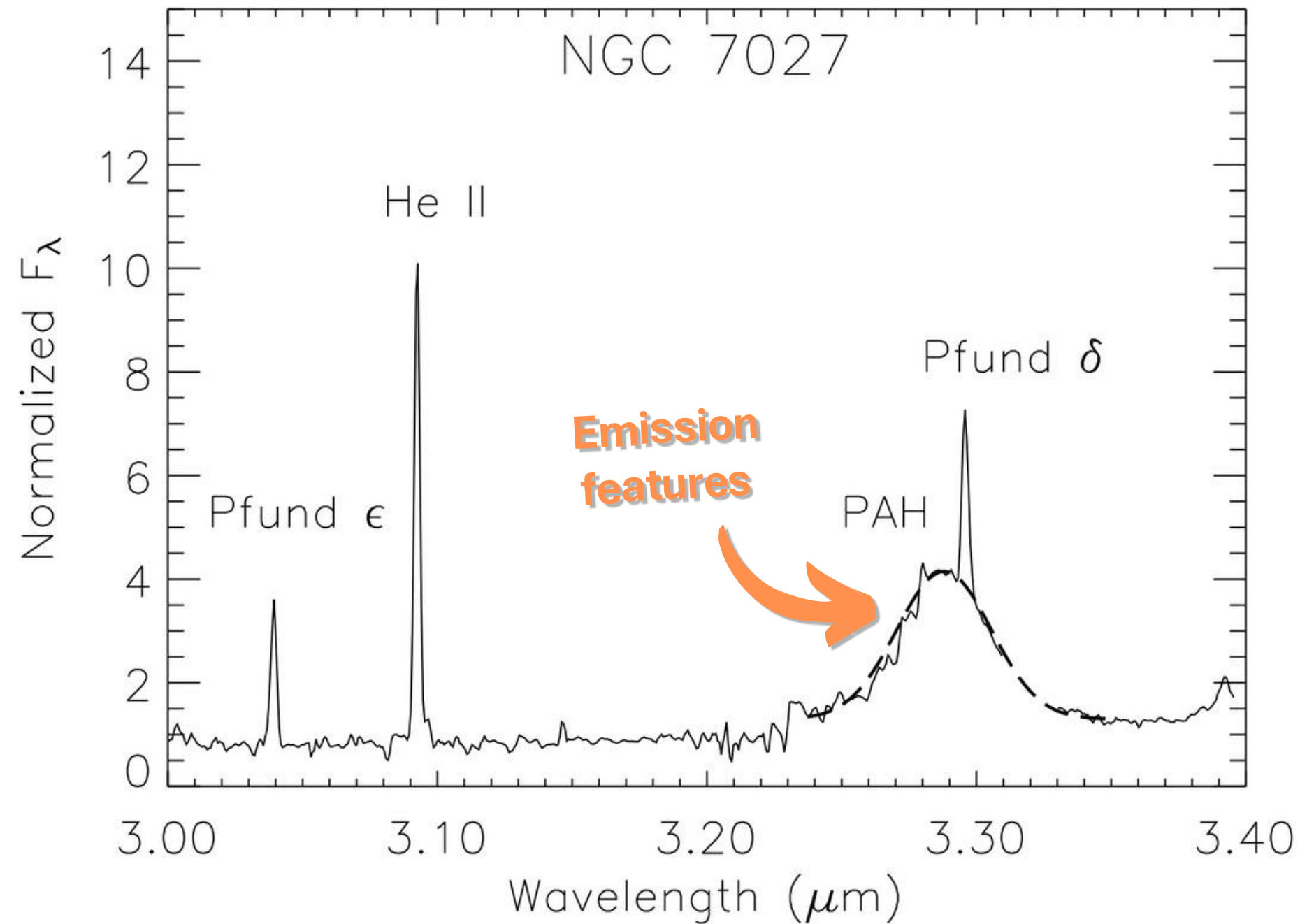
Smith, E.C.D., & McLean, I.S. 2008, ApJ, 676:408-415.

Young
Star



Ultra-violet
Radiation

Emission Features



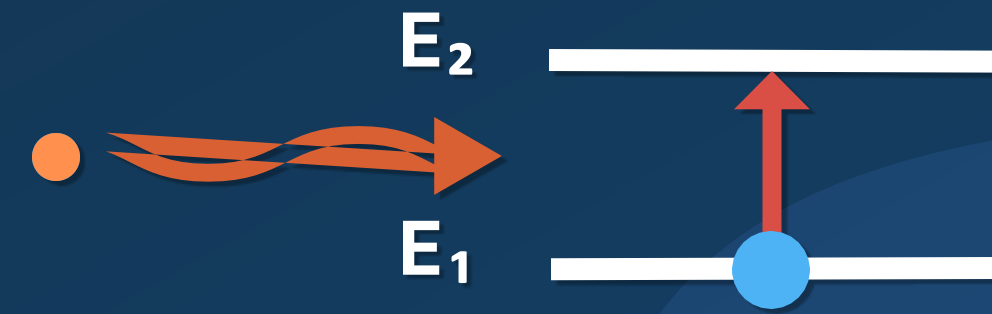
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Young
Star

