Formation of Dust in Astrophysical Environments

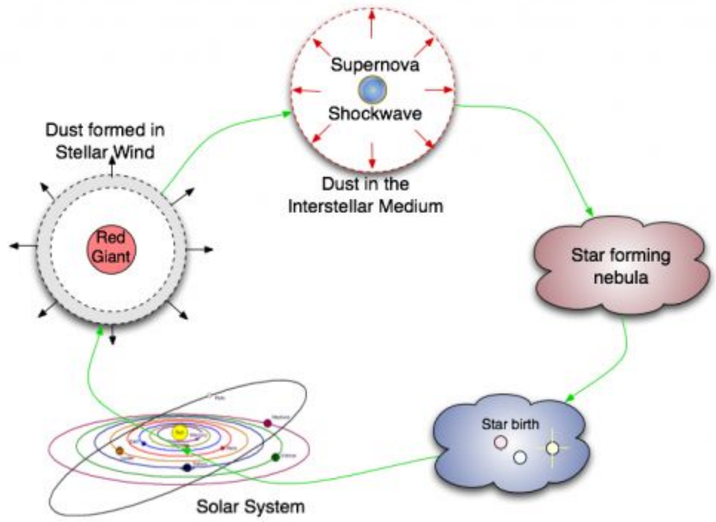
Christopher Michael Mauney

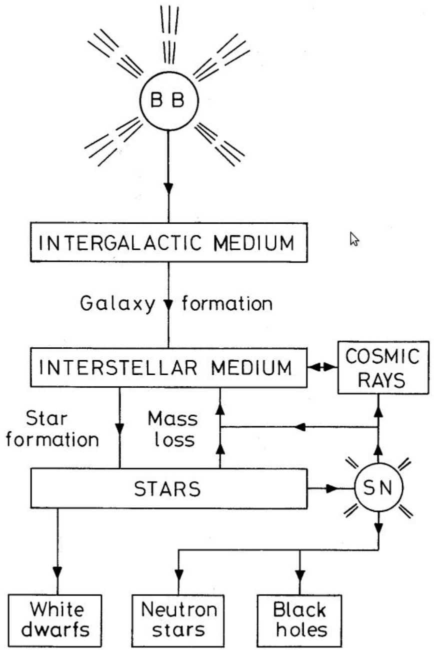
LA-UR-22-25004

- Overview
- Observational Models
- Computational Modelling of Formation and Growth
- Dust Formation in Common Envelope Ejecta

