How Collapse Dynamics Shape the Dusty Chemical Inventory of Star Forming Regions

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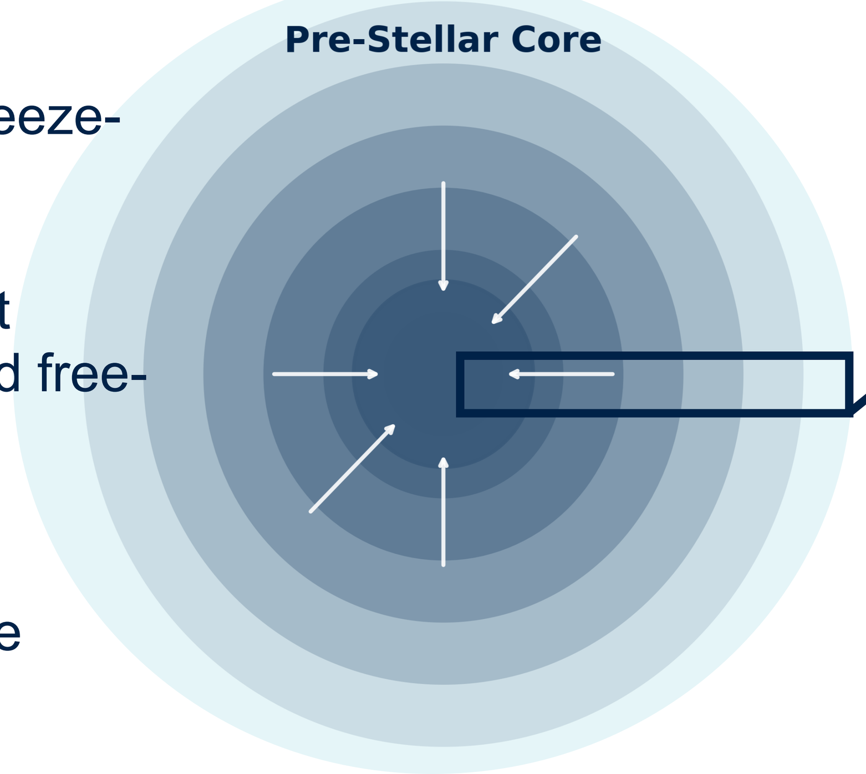
Abstract We present monolayer-resolved modelling of molecular ice freeze-out on dust grains. Our approach tracks dust and gas phase species as they evolve through core contraction, allowing us to predict how different collapse scenarios affect the dust grain chemical inventory available to later protoplanetary systems. Our results demonstrate that collapse dynamics drive chemical differentiation between cores with identical initial compositions.

Introduction

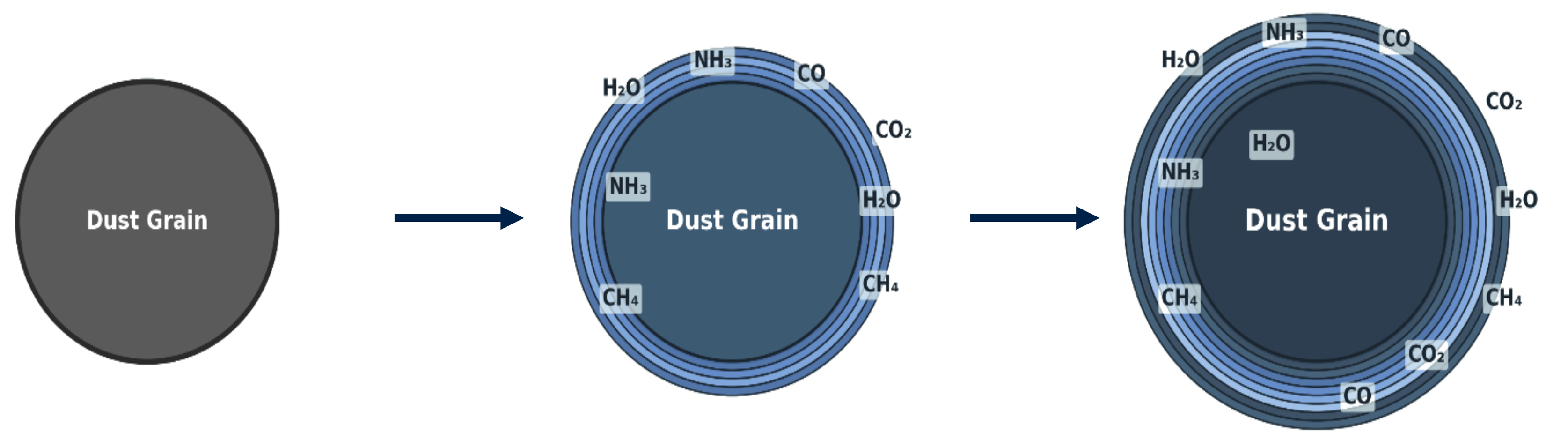
•Layer-by-layer modelling shows how collapse dynamics shape molecular freeze-out and the build-up of icy mantles.

