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# Molecule formation in the ejecta of SN 1987A: the impact of effective matter mixing based on 3D hydrodynamical models

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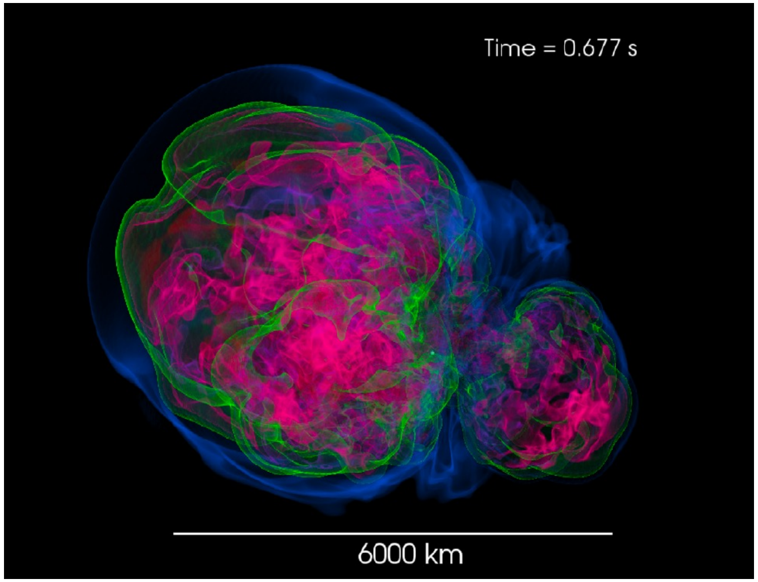
[MO+2023, submitted to ApJS (arXiv:2305.02550)]

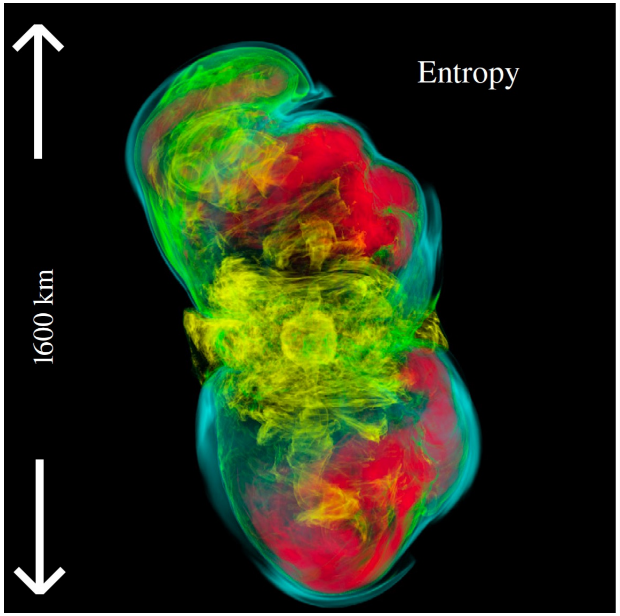
# What are the explosion mechanisms and morphologies of core-collapse supernovae (CCSNe)?

Delayed neutrino heating mechanism
aided by <u>SASI</u> and/or convection
<u>S</u>tanding <u>A</u>cretion <u>S</u>hock <u>I</u>nstability




[Vartanyan+19, MNRAS, 482, 351]

Magnetorotationally-driven
explosion (and/or neutrino heating)

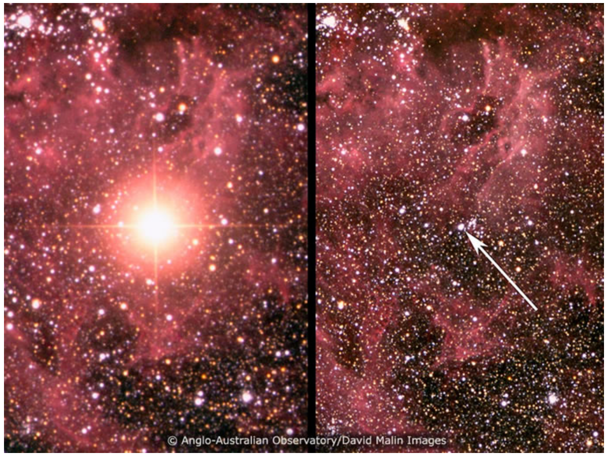



[Mösta+14, ApJL, 785, L29]

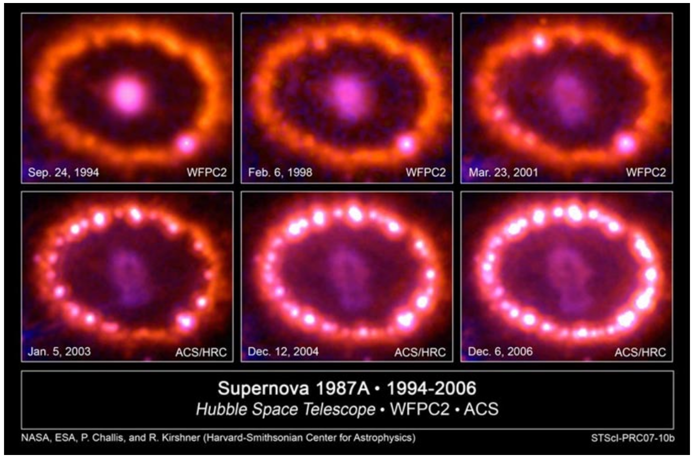
Volume rendered distributions of entropy

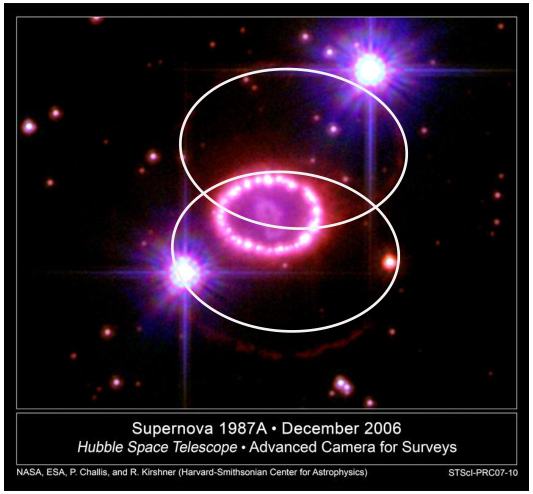
Core-collapse supernova explosions are essentially non-spherical?