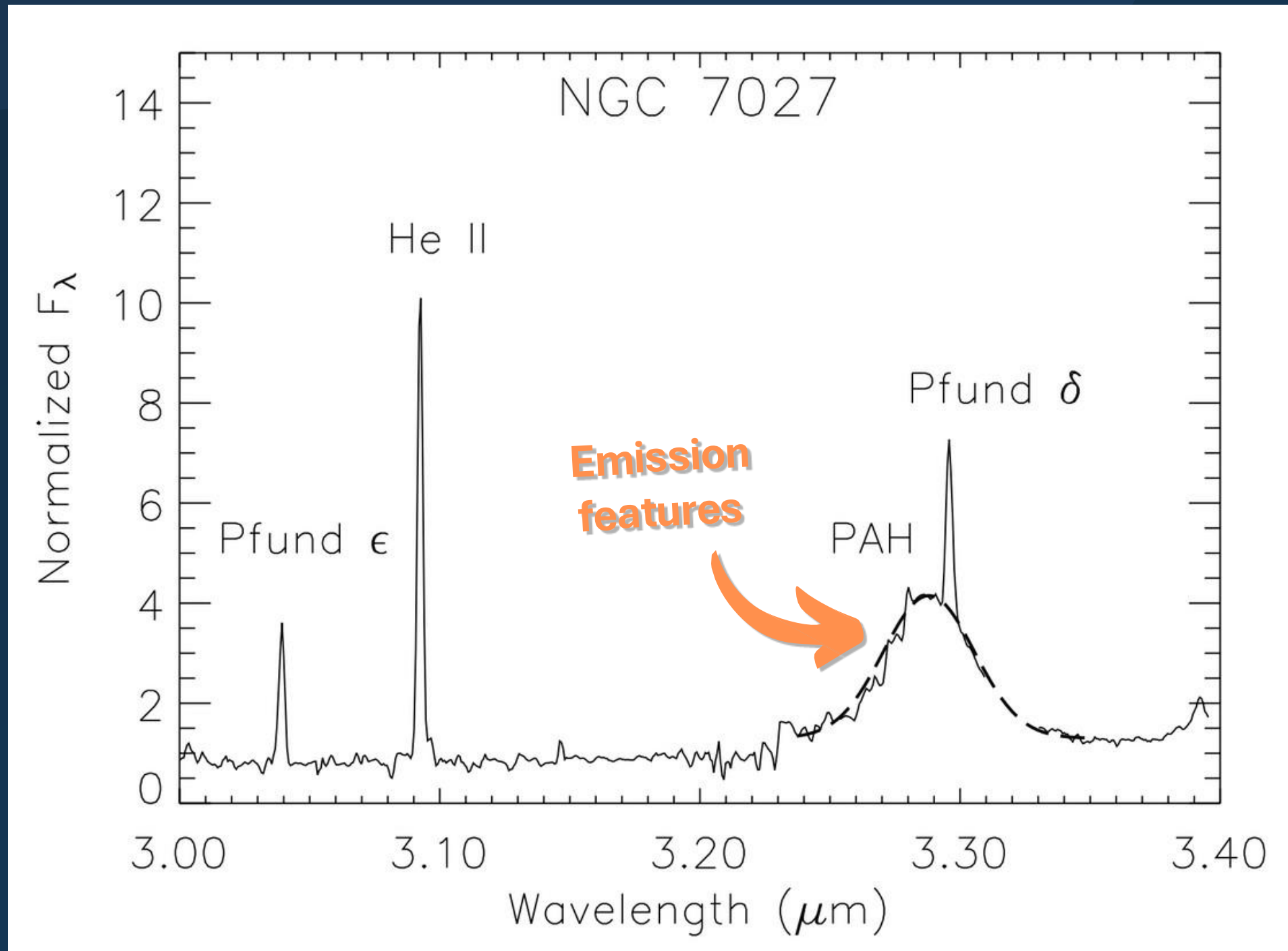


Ultra-violet
Radiation

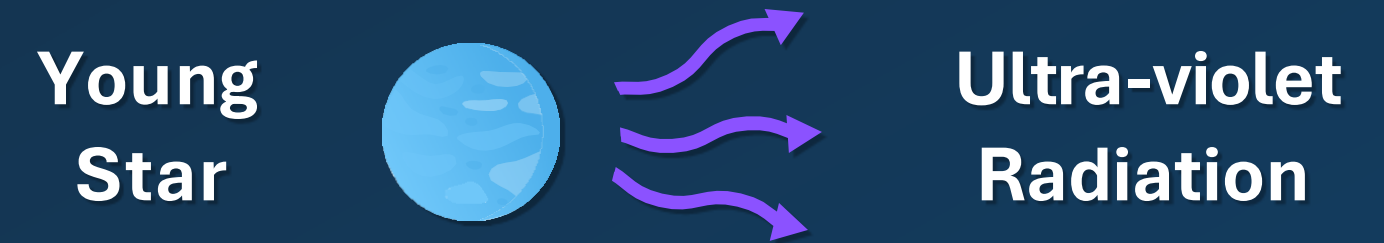
Absorption:



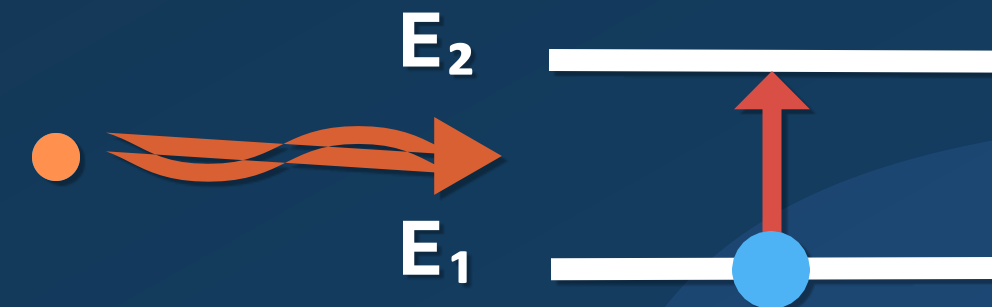
Emission Features



Smith, E.C.D., & McLean, I.S. 2008, ApJ, 676:408-415.



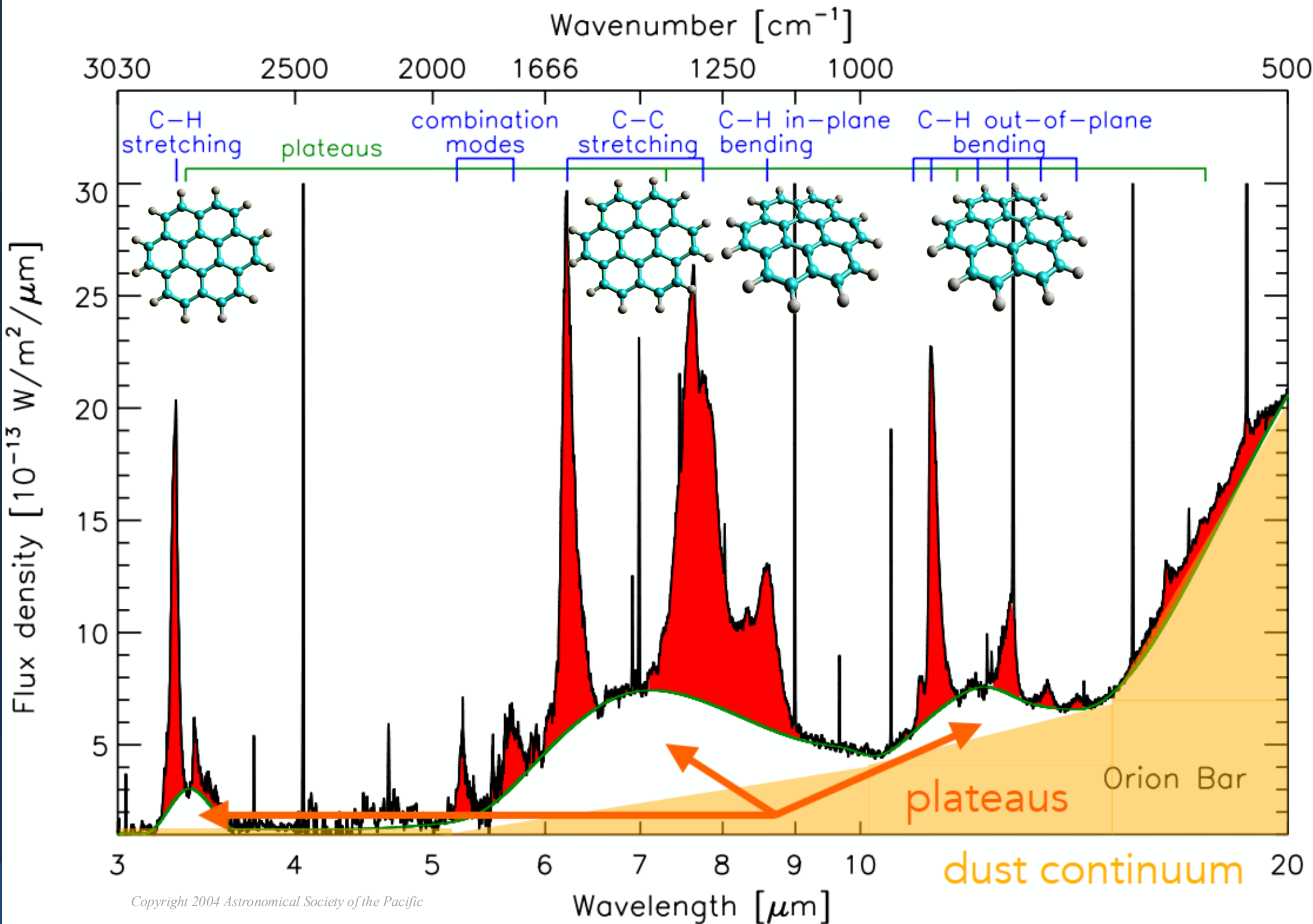
Absorption:



Emission:



$$\lambda = hc / E_{\text{photon}}$$



PAH Emission

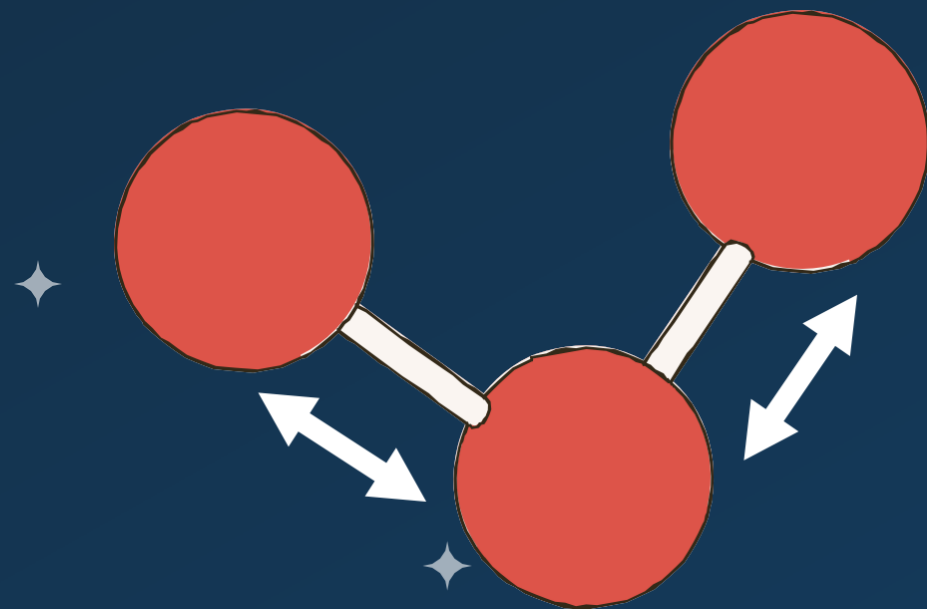
Broad features at:
3.3, 6.2, 7.7, 8.6,
11.3, and 12.7 μm

