Can Heavy-Element Molecules Probe *r*-process Nucleosynthesis?

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Xiao Zhang[a,b], Gabriel Martínez-Pinedo[a,b], Andreas Flörs[a], Zewei Xiong[a]

[a]GSI Helmholtzzentrum für Schwerionenforschung, [b]Technische Universität Darmstadt

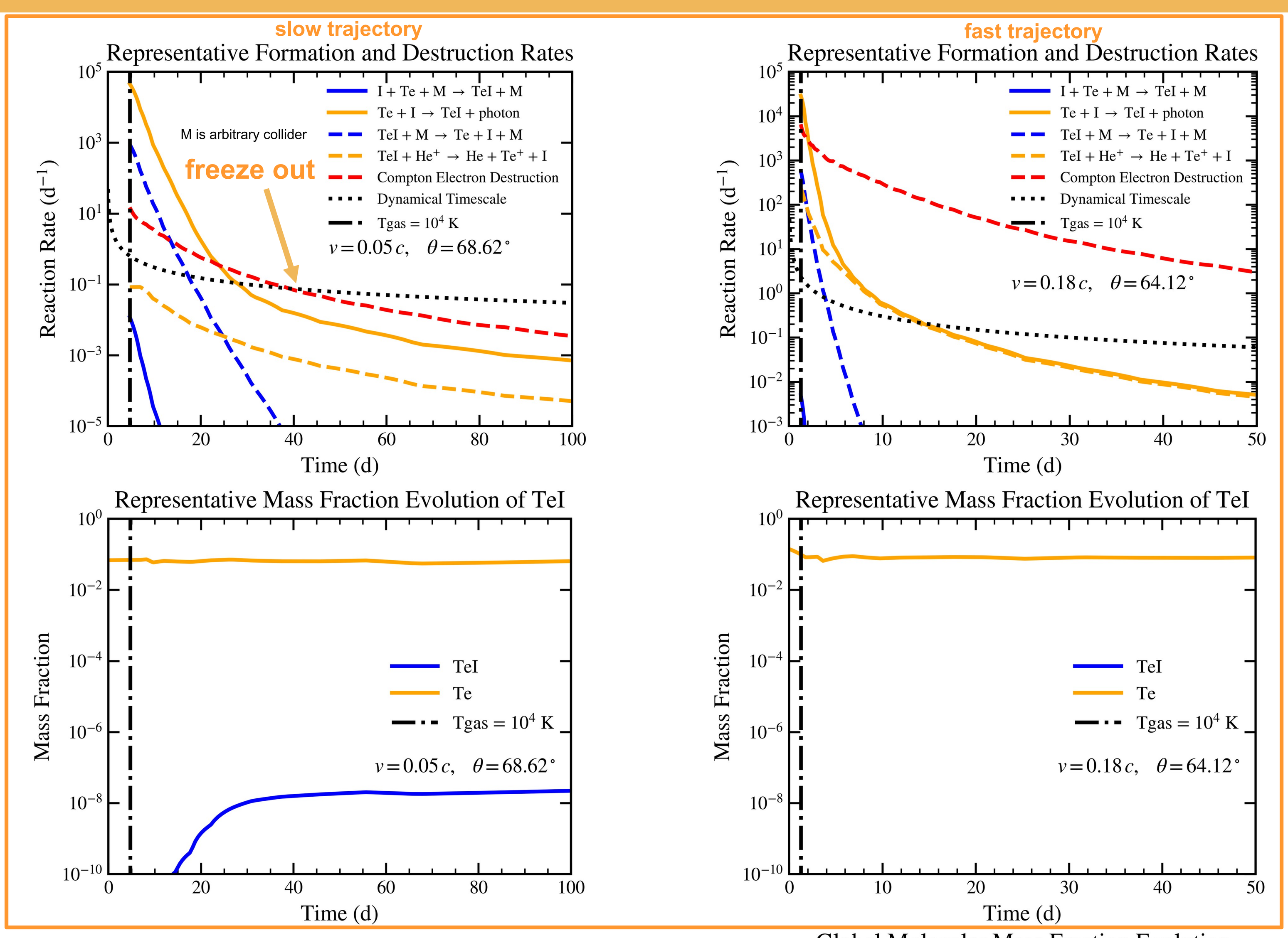
Introduction

- Binary neutron-star (BNS) mergers synthesize and eject ***r*-process elements**, powering kilonovae and enriching merger remnants.
- **Can atoms and ions efficiently form molecules and clusters before the ejecta becomes too dilute?** Their isotopic signatures may provide a new probe of *r*-process nucleosynthesis.
- **As a first case study, we investigate tellurium-bearing molecules and clusters in BNS merger ejecta.** Tellurium lies near the **second *r*-process peak;** combining Te with abundant light and halogen species motivates candidate molecules such as **TeI, TeBr, and TeH**, while **Te clusters** probe the first steps toward condensation.