•**Four collapse models**: Bonnor-Ebert (L1544), Inside-out, transient wave and free-fall linked with gas–grain chemistry.

•Inner ice layers record local chemical history; these vary among the collapse models **even with the same initial conditions.**

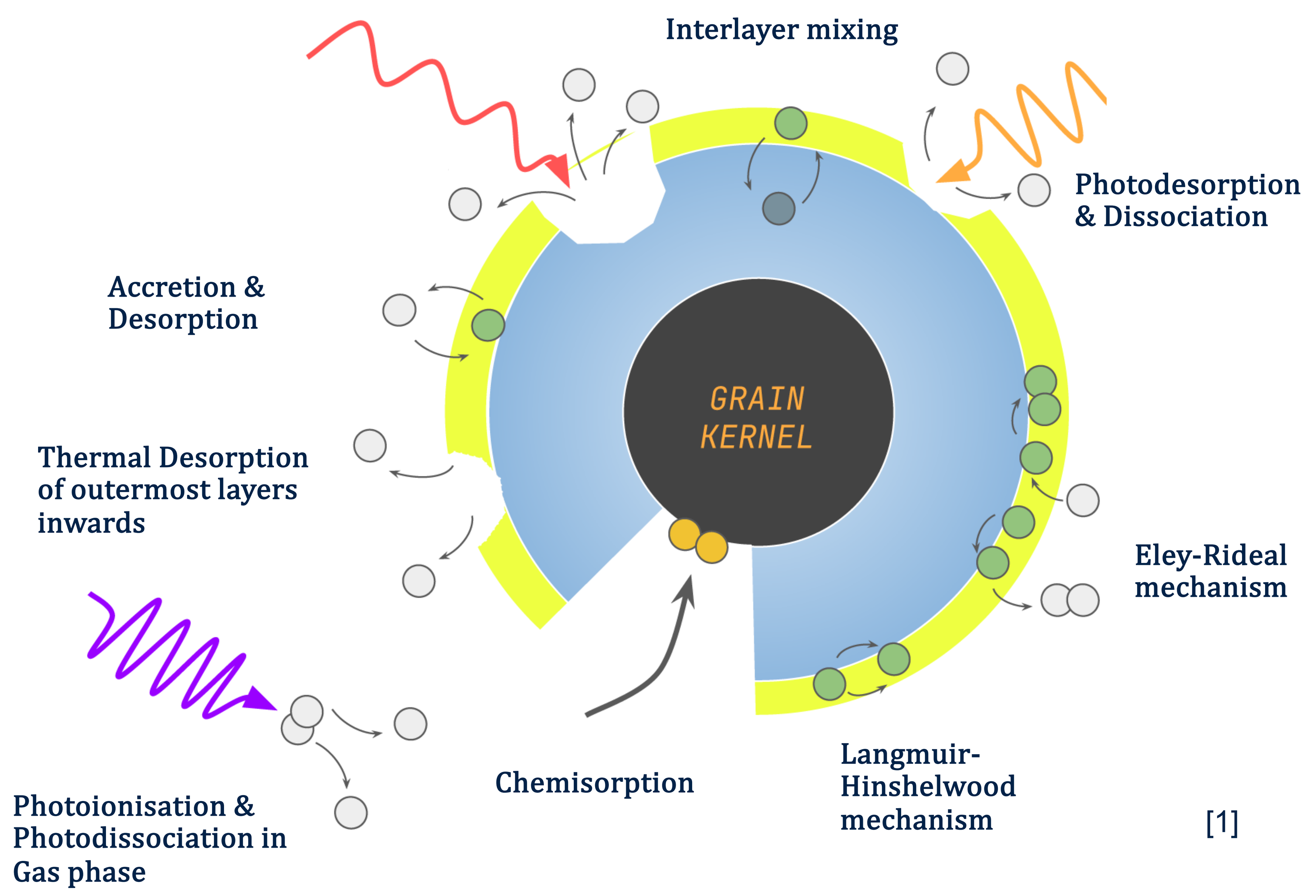


Edge ***Core***



$A_V < 0.5$	$A_V \approx 1.5$	$A_V > 20$
$n_H \sim 10^2$	$n_H \sim 10^3$	$n_H \sim 10^6$
0.300 pc	0.110 pc	0.008 pc