# Supernova 1987A (SN 1987A)




- Basic observational features of SN 1987A
  - SN @ LMC on 23 Feb., 1987
  - Neutrinos from the SN were detected by Kamiokande
  - Triple-ring nebula



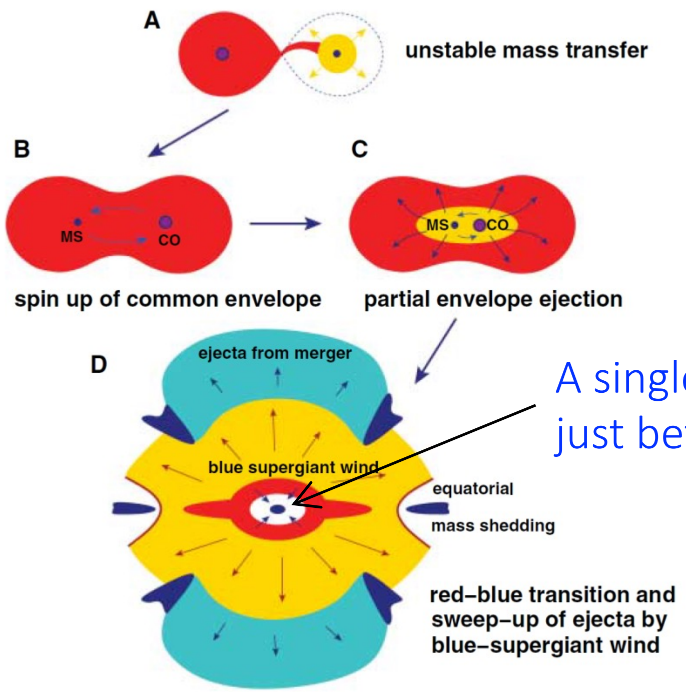



# The progenitor of SN 1987A was the outcome of a binary merger?

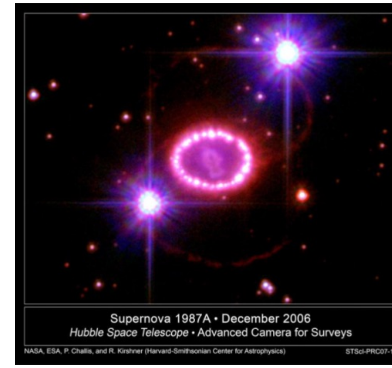
[Morris & Podsiadlowsky 2007, Science, 315, 1103]

- 3D smoothed particle hydrodynamic (SPH) simulations

~ 15 $M_\odot$ RSG ~ 5 $M_\odot$ MS star




A single blue supergiant (BSG) just before the explosion

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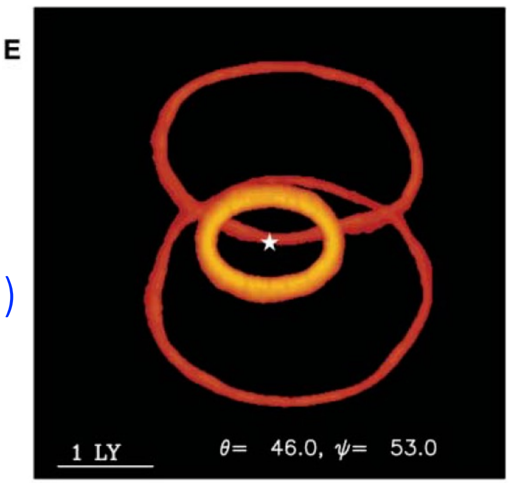
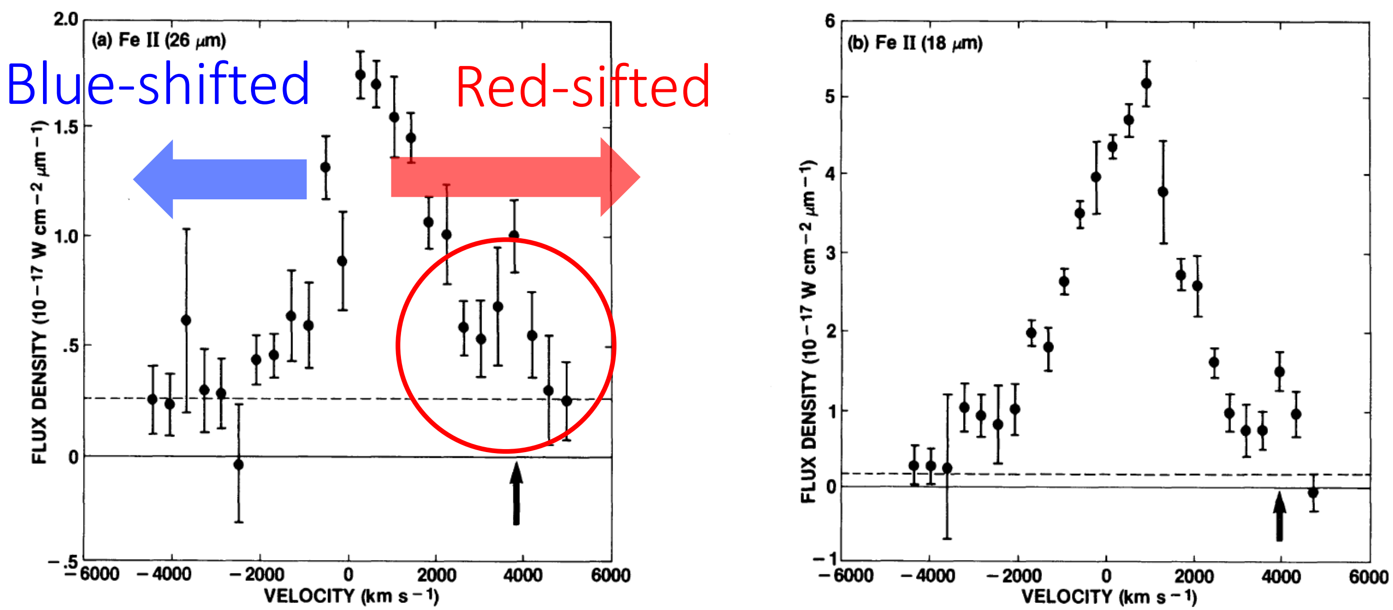



- We use a 18.3 $M_\odot$ binary merger progenitor model (14 $M_\odot$ + 9 $M_\odot$) (Urushibata+2018, MNRAS, 473, L101) in our simulations (shown later)

# SN 1987A: High velocity iron: Matter mixing?

[Fe II] line profiles

[Haas+1990, ApJ, 360, 257]
(observations at ～ 400 days after the explosion)