*Each corresponds
to different
vibrational modes!*

Vibrational Modes

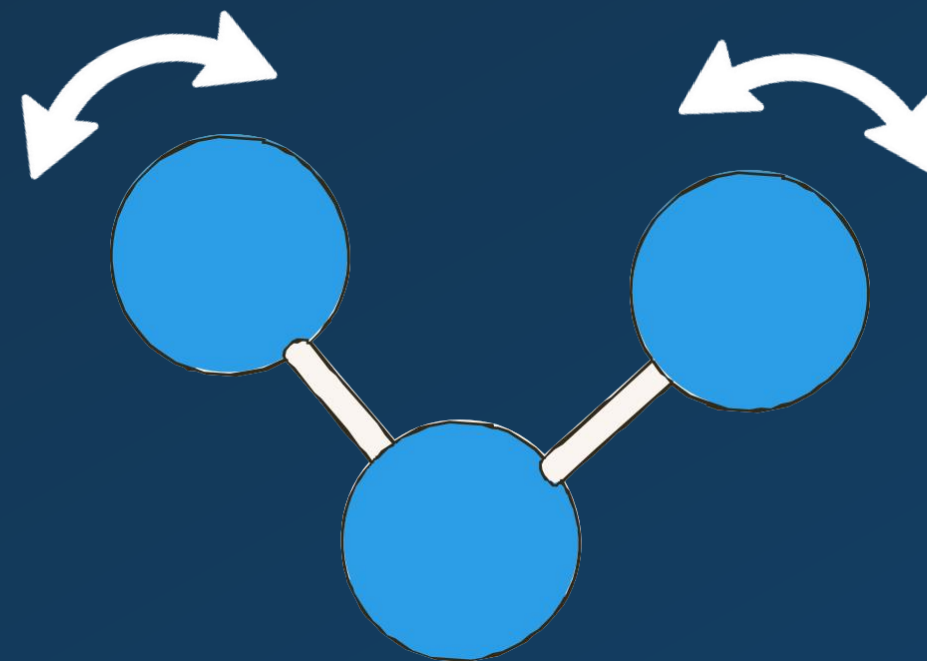
Stretching

Bond *length* changes

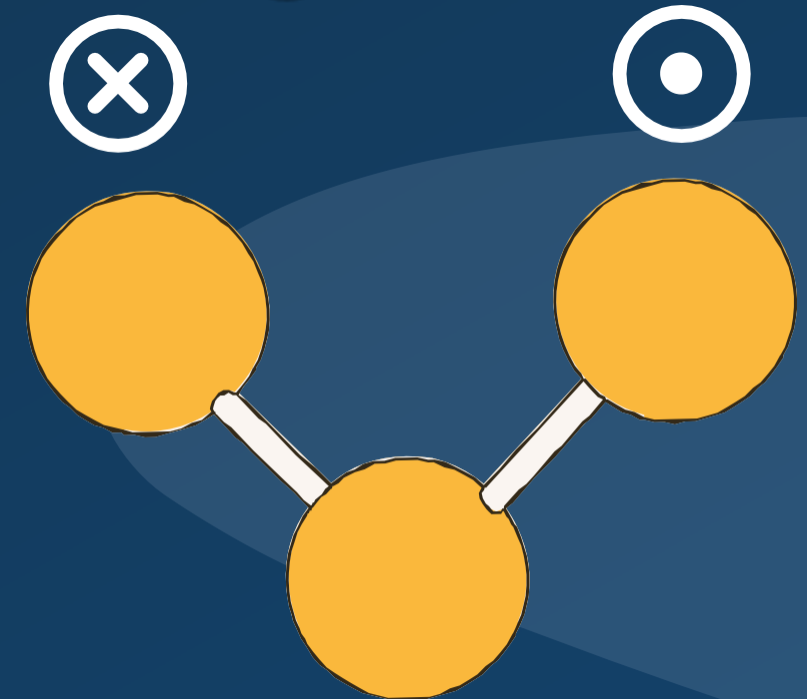


Bending

Bond *angle* changes

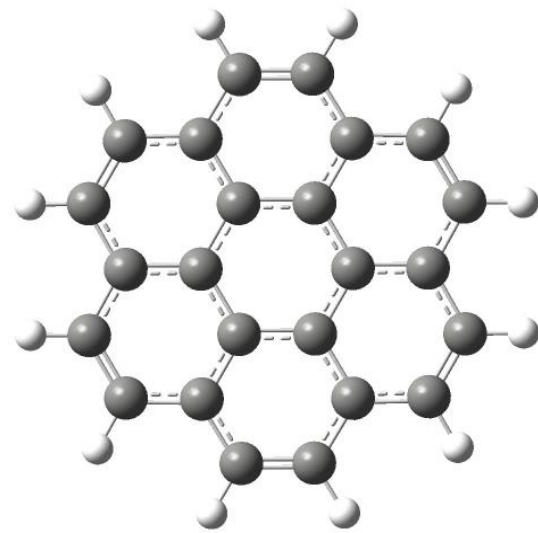


In-Plane

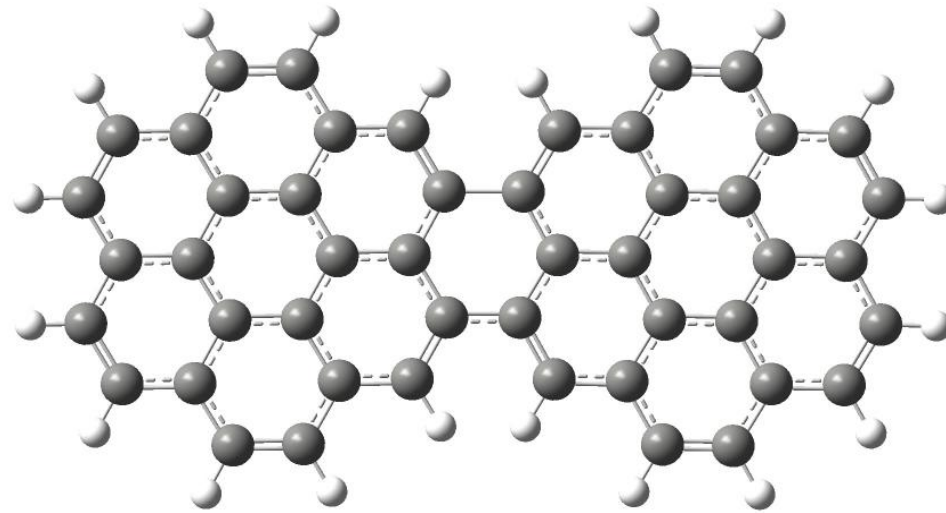


Out-of-Plane

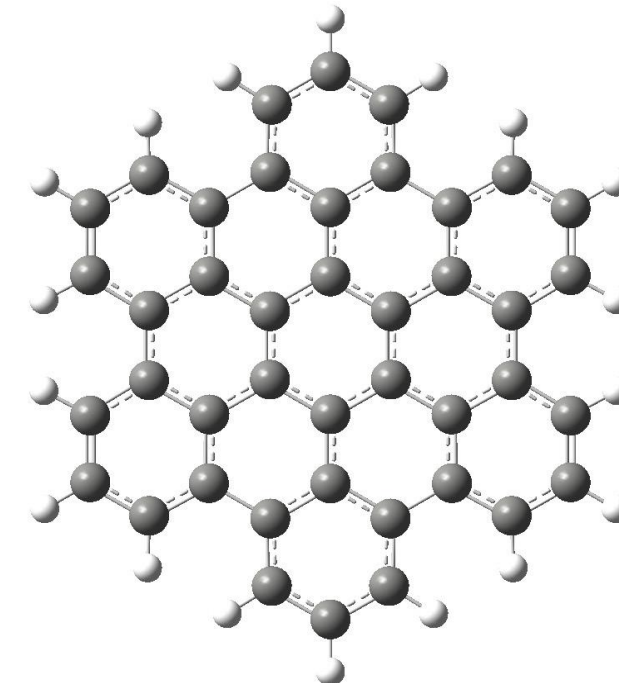
The molecular structures of PAHs



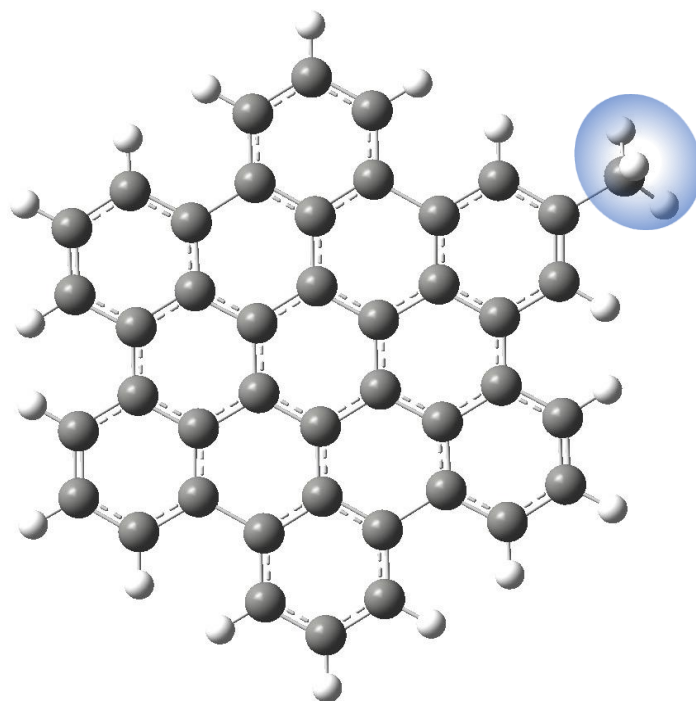