Chemistry *Methodology*



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- 79 Gas-phase Species
- 17 Ice Species
- 1200+ reactions (KIDA,UMIST databases)

Dynamics *Methodology*

BE (Bonnor-Ebert) Sphere
- Quasi-equilibrium contraction of an unstable BE sphere
- QE-BES resembles a BES except in the centre which evolves out of equilibrium most rapidly

SIS (Singular Isothermal Sphere)
- Self-similar solution of the collapse of a singular isothermal sphere
- Central singularity collapses first (inside-out); rarefaction wave (expansion wave) propagates outward at local sound speed

Freefall
- Collapse of a uniform density sphere under self-gravity
- All shells fall simultaneously with acceleration proportional to enclosed mass. Free-fall time = $\sqrt{(3\pi/32G\rho_0)}$

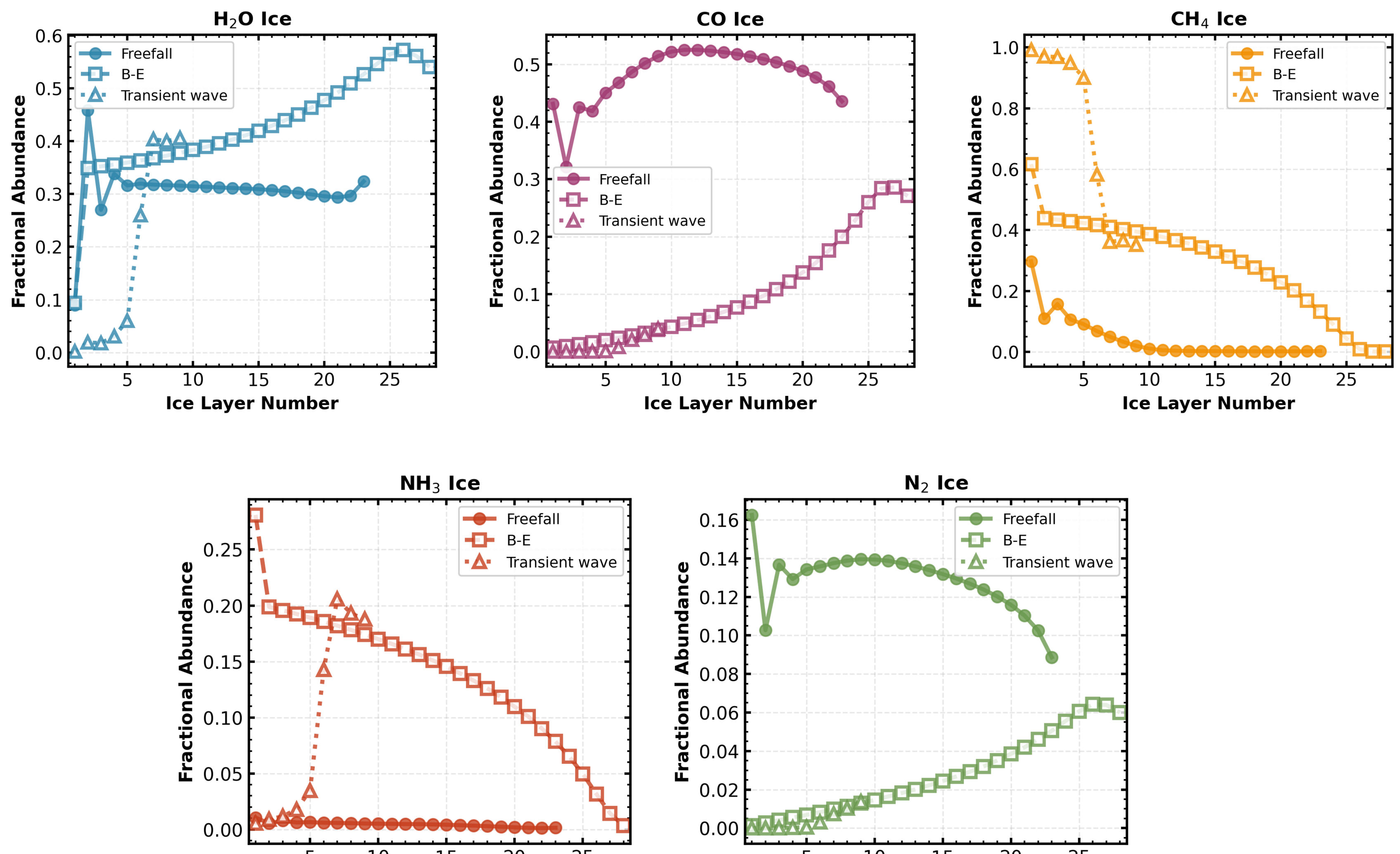
Transient wave
- Passage of compression wave through static core
- External shock/perturbation causes transient density increase; density rises, then declines; core collapse fails