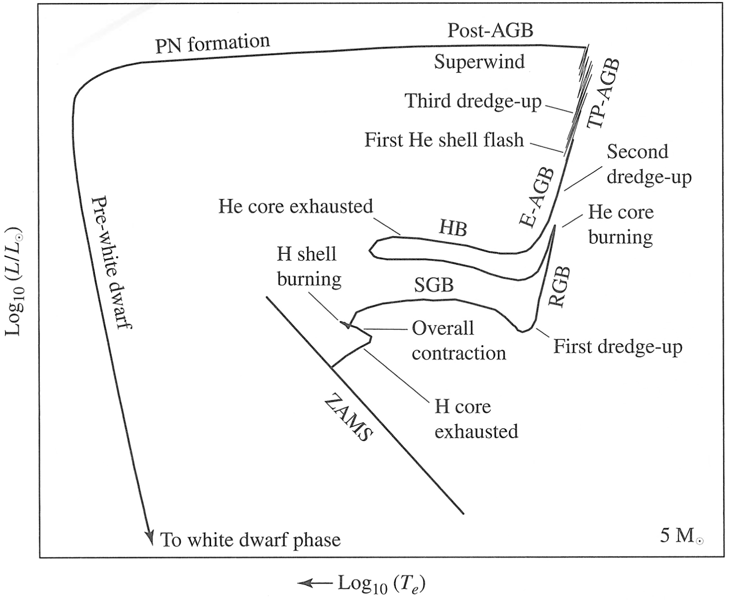
Overview

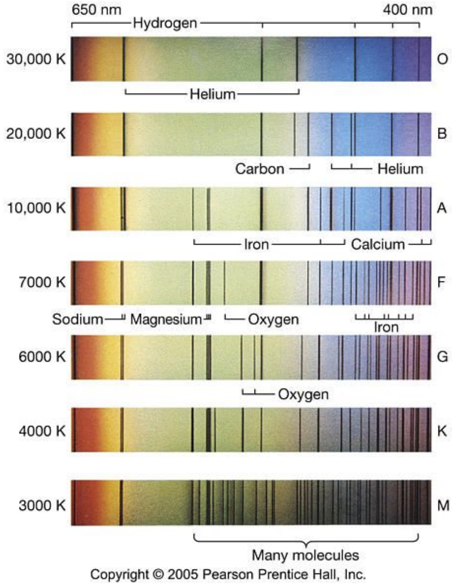
Galactic Cycle of Matter





Stellar Chemical Buildup





The most common channel of dust production* is through mass loss from evolved stars

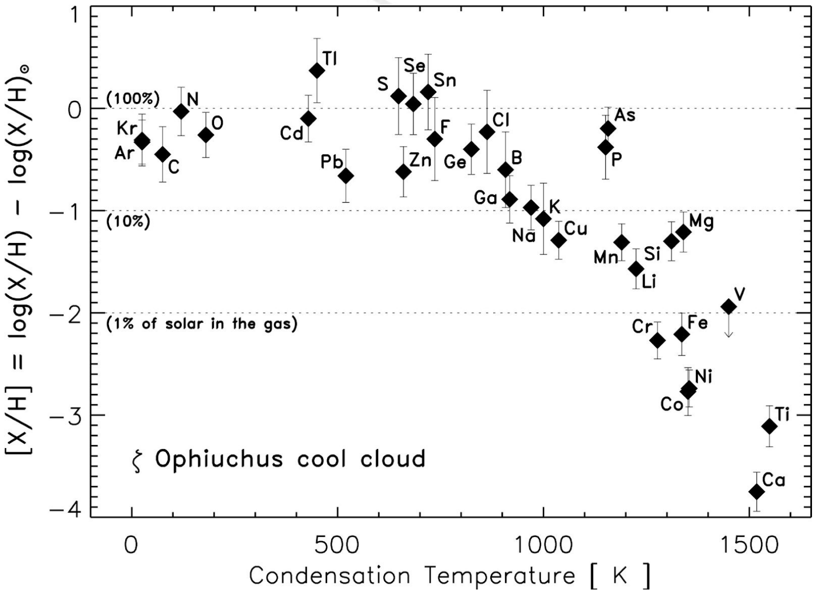
**dust abundance and ubiquity in the ISM is debated*

ISM Depletion

Savage & Sembach 1996

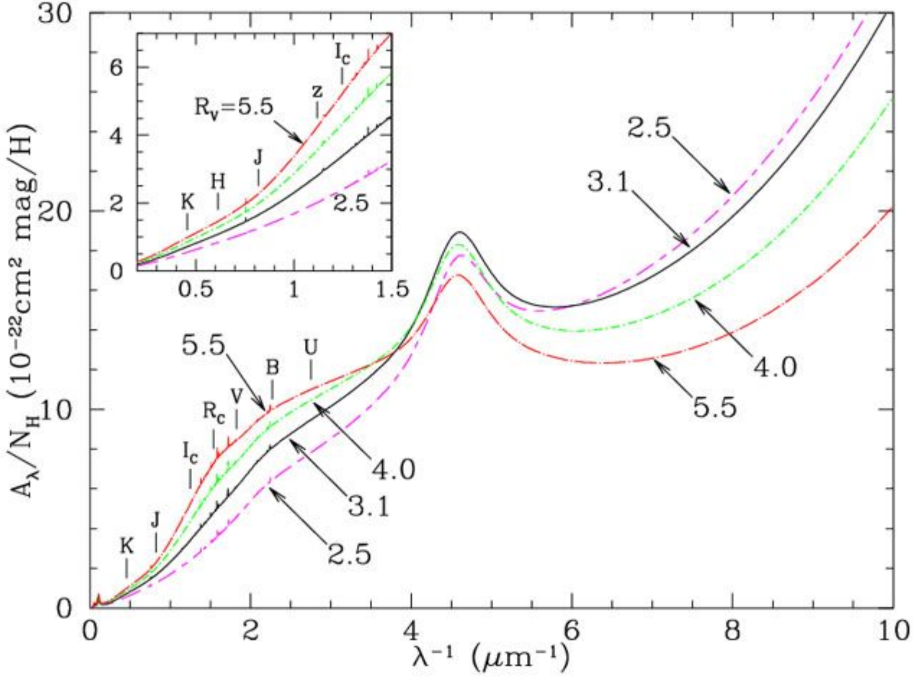
In the ISM, heavy elements are missing from the gas phase (relative to solar abundances).