Coronene
($\text{C}_{24}\text{H}_{12}$)



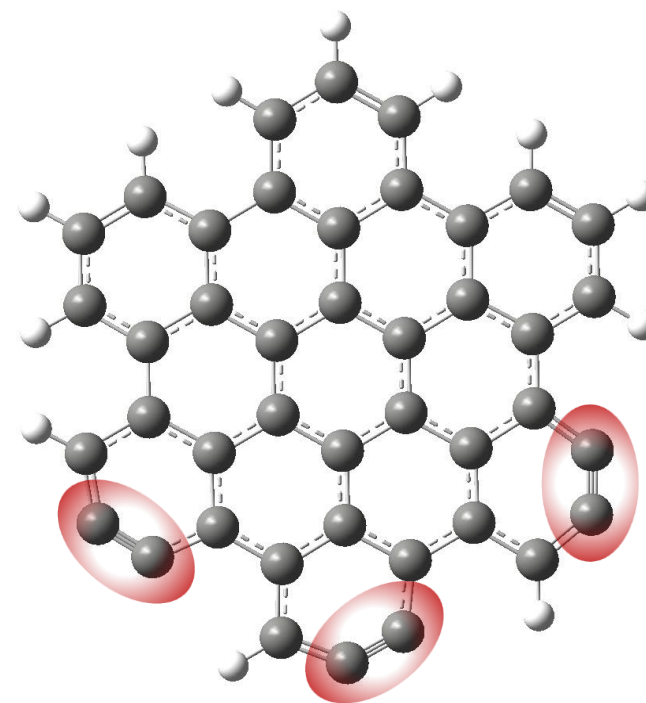
Dicoronene
($\text{C}_{48}\text{H}_{20}$)



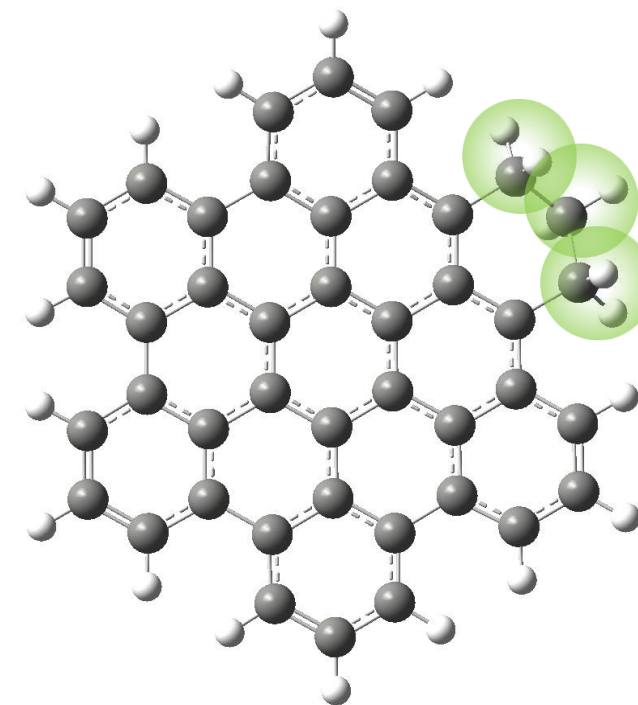
**Hexabenzocoronene
HBC** ($\text{C}_{42}\text{H}_{18}$)



(-CH₃) Substituted HBC
($\text{C}_{42}\text{H}_{21}$)



Dehydrogenated HBC
($\text{C}_{42}\text{H}_{12}$)



Superhydrogenated HBC
($\text{C}_{42}\text{H}_{21}$)

PAH Emission Varies With....