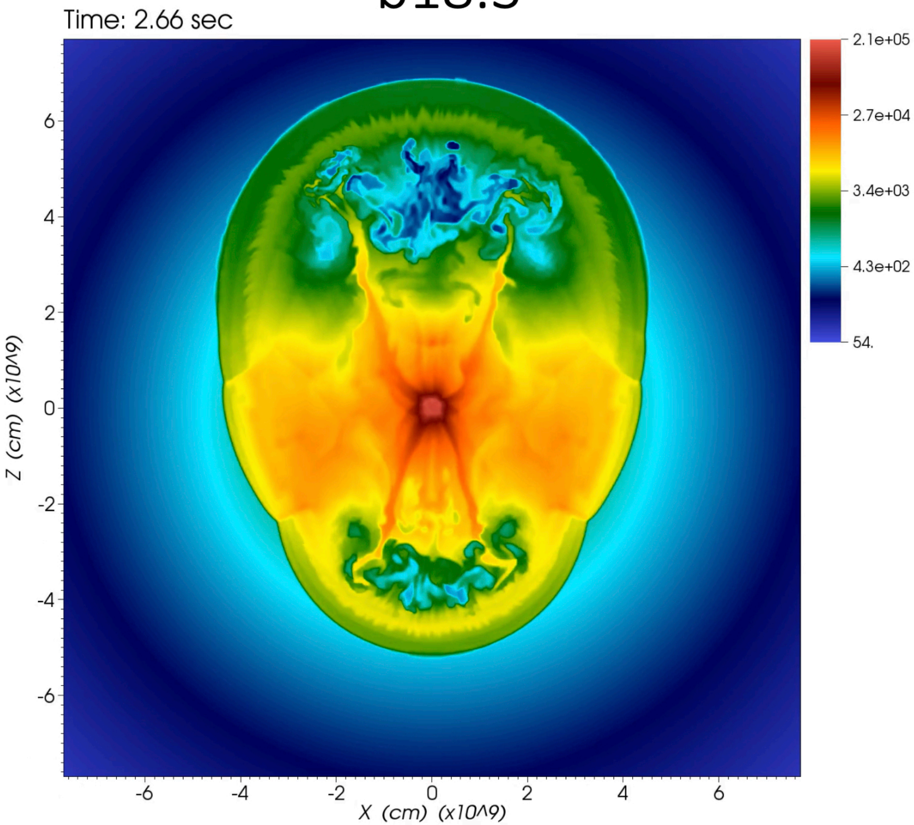

- High velocity tails of [Fe II] line profiles reach (> 4,000 km/s)

Fast $^{56}$Fe ($^{56}$Ni → $^{56}$Co → $^{56}$Fe) velocity → Matter mixing ?
radio active decay
Red-shifted side is dominated → Asymmetric explosion?

# Time evolution of 2D slices of the density : binary merger model vs single star model (Movies)

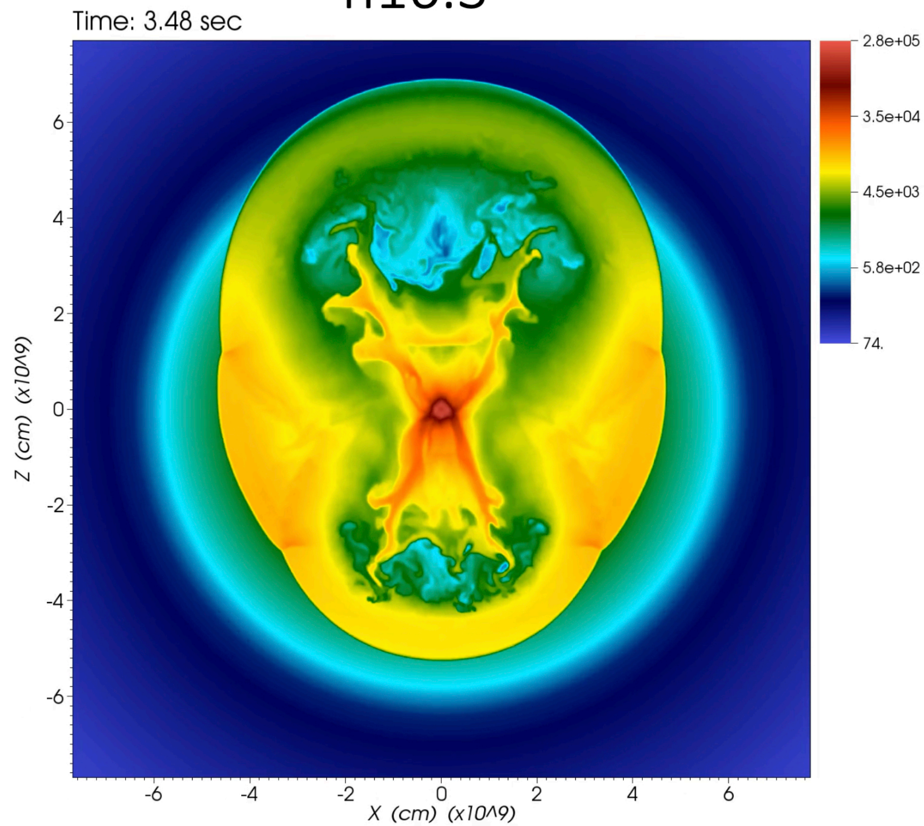
[MO+20, ApJ, 888, 111]

b18.3




Binary merger progenitor

n16.3

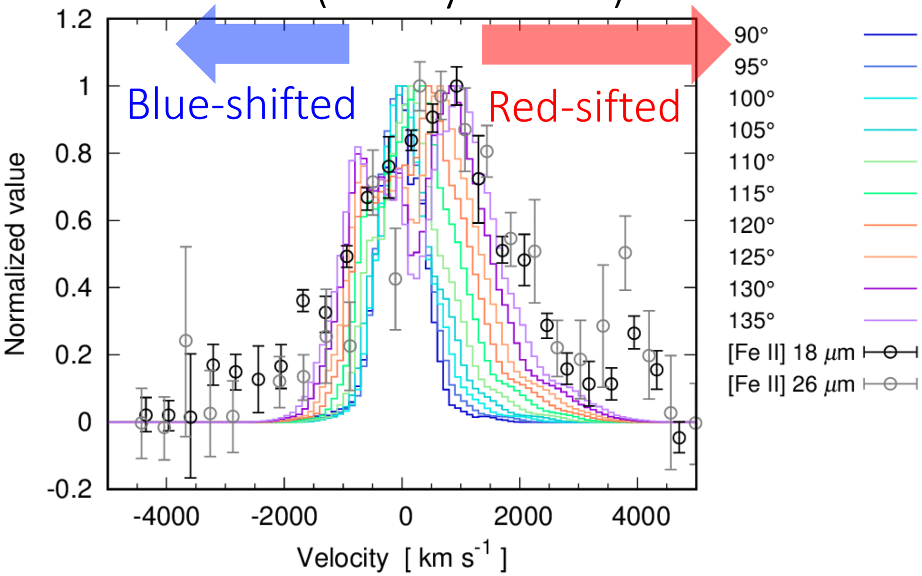



Single star progenitor

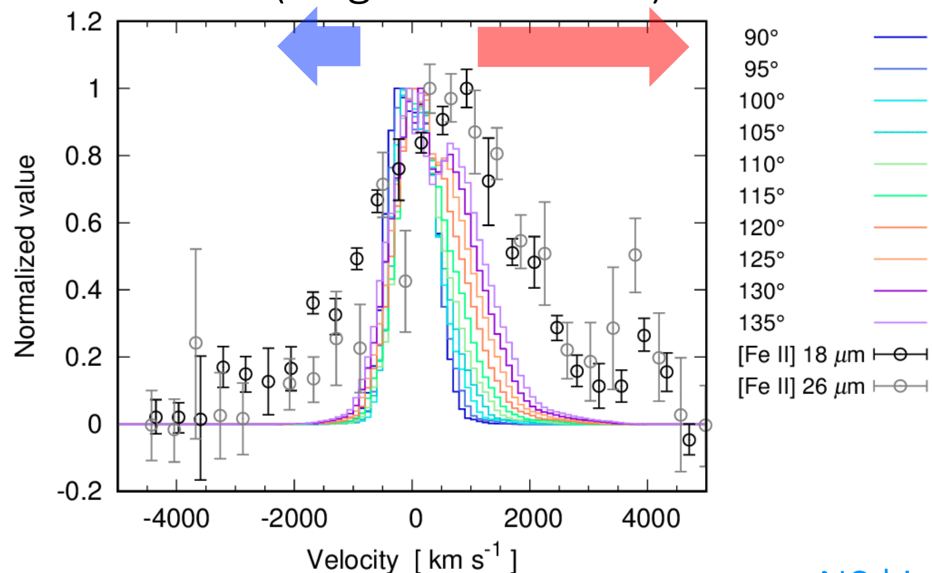
[MO+20, ApJ, 888, 111]