Depletion has been seen to locally decrease in clouds following the passage of interstellar shocks.



Extinction of light

Draine 2011

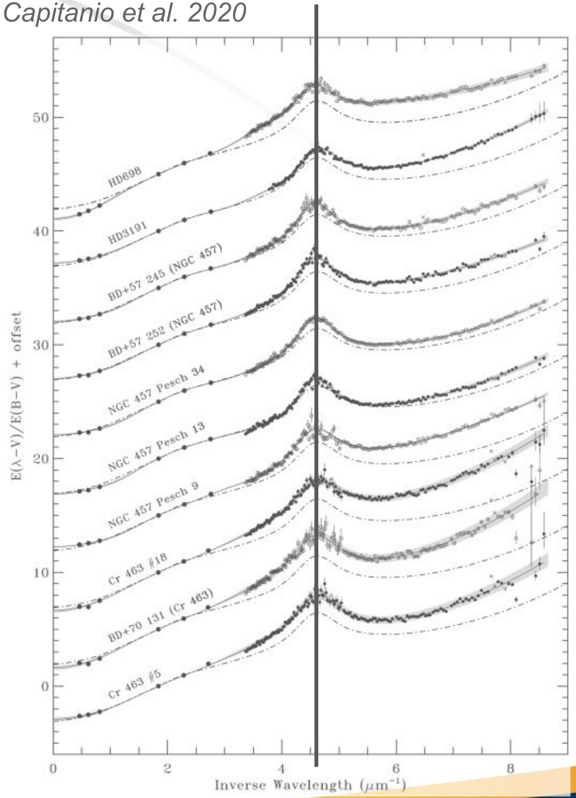


- Abundant lines across high-λ regime
- Broad “bump” feature at 2175.
- Strong UV extinction

2175 Å feature

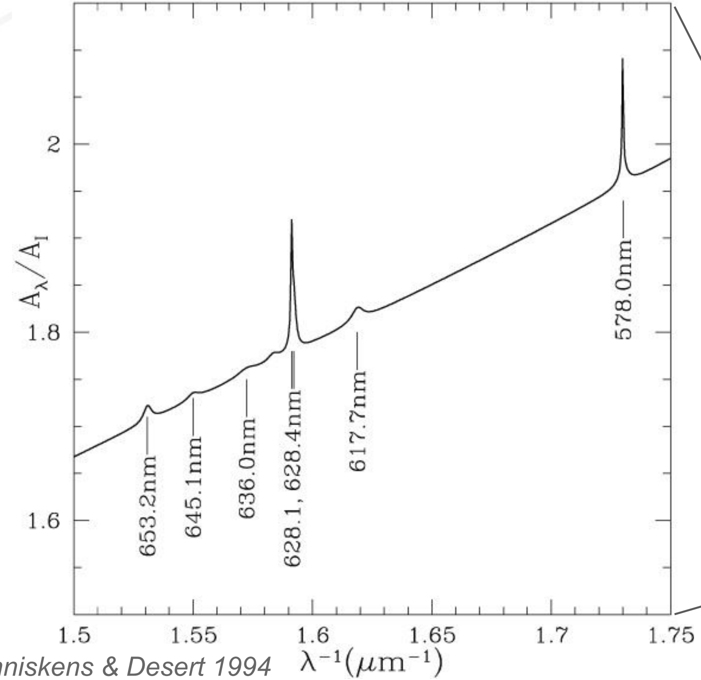
- The “bump” is ubiquitous
- Usually attributed to some form of carbon dust, though no definitive candidate for source