1. Grain Size
2. Molecular Edge Structure
3. Charge State

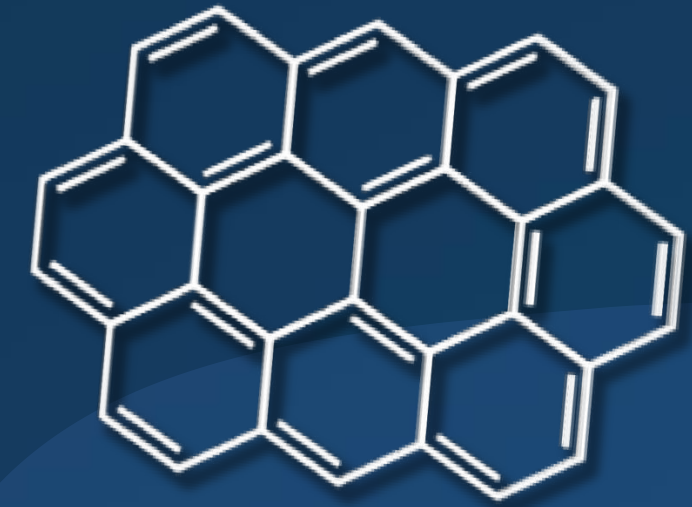
Relative intensities of PAH features gives insight into the physical properties of the PAH population!

1. Grain Size

- Larger molecules have more vibrational degrees of freedom
- Average energy per mode is lower
- Photons emitted will have lower energy — longer wavelength!



Small



Large

More large molecules = Stronger long-wavelength emission relative to short-wavelength emission

2. Edge Structure

Influences the relative strengths of the features associated with the C-H out-of-plane bending mode:

11.3 μm : Smoother, straighter edges

12.7 μm : More corners

* either smaller or have more irregular edges



Irregular



Smooth

Strength of the 12.7 μm feature relative to the 11.3 μm feature is a reflection of PAH molecular edge structure

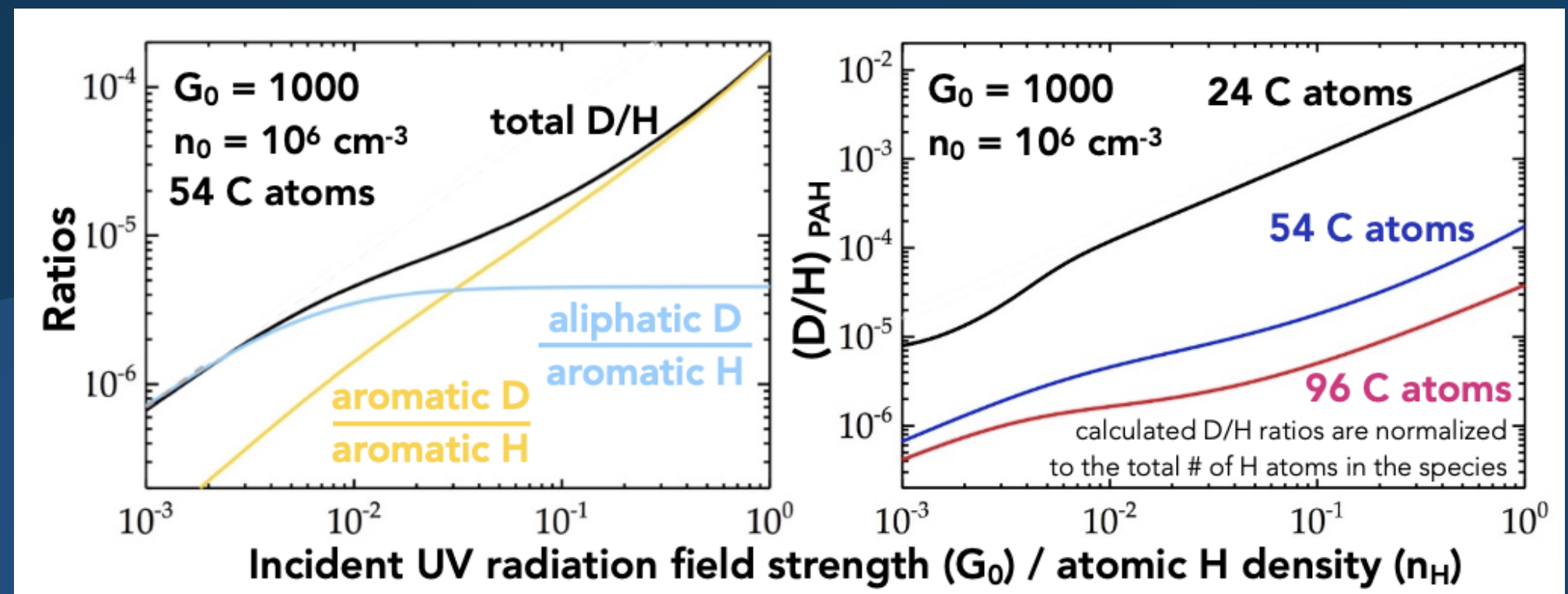
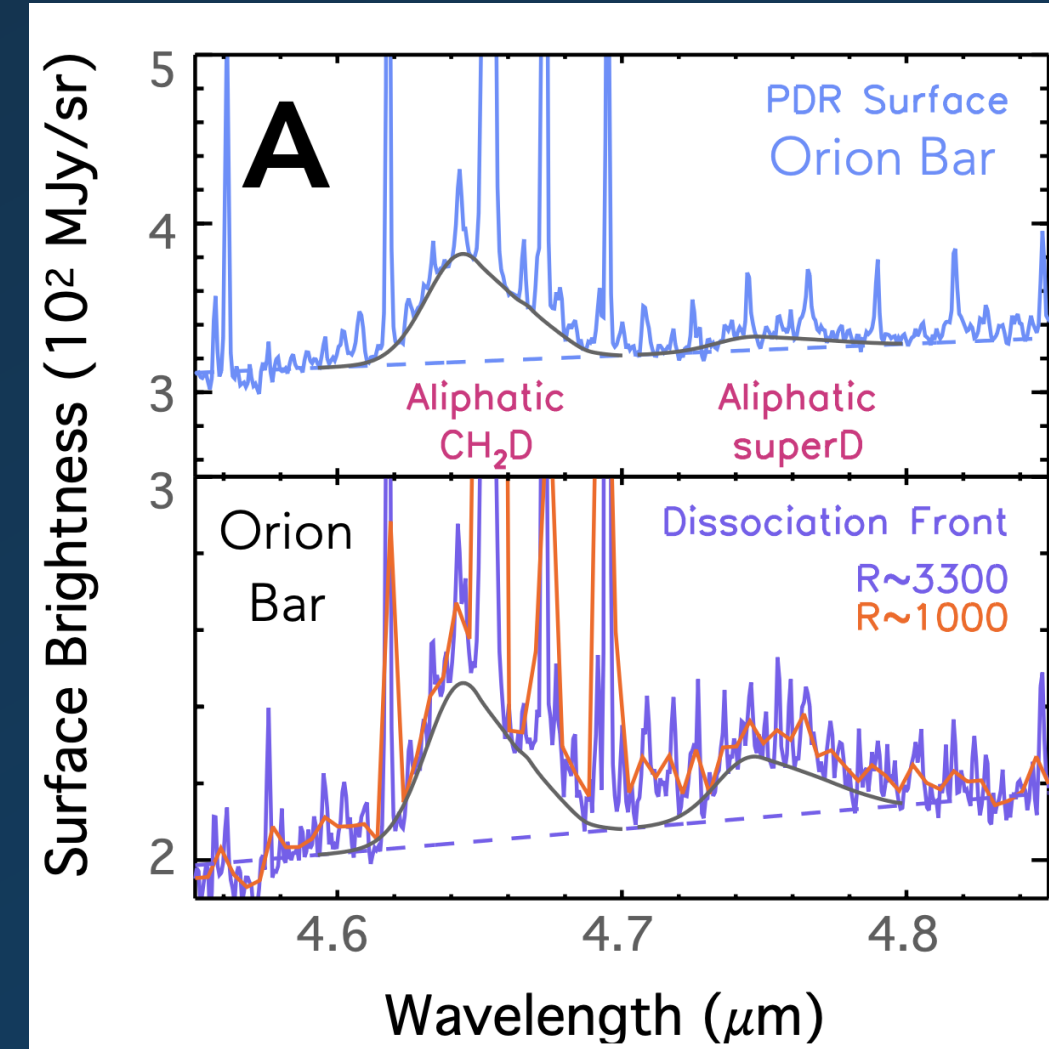
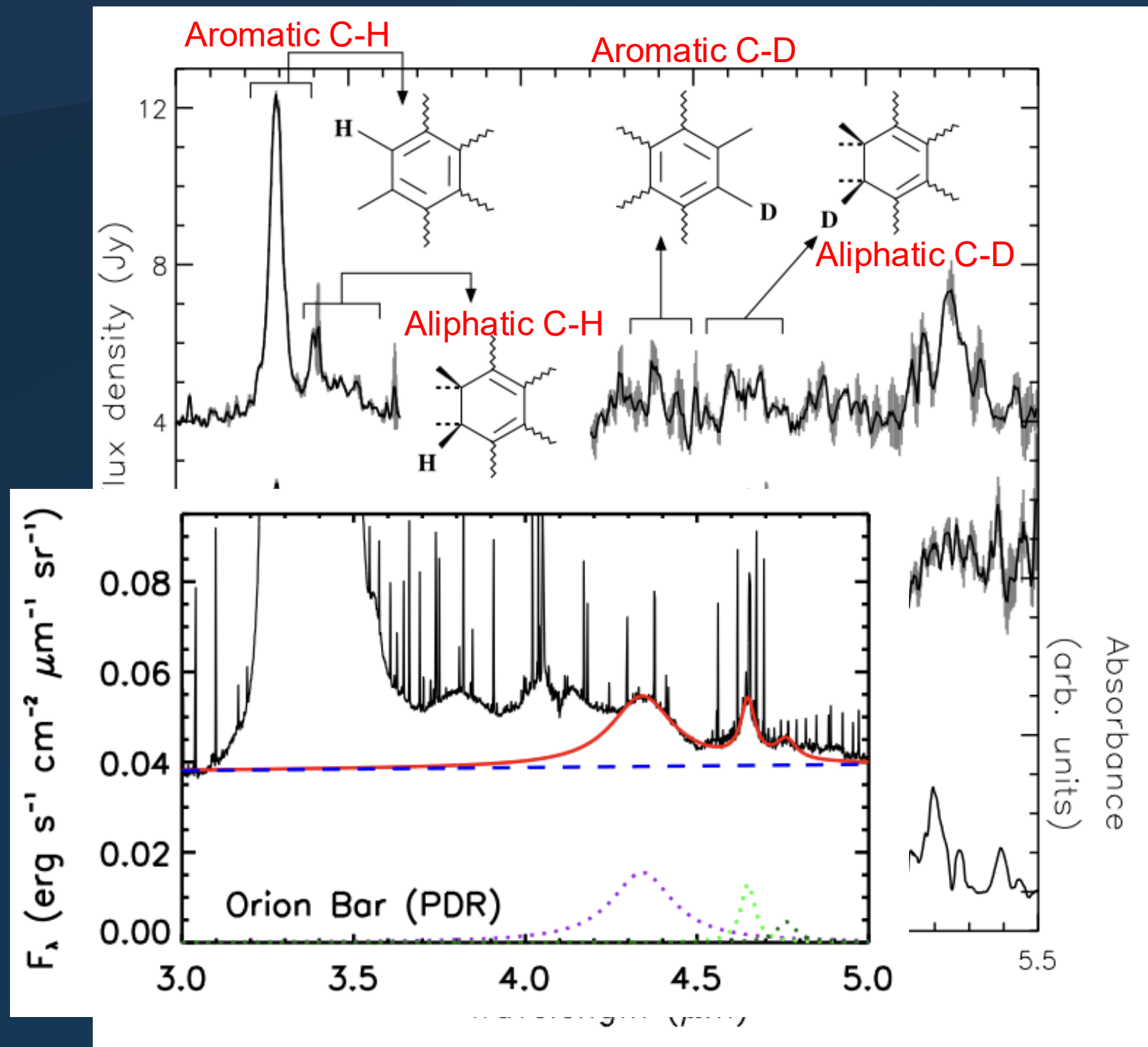
3. Charge State