# Line of sight (LoS) velocity distributions of $^{56}$Ni

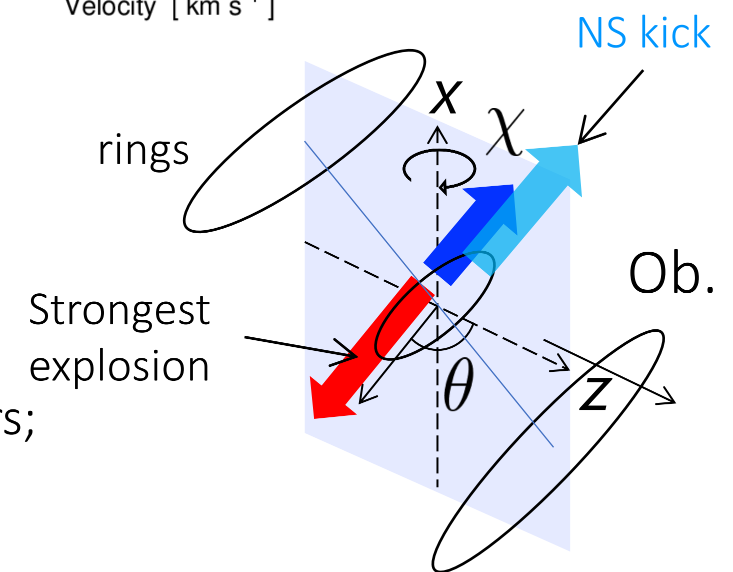
b18.3 (binary model)




n16.3 (single star model)



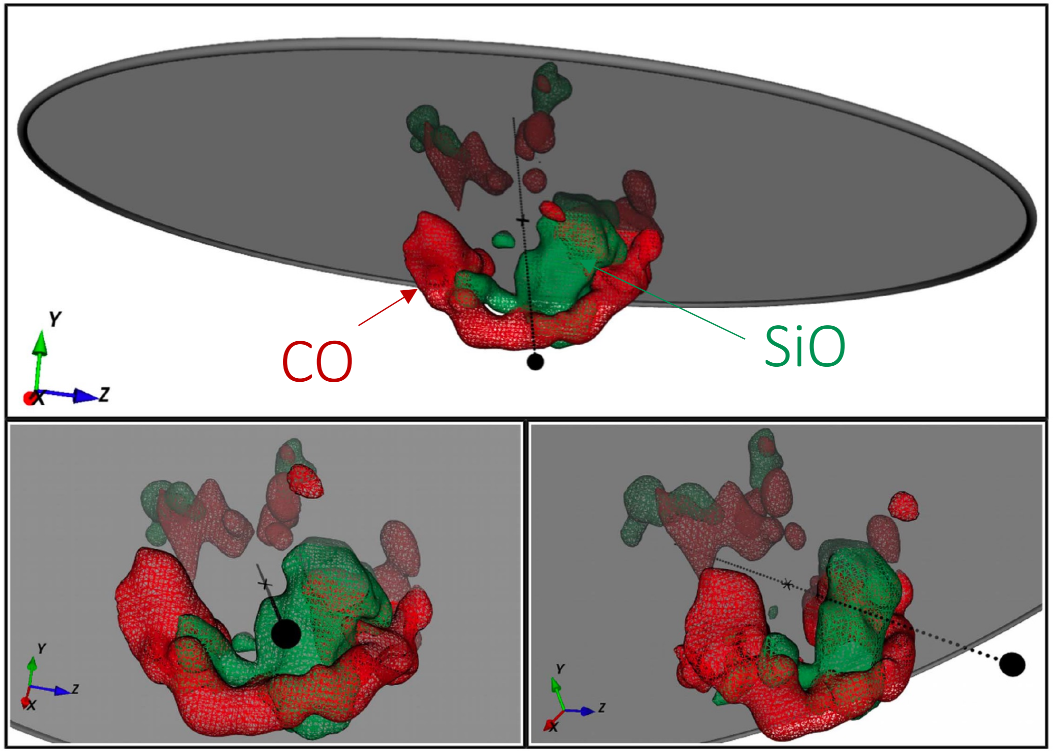

- The best model:
  - Progenitor model: b18.3 (binary merger)
  - ($E_{in}$, α, β) = (2.5 x $10^{51}$ erg, 1.5, 16.0)
  - θ = 130° , χ = 10°
  - Estimated NS kick velocity: 285 km s$^{-1}$
    (consistent with kick velocities of young pulsars; e. g. Faucher-Giguère & Kapsi 2006)



# Distribution of molecules in the ejecta of SN 1987A seen in 3D

[Abellán+2017, ApJ, 842, L24]

ALMA observations of CO $J$ = 2 -1, SiO $J$ = 5 – 4, 6 -5 rotational transitions



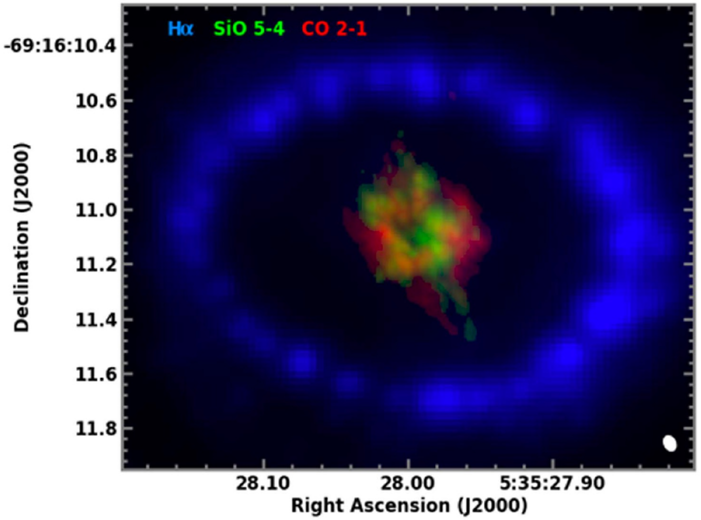




**Figure 1.** Molecular emission and Hα emission from SN 1987A. The more compact emission in the center of the image corresponds to the peak intensity maps of CO 2−1 (red) and SiO 5−4 (green) observed with ALMA. The surrounding Hα emission (blue) observed with *HST* shows the location of the circumstellar equatorial ring (Larsson et al. 2016).