- We **post-process BNS merger trajectories** to **model molecular formation** and **predict rotational emission** at radio and submillimeter wavelengths to assess its detectability with ALMA.

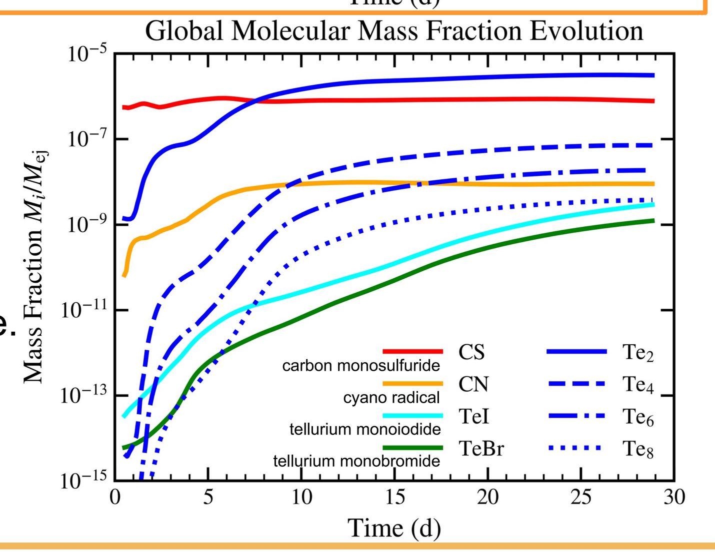
Model Pipeline

- **BNS merger trajectories**
  - Asymmetric BNS-merger model **asy-n1-a6** [1]
  - Temperature, density, nuclear abundances
- **Chemical reaction network:** **155 species** (atoms, ions, molecules, clusters) and **1155 reactions**
  - Benchmark supernova chemistry [2, 3] (H, He, O, C, Si, S, Mg, Fe, Al)
  - Extended with halogens (F, Cl, Br, I), Te-bearing molecules (e.g. TeI, TeH, TeO), Te_n clusters ($n \leq 15$)
  - Compton electron destruction from **radioactive decay**
- **Quantum chemistry calculations** [4] for missing molecular data
  - Bond energies → estimated destruction rates
  - Molecular constants → rotational spectra
- **From chemistry to observables**
  - Post-process trajectories from 10^4 K to 400 K [5] → molecular number density distribution $n_i(t,r,\theta)$
  - Number density distribution + spectroscopy → **rotational line flux**