Capitanio et al. 2020

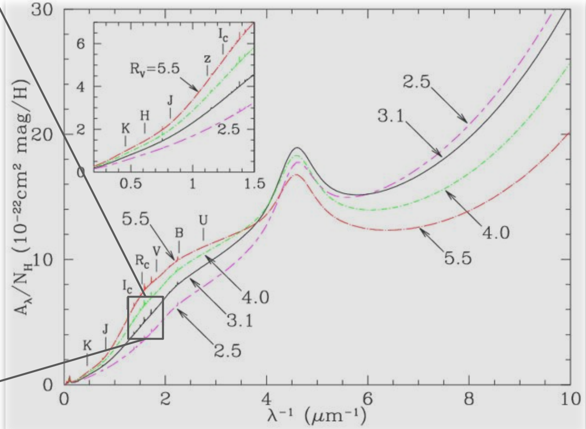


Diffuse Interstellar Bands

No conclusively identified source (molecule/grain) associated to any line(many proposed)



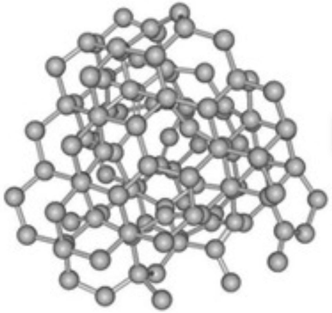
Jenniskens & Desert 1994

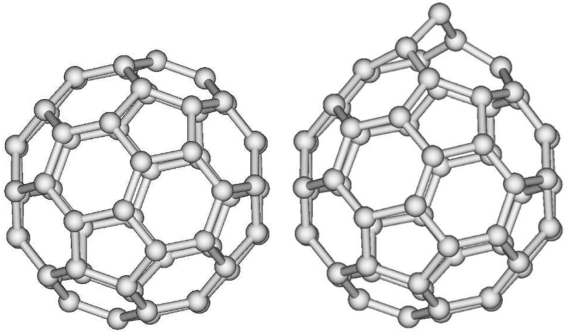


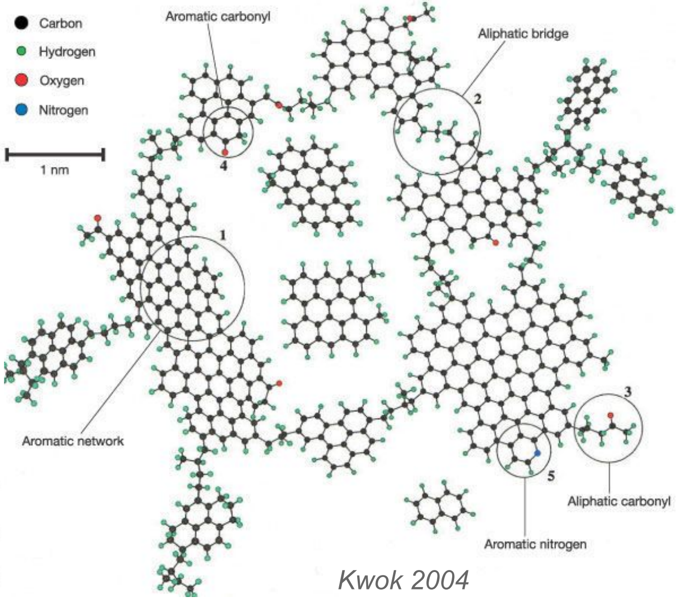
Components

Carbon dust may be any/some/all of:

- Amorphous
- Chains
- Fullerene/”fullerene-like”
- PAH





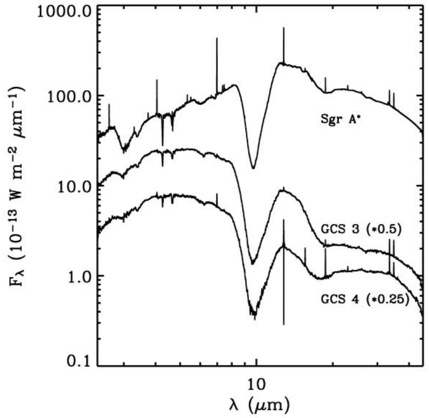


Kwok 2004

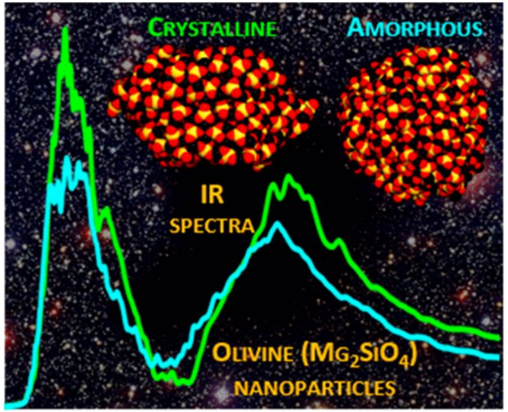
Components

Silicate grains

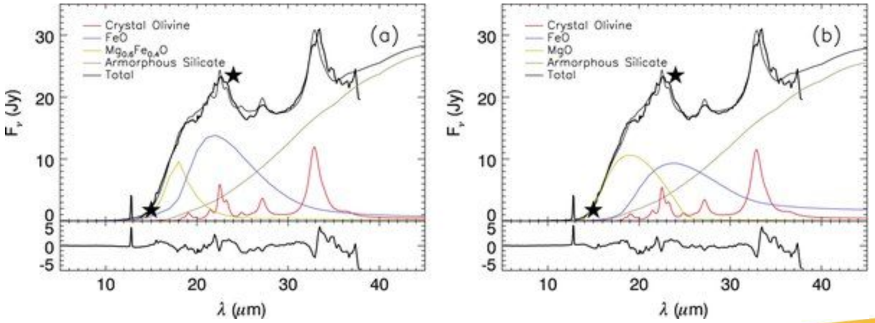
- Range of stoichiometry
- Likely amorphous in ISM (broad lines)
- Evidence of highly-structured crystal features in "processed" environs (PPN, AGN)



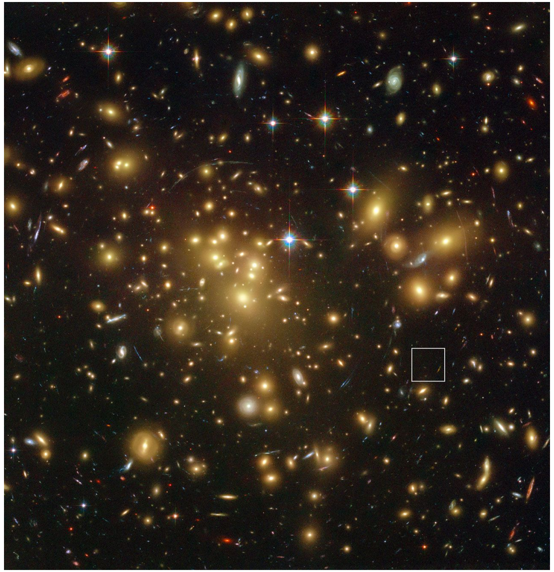
Kemper et al. 2004



Zamirri et al. 2019



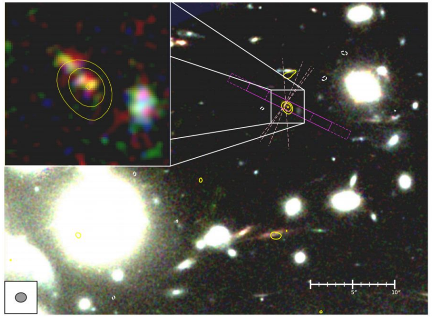
Dust in High-z galaxies

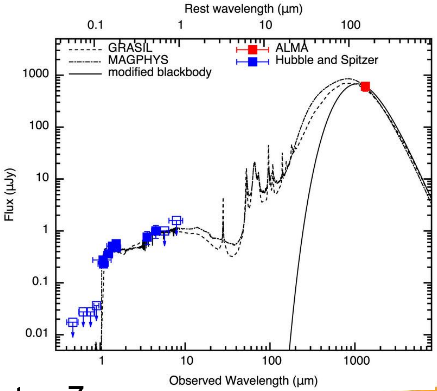


Watson 2015

Population of galaxies is generally high gas/dust, but some galaxies are quite dusty, similar to MW.