3D spatial distribution in a SN ejecta for the first time!

[MO+2023, submitted to ApJS (arXiv:2305.02550)]

# Calculations of molecule formation in the ejecta of SN 1987A — Impact of matter mixing on molecule formation —

**There has been no numerical study on molecule formation in the core-collapse supernova ejecta based on 3D hydrodynamical models**

This study — The impact of matter mixing on the molecule formation

- Ejecta models: one-zone/1D models based on 3D hydrodynamical models of the bipolar-like explosions [MO+2020, ApJ, 888, 111]
- Calculations of rate equations with a chemical reaction network
  - 75 species (11 atoms, 24 diatomic molecules, electron, and 39 ions)
- Calculations of rate equations for CO rotational-vibrational transitions
  - Contribute to the cooling of the gas
  - Diagnostic of the models through the comparison with observations
- Other effects taken into account
  - Heating of the gas due to the decay of $^{56}$Ni and/or $^{56}$Co
  - Ionizations and/or dissociation of atoms and molecules by Compton electrons from the decay of $^{56}$Ni and/or $^{56}$Co

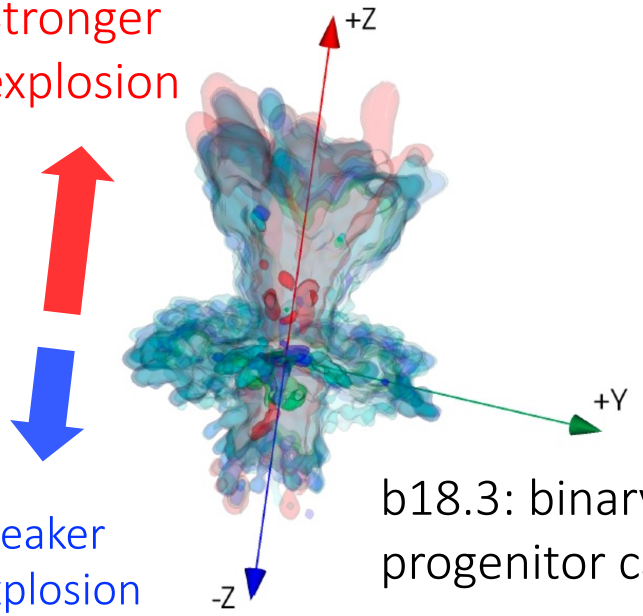
Figures from MO+2023, submitted to ApJS (arXiv:2305.02550)]

# Elemental distributions in the 3D hydrodynamical models (initial conditions)

- 3D models of asymmetric bipolar-like explosions with two progenitor stars [MO et al. 2020, ApJ, 888, 111]

Initial distribution of elements in the inner ejecta

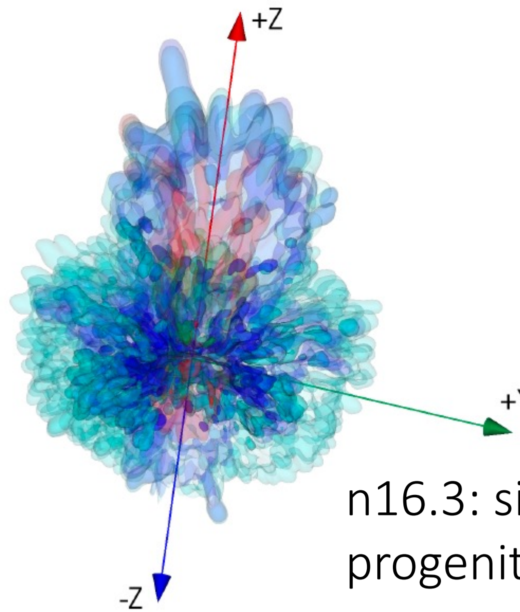
Stronger explosion




Weaker explosion

b18.3: binary merger progenitor case

[Urushibata+2018]




n16.3: single-star progenitor case

[Nomoto & Hashimoto 1998]

$^{56}$Ni (red), $^{28}$Si (green), $^{16}$O (blue), $^{12}$C (cyan)

# Roles of the radioactive decay of $^{56}$Ni

$$^{56}\mathrm{Ni} \longrightarrow {}^{56}\mathrm{Co} \longrightarrow {}^{56}\mathrm{Fe}$$

Compton scattering

$$\mathrm{e}^- + \gamma \longrightarrow \mathrm{e}^-_\mathrm{C} + \gamma'$$

- Heating of gas $\longrightarrow$ delays the start of molecule formation
- Ionization and destruction of molecules (atoms) by Compton electrons

| | | |
| --- | --- | --- |
| $\mathrm{CO} + \mathrm{e}^-_\mathrm{C} \longrightarrow \mathrm{C} + \mathrm{O}^+ + \mathrm{e}^- + \mathrm{e}^-_\mathrm{C}$ | Dissociative ionization | Decrease the amount of CO and SiO |
| $\mathrm{CO} + \mathrm{e}^-_\mathrm{C} \longrightarrow \mathrm{C}^+ + \mathrm{O} + \mathrm{e}^- + \mathrm{e}^-_\mathrm{C}$ | Dissociative ionization | |
| $\mathrm{CO} + \mathrm{e}^-_\mathrm{C} \longrightarrow \mathrm{C} + \mathrm{O} + \mathrm{e}^-_\mathrm{C}$ | Dissociation | |
| $\mathrm{CO} + \mathrm{e}^-_\mathrm{C} \longrightarrow \mathrm{CO}^+ + \mathrm{e}^- + \mathrm{e}^-_\mathrm{C}$ | Ionization | |
| $\mathrm{X} + \mathrm{e}^-_\mathrm{C} \longrightarrow \mathrm{X}^+ + \mathrm{e}^- + \mathrm{e}^-_\mathrm{C}$ | Ionization of atoms | |

[Cherchneff & Dwek 2009; Sluder+2018; Liljegren+2020]

- Indirect effects of the above through a sequence of other reactions

| | | |
| --- | --- | --- |
| $\mathrm{C}^+ + \mathrm{SiO} \longrightarrow \mathrm{CO} + \mathrm{Si}^+$ | Ion-neutral reaction (IN) | Ion involving reactions |
| $\mathrm{He}^+ + \mathrm{CO} \longrightarrow \mathrm{O} + \mathrm{C}^+ + \mathrm{He}$ | Ion-neutral reaction (IN) | |
| $\mathrm{He}^+ + \mathrm{SiO} \longrightarrow \mathrm{Si} + \mathrm{O}^+ + \mathrm{He}$ | Ion-neutral reaction (IN) | |
| $\mathrm{H}^+ + \mathrm{SiO} \longrightarrow \mathrm{SiO}^+ + \mathrm{H}$ | Charge Exchange (CE) | |