- When a PAH molecule becomes charged, an oscillating electric dipole is induced
- Increases the intensity of the C-C stretching modes
- As a result, features between 5-10 μm are weak in the spectra of neutral PAHs, but dominant in the spectra of ionized PAHs



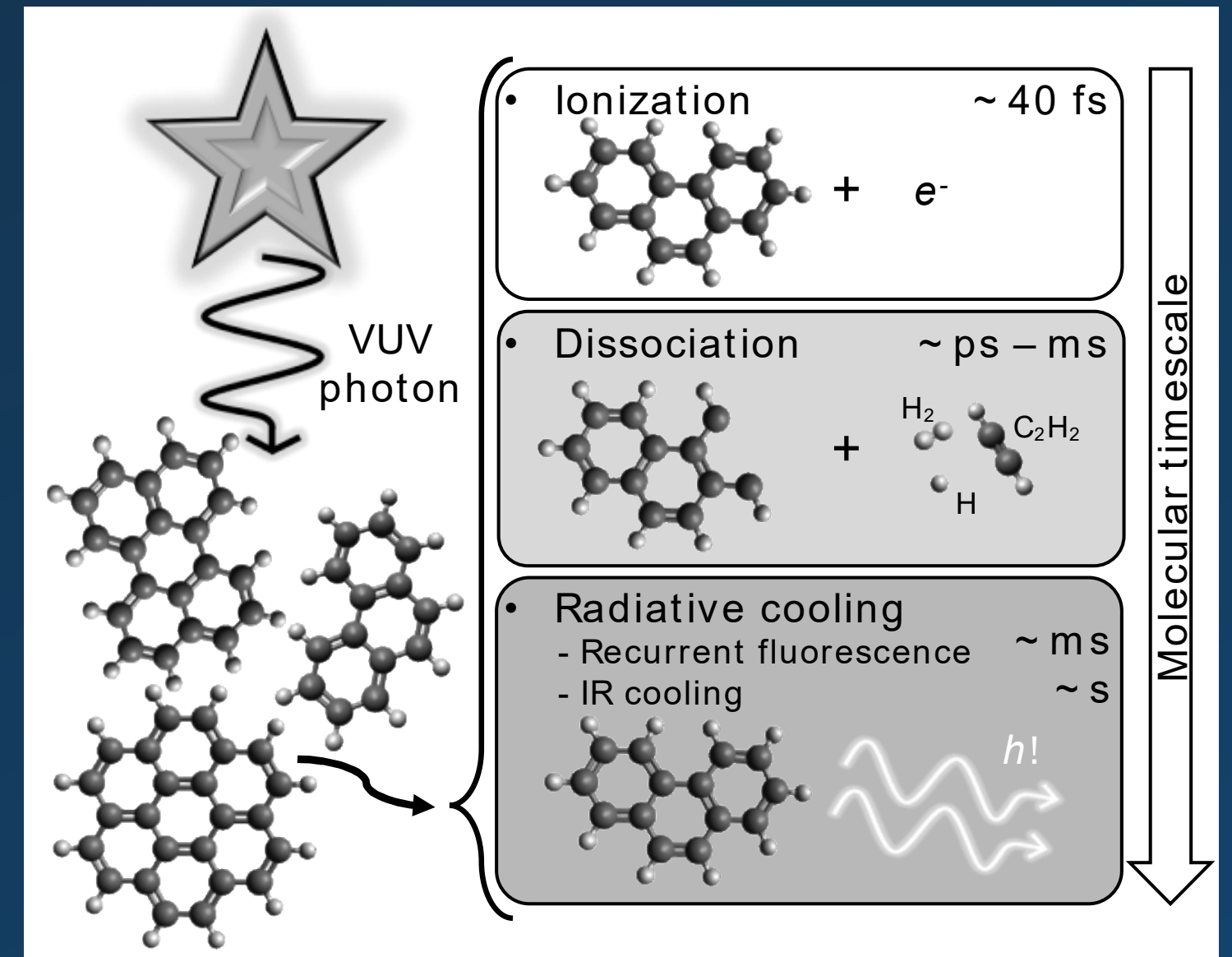
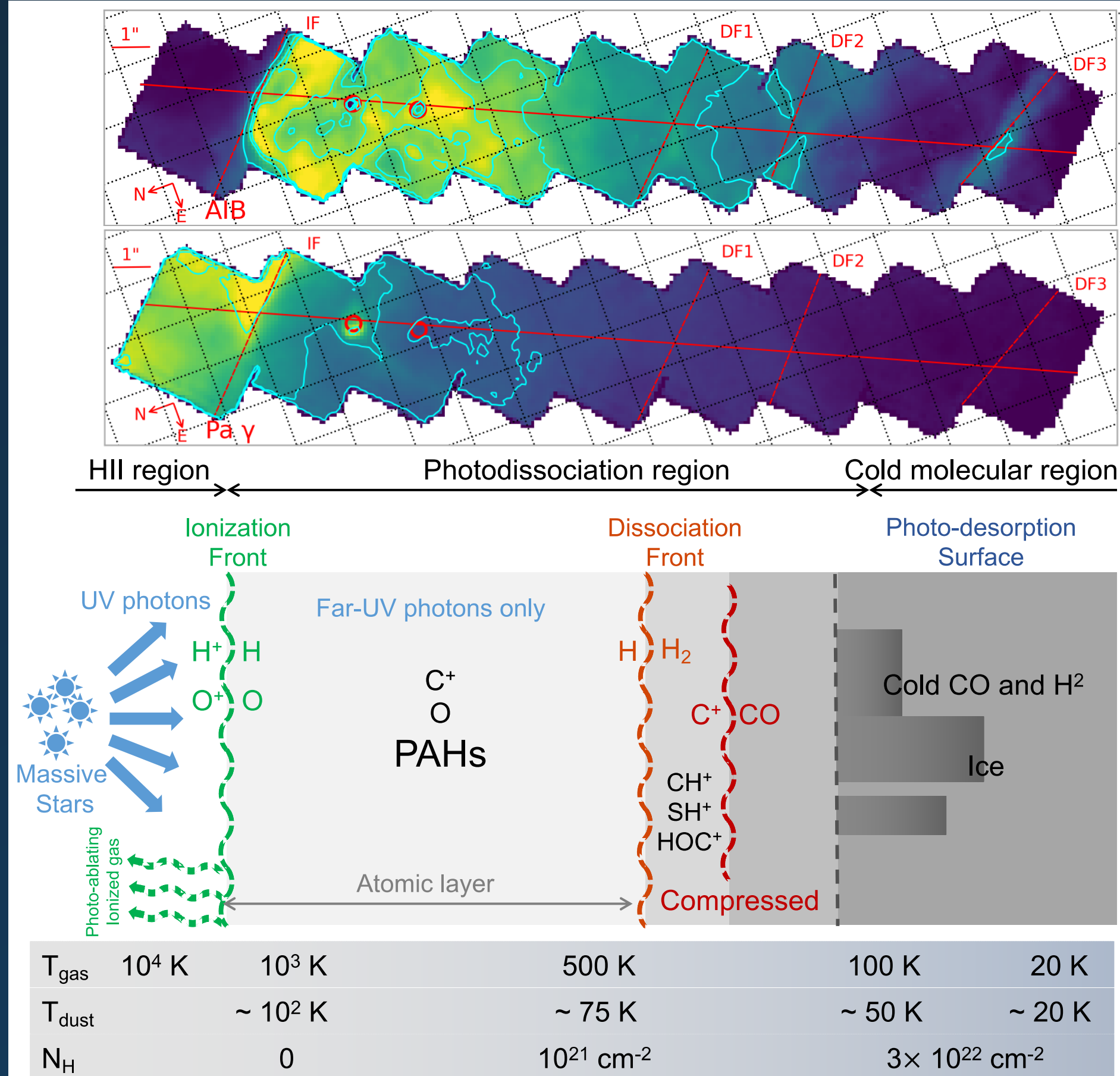
Relative intensity of the features between 5-10 μm is an indication of the ionization fraction