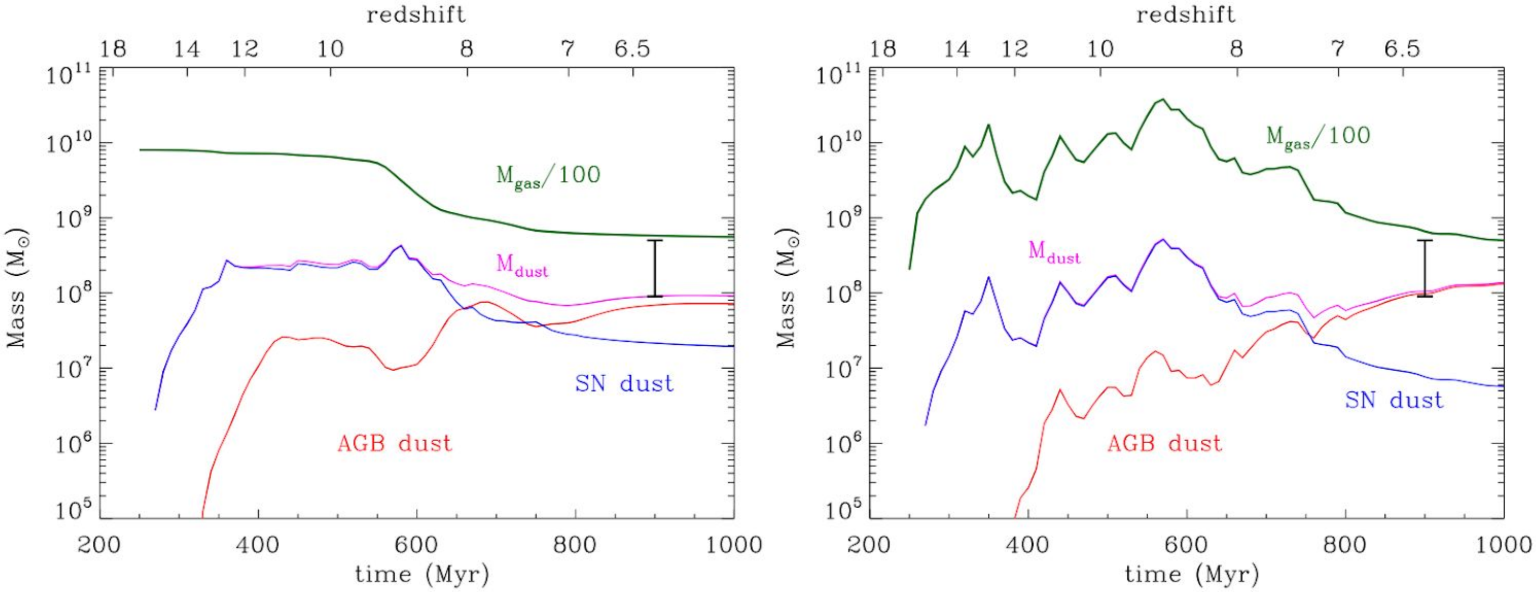
How do these galaxies get dusty?