[Lepp+1990; Liu & Dalgarno 1996; Cherchneff & Dwek 2009]

| | | |
| --- | --- | --- |
| $\mathrm{H} + \mathrm{e}^- \longrightarrow \mathrm{H}^- + \gamma$ | Radiative Electron Attachment (REA) | Increase the amount of CO and SiO |
| $\mathrm{H}^- + \mathrm{H} \longrightarrow \mathrm{H}_2 + \mathrm{e}^-$ | Associative electron Detachment (AD) | |
| $\mathrm{O} + \mathrm{H}_2 \longrightarrow \mathrm{OH} + \mathrm{H}$ | Neutral-neutral reaction (NN) | |
| $\mathrm{C} + \mathrm{OH} \longrightarrow \mathrm{CO} + \mathrm{H}$ | Neutral-neutral reaction (NN) | |
| $\mathrm{Si} + \mathrm{OH} \longrightarrow \mathrm{SiO} + \mathrm{H}$ | Neutral-neutral reaction (NN) | |

This sequence for increasing CO and SiO is newly pointed

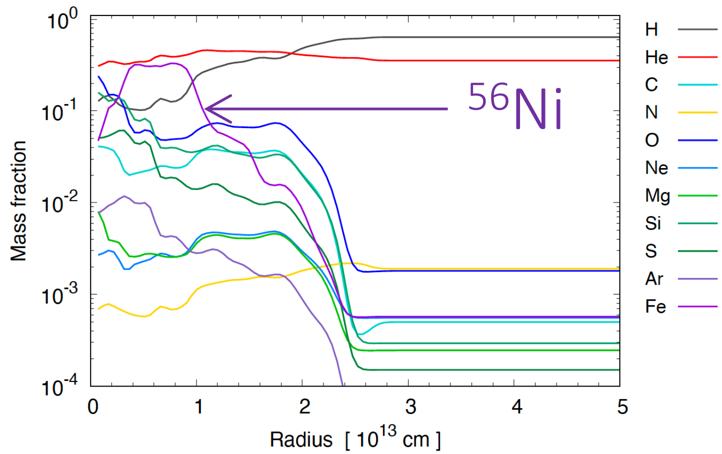
[MO+2023, submitted to ApJS (arXiv:2305.02550)]

# Calculations of different specified directions

[MO+2023, submitted to ApJS (arXiv:2305.02550)]

- Dependence of molecule formation on directions for the binary merger progenitor model (b18.3-high: MO+2020)

+Z

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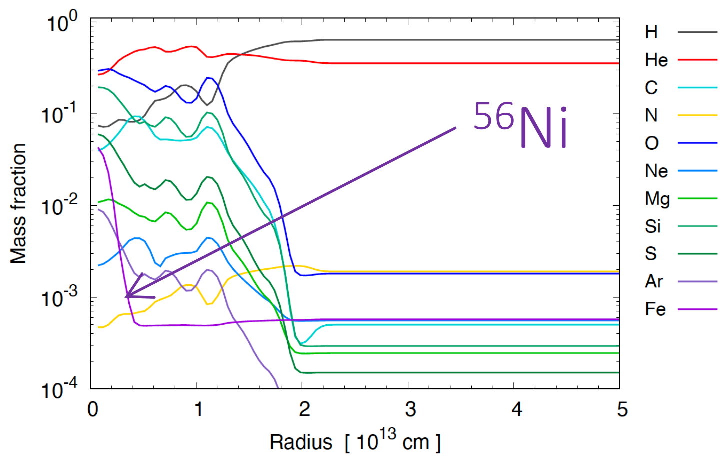
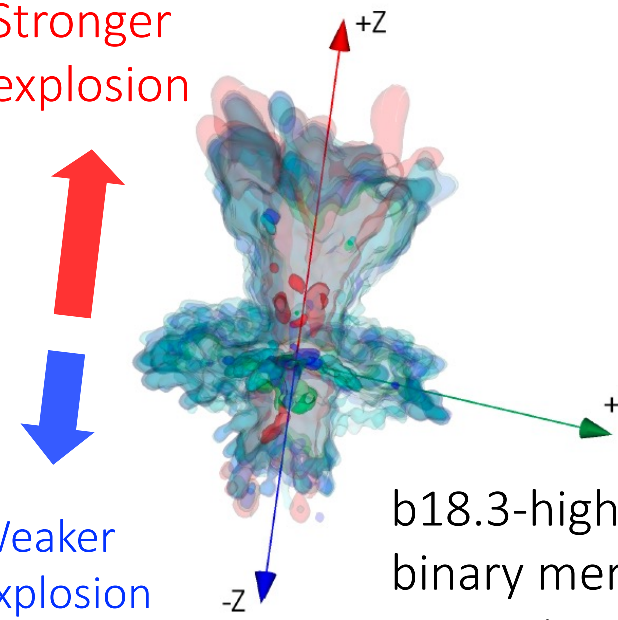



Stronger explosion




Weaker explosion

b18.3-high: binary merger progenitor case

$^{56}$Ni (red), $^{28}$Si (green), $^{16}$O (blue), $^{12}$C (cyan)

# Calculations of different specified directions

[MO+2023, submitted to ApJS (arXiv:2305.02550)]