The aromatic/aliphatic C-H/C-D stretches

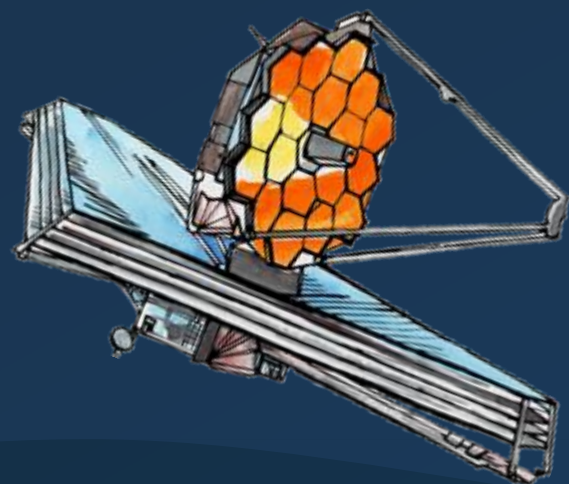


E. Peeters *et al* 2004 *ApJ* 604 252
 E. Peeters *et al* *A&A*, 685, A74 (2024)
 X. J. Yang, & Aigen Lin, *ApJ*, 2025

PAH Co-evolution with UV photon



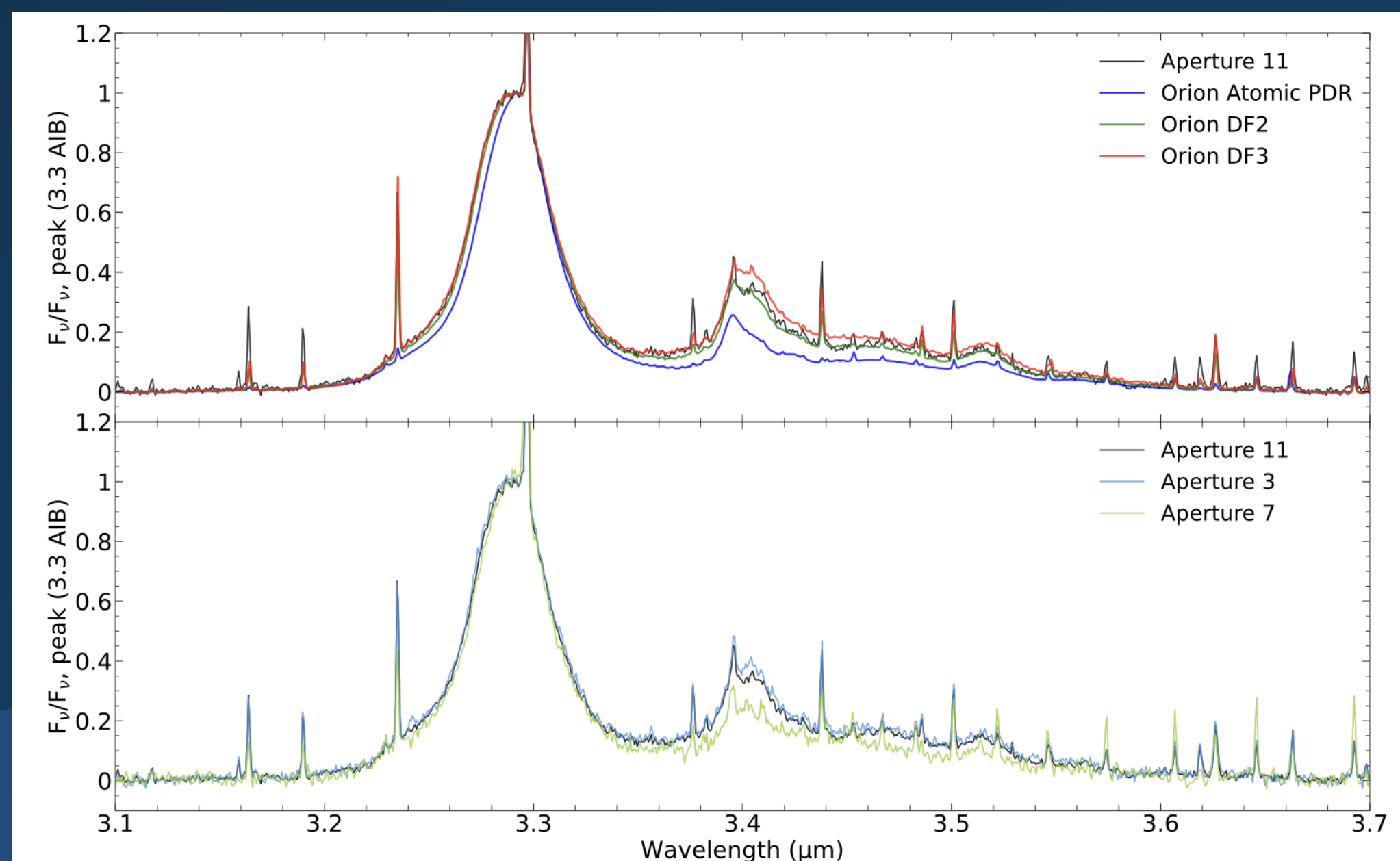
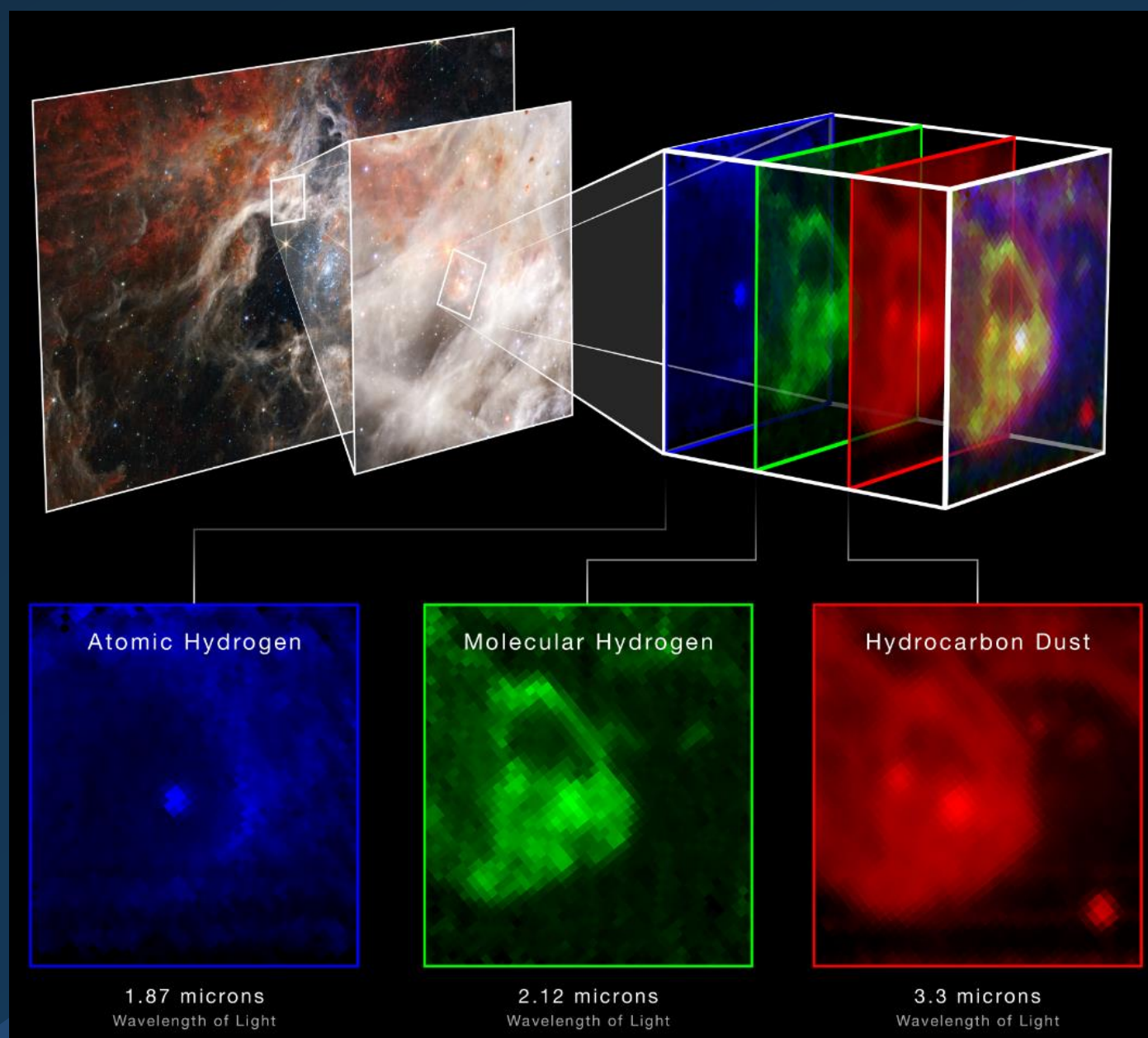
Congcong Zhang, Doctoral thesis, 2025



JWST & SPHEREx



- Image: NIRCarn
- Spectrum: NIRSpec IFU



The background is a solid dark red color. It is decorated with numerous white line-art chemical structures of polycyclic aromatic hydrocarbons (PAHs). These structures include single benzene rings, fused ring systems like naphthalene and anthracene, and larger, more complex clusters of fused hexagons. They are scattered across the entire background, with a higher density around the central oval.

Thank you