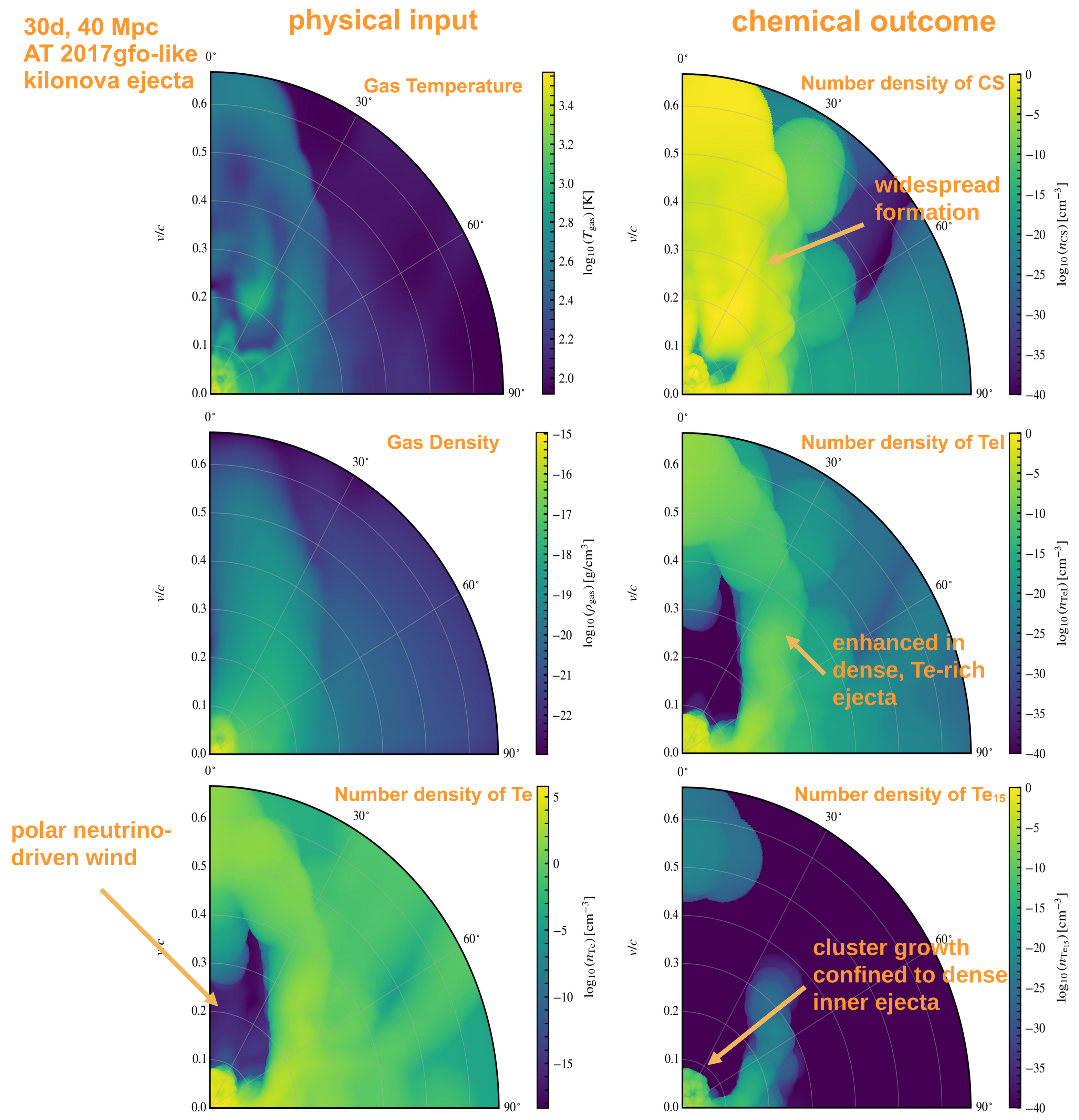
Chemical outcome



- **Dominant processes**
  - Formation: radiative association
  - Early destruction: thermal fragmentation
  - Late destruction: Compton electron destruction
- **Chemical outcome**
  - Te_2 dominates the Te-bearing molecules, but **lacks electric-dipole transitions** as mononuclear molecule.
  - The initial Te mass fraction is **0.067**; **~0.01%** forms molecules and clusters.
  - **CS** forms efficiently.
  - Molecular abundances **freeze out by ~40 d**.



Molecular Distribution



Detectability of TeI

Scenario	Strongest TeI line	Peak flux density (mJy)	ALMA Band 5σ sensitivity, 1 hr (mJy)
AT 2017gfo-like kilonova 30 d, 40 Mpc	J = 273→272 (602.85 GHz)	2.64×10^{-15}	ALMA Band 9 2.25
Nearby remnant 1000 yr, **10 pc**	J = 50→49 (110.82 GHz)	**0.096**	**ALMA Band 3 0.065**

- **AT 2017gfo-like kilonovae:** At 40 Mpc, TeI rotational emission remains **~15 orders of magnitude below** current ALMA sensitivity.
- **Nearby remnants:** For remnants within **10 pc**, TeI may provide **detectable** rotational emission with ALMA.

Conclusions & Outlook

Conclusions
- Te-bearing molecules preferentially form in **slow, dense, Te-rich BNS ejecta**.
- **Te_2 dominates** the Te-bearing molecules, but **lacks electric-dipole transitions**.
- A framework for predicting **molecular rotational emission** and evaluating its **radio detectability** has been developed and applied to **TeI**.

Outlook
- Extend to **other *r*-process elements and molecular emission bands**.
- Introduce **non-LTE excitation**.
- Explore **molecular isotopic signatures** and **radioactive molecules**.

References

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