- Dependence of molecule formation on directions

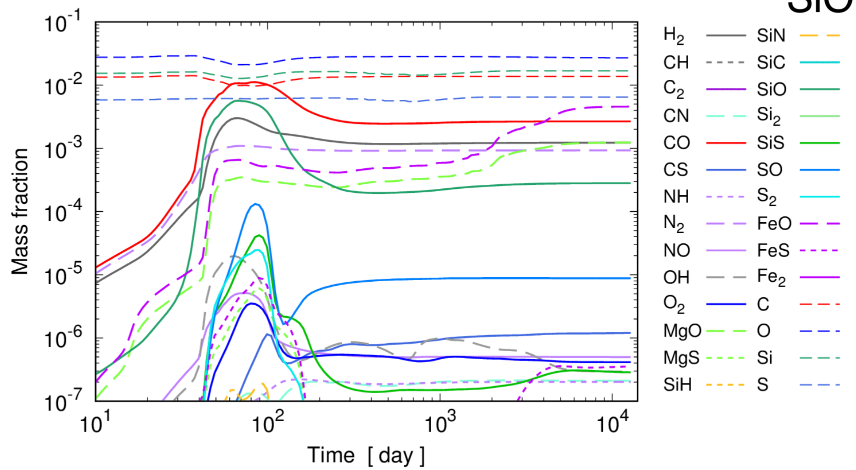
Evolution of mass fractions of moleules

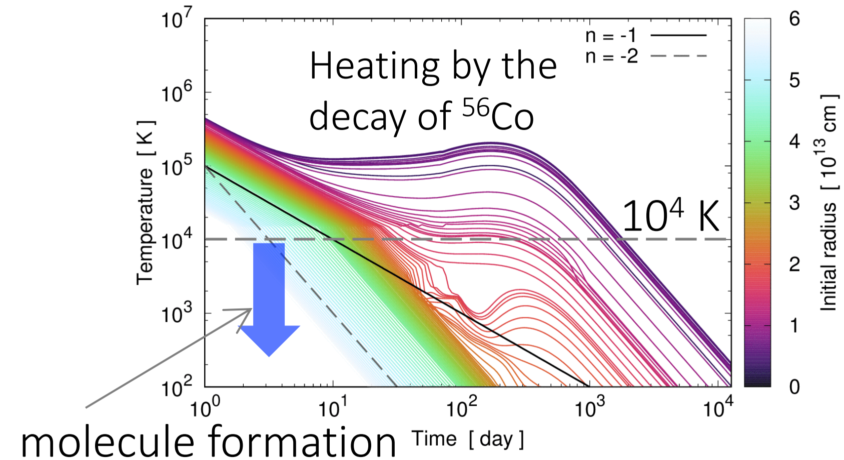
CO

SiO

Evolution of temperatures of gas

+Z

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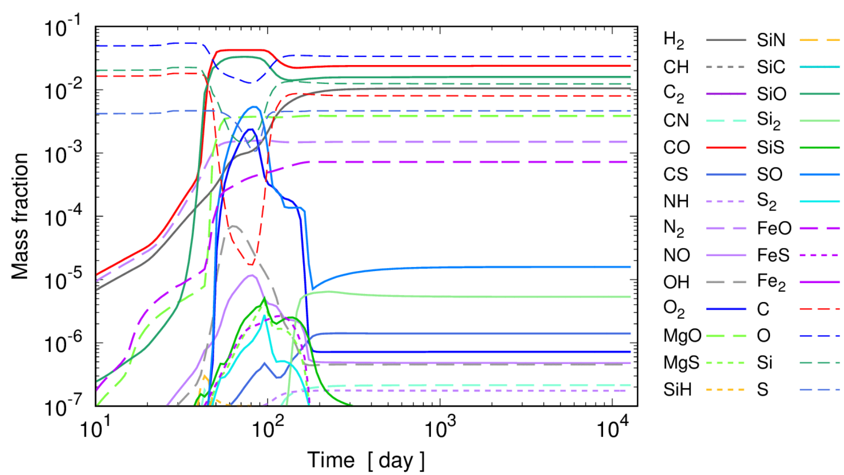
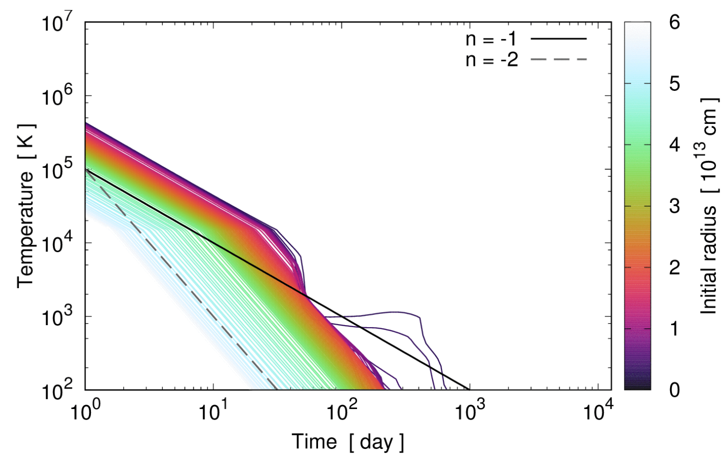


# Radial distribution of molecules

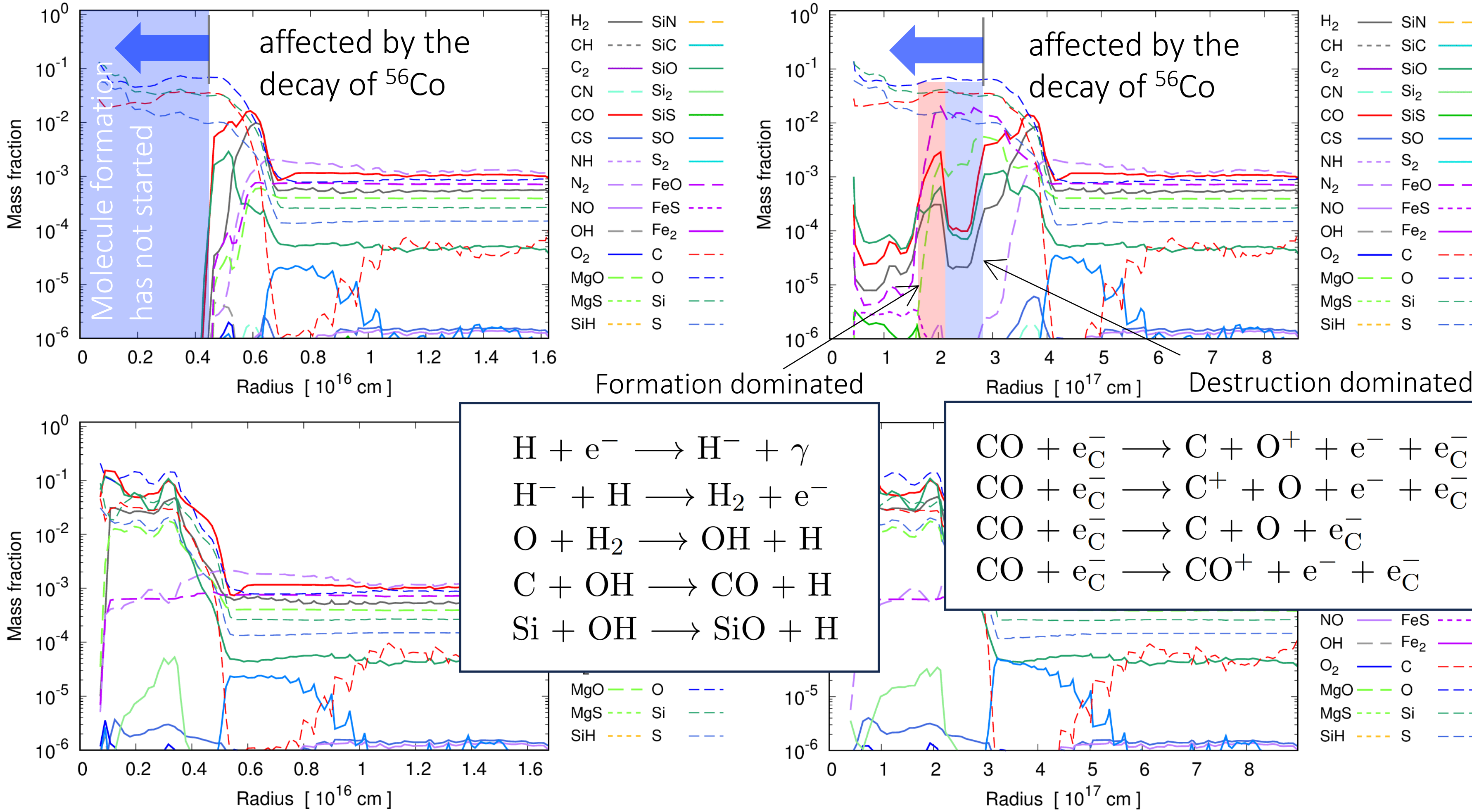
[MO+2023, submitted to ApJS (arXiv:2305.02550)]