A1689-zD1, a dusty galaxy at z~7

Dust Origins across Time



Dwek & Cherchneff 2010

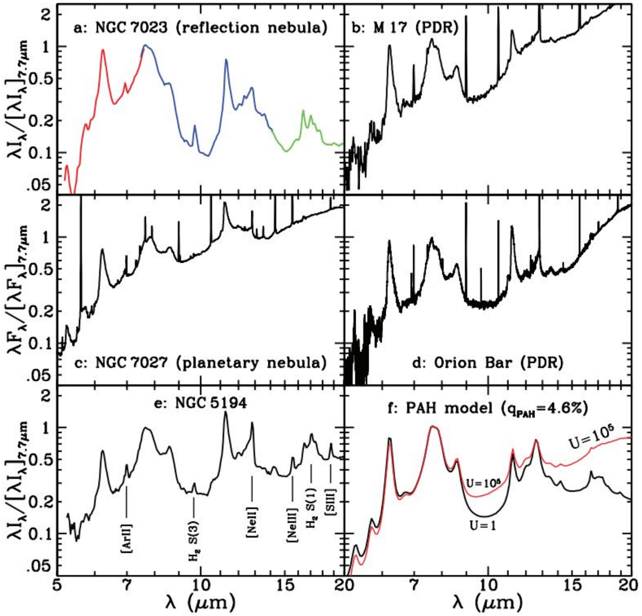
Observational Modelling

Dust Modelling

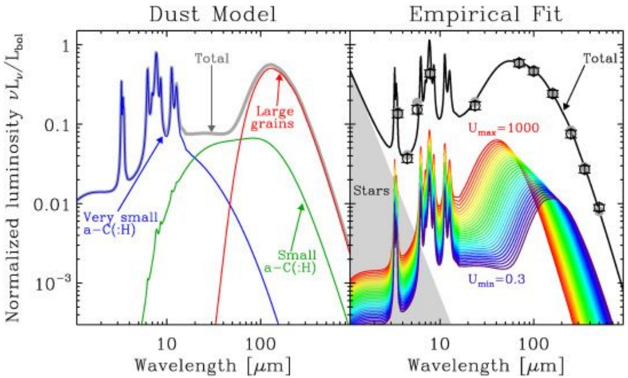
Separate dust components modelled with modified BB.
Free parameters of fits:

- Dust mass
- Dust temperature
- Dust composition/structure

Draine 2007

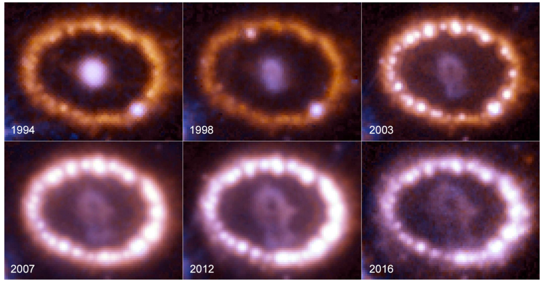


Galliano 2017



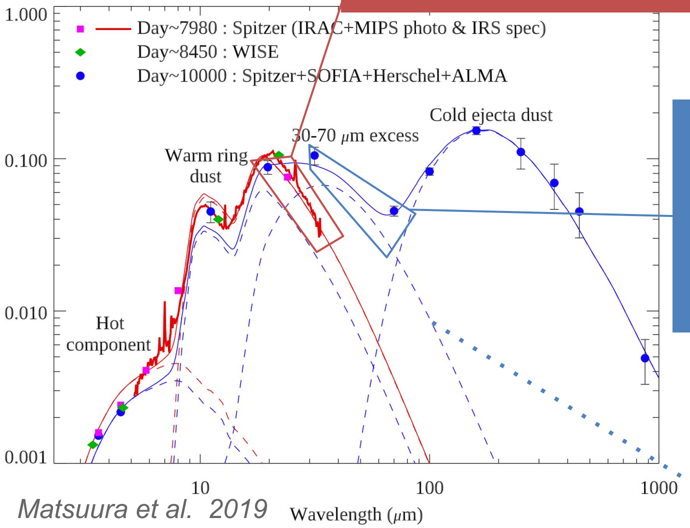
Observational Modelling Example

Hubble 2017



Forward shock passage through the circumstellar ring of 1987A (Hubble)

Shock passes through dusty clump around day ~7900. Dust grains are heated and large grains are sputtered



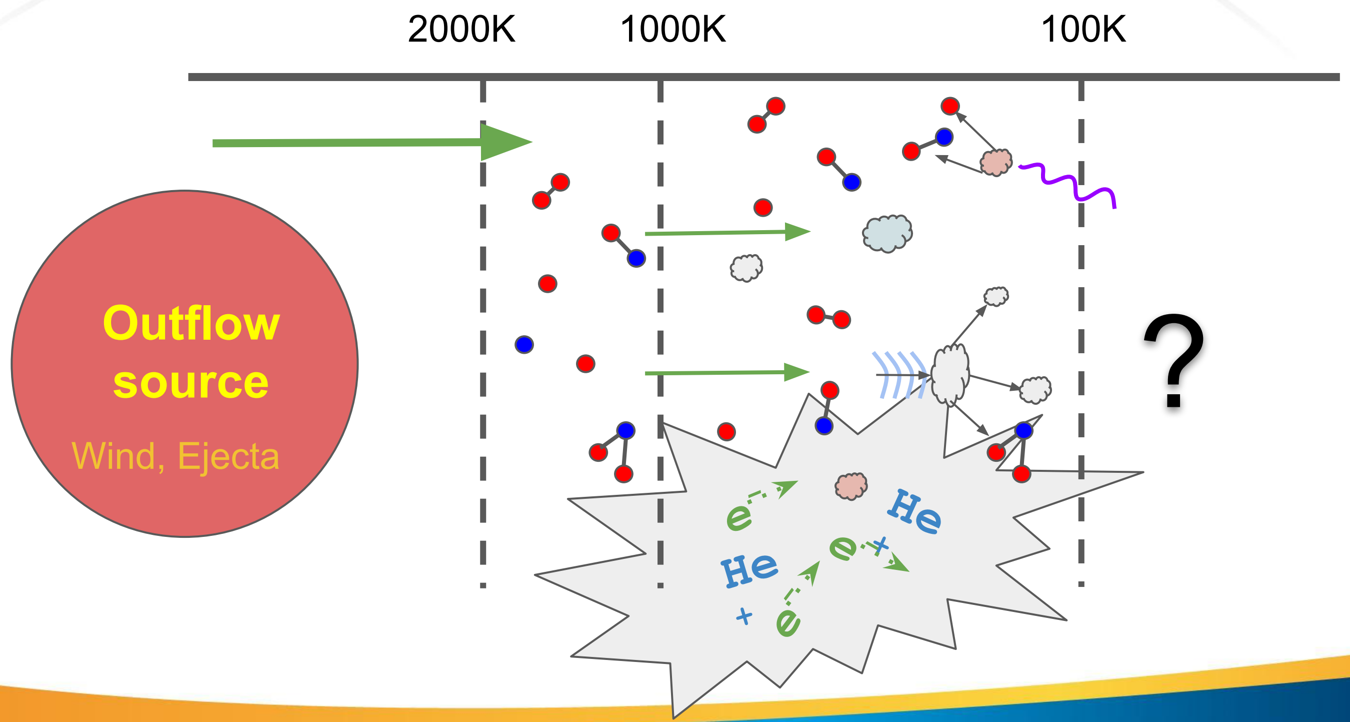
Matsuura et al. 2019

5 yrs later, excess emission at 30-70um, implying an increase in dust mass. A possible explanation is the reformation of dust, or the growth of surviving grains.

Excess modelled as a modified blackbody fitted to data.

Dust Formation Modelling

Formation in Outflow

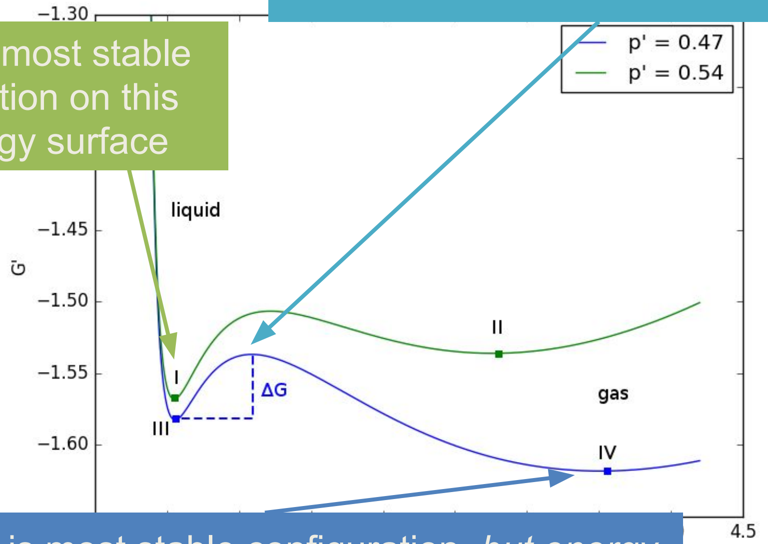


First-order Phase Transition

- Nomenclature