Summary

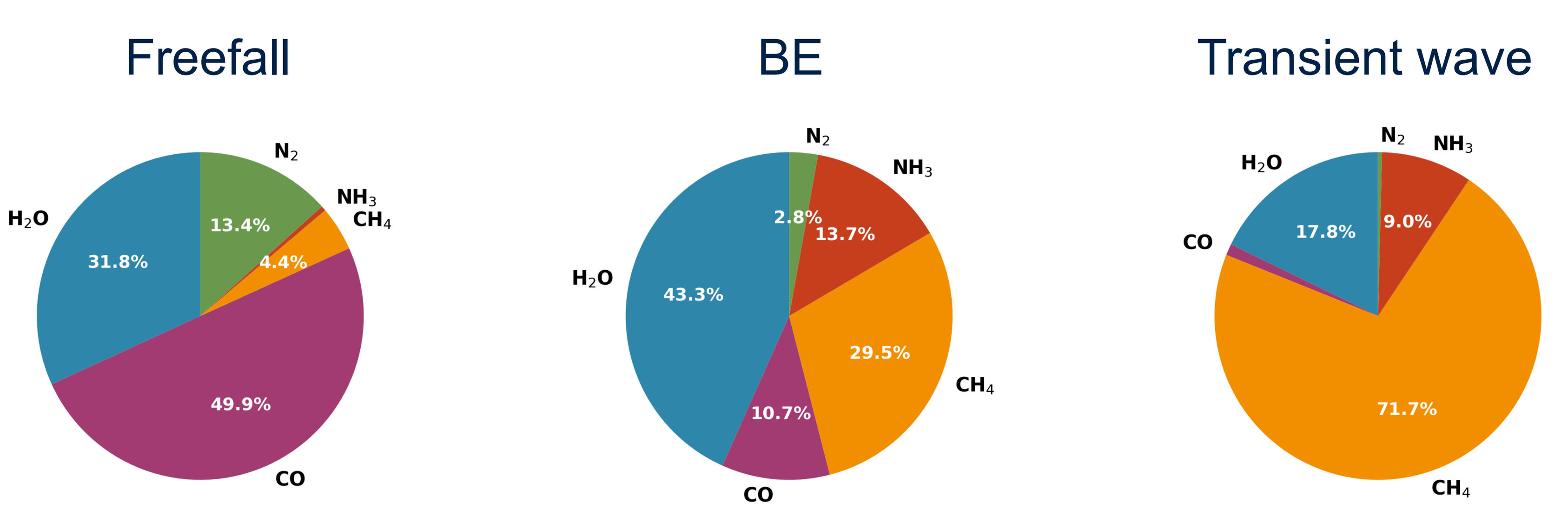
Warm carbon-chain vs hot oxygen-rich mature cores arise from identical starting conditions. Formation of carbon-rich ices with complex organics or oxygen-dominated ices depends on the collapse pathway, highlighting the role of physical evolution in shaping chemical diversity.

Results

Layer-by-layer ice composition at inner most radius



Total ice compositions



When the main carbon reservoir remains in CO, this keeps a more primitive composition and stops carbon from forming CH_4 which sequentially stops the formation of longer carbon chains, when CH_4 dominates, longer carbon chains can readily form

Different core collapse models follow unique paths through temperature and density space, directly influencing which molecules freeze onto dust grains at each stage.

[1] adapted from: Maitrey S, Majumdar L, Manilal V, Srivastava B, Rayalacheruvu P, Willacy K, et al. Insights from the PEGASIS three-phase astrochemical model. *Astron Astrophys.* 2025;699:A332. doi:10.1051/0004-6361/202554717.