- Evolution (two epochs) of radial distribution of molecules

~ 200 days after the explosion | ~10,000 days after the explosion

+Z

+Y




$$\mathrm{H} + \mathrm{e}^- \longrightarrow \mathrm{H}^- + \gamma$$
$$\mathrm{H}^- + \mathrm{H} \longrightarrow \mathrm{H}_2 + \mathrm{e}^-$$
$$\mathrm{O} + \mathrm{H}_2 \longrightarrow \mathrm{OH} + \mathrm{H}$$
$$\mathrm{C} + \mathrm{OH} \longrightarrow \mathrm{CO} + \mathrm{H}$$
$$\mathrm{Si} + \mathrm{OH} \longrightarrow \mathrm{SiO} + \mathrm{H}$$

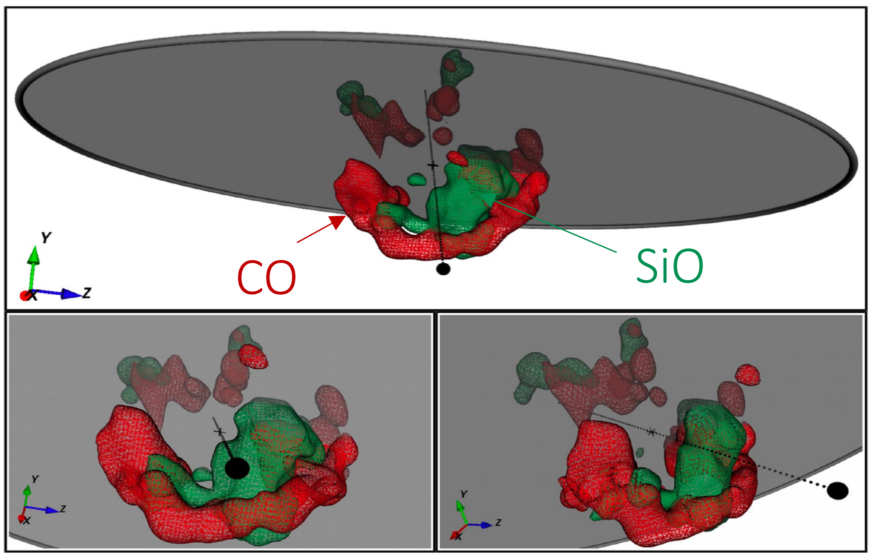
$$\mathrm{CO} + \mathrm{e}^-_{\mathrm{C}} \longrightarrow \mathrm{C} + \mathrm{O}^+ + \mathrm{e}^- + \mathrm{e}^-_{\mathrm{C}}$$
$$\mathrm{CO} + \mathrm{e}^-_{\mathrm{C}} \longrightarrow \mathrm{C}^+ + \mathrm{O} + \mathrm{e}^- + \mathrm{e}^-_{\mathrm{C}}$$
$$\mathrm{CO} + \mathrm{e}^-_{\mathrm{C}} \longrightarrow \mathrm{C} + \mathrm{O} + \mathrm{e}^-_{\mathrm{C}}$$
$$\mathrm{CO} + \mathrm{e}^-_{\mathrm{C}} \longrightarrow \mathrm{CO}^+ + \mathrm{e}^- + \mathrm{e}^-_{\mathrm{C}}$$

# Comparison with the CO and SiO distribution by ALMA observations

[MO+2023, submitted to ApJS (arXiv:2305.02550)]

- Comparison of calculations for specified directions with the ALMA observations

ALMA observations




[Abellán+2017, ApJ, 842, L24]

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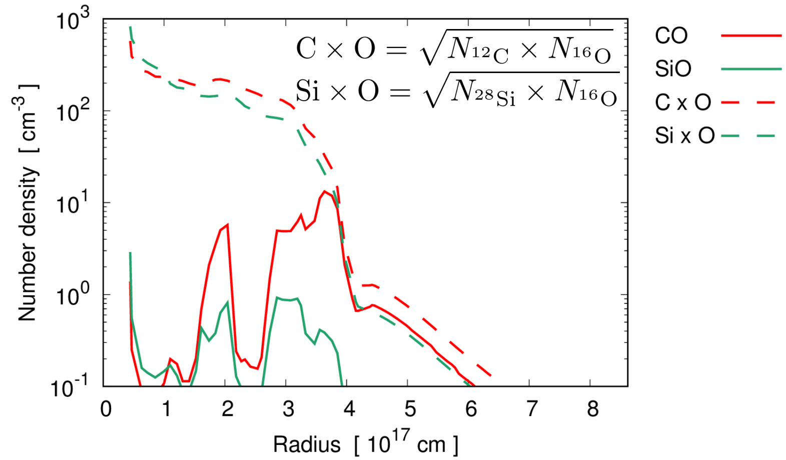


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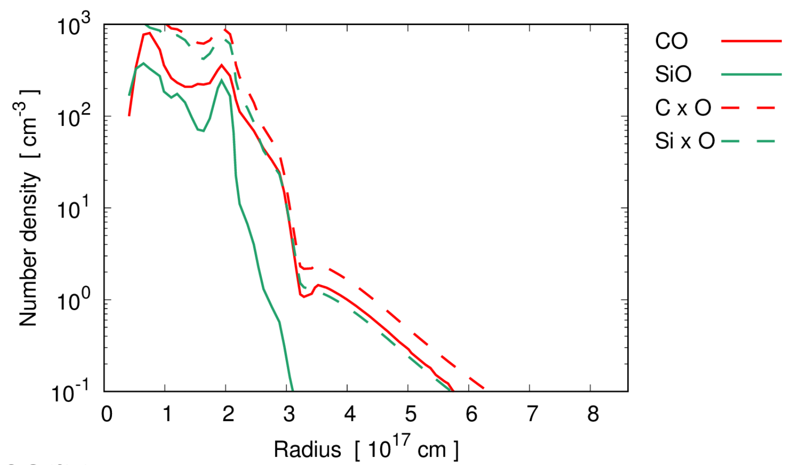


- Calculated CO distribution may look like a ring?; more direct applications to 3D models are necessary
- The observed ring-like structure may be a support for a bipolar-like explosion?

# Summary

**Molecule formation in the ejecta of SN 1987A based on 3D hydrodynamical models**

- Matter mixing affect the distributions of $^{56}$Ni and seed atoms and the resulting molecule formation
- The decay of $^{56}$Ni plays a non-negligible role in molecule formation through the heating of gas and ionization/destruction by Compton electrons
- Under some conditions, the decay of $^{56}$Ni could locally increase the amounts of CO and SiO
- The bipolar-like explosion results in a very different distribution of $^{56}$Ni along the bipolar axis and the equatorial plane
- The above results in very different amounts of molecules between the two
- The 3D model may qualitatively reproduce the observed ring-like structure of CO

**Problems and future work**

- Observed CO vibrational bands are difficult to explain with the current model
- More realistic treatments of the gas temperature, the energy deposition, and the excitation processes of vibrational levels of CO may be crucial
- Application of a dust formation theory (near future work)
- Isotope-dependent calculations? — e.g., $^{28,30}$SiC (for presolar Type-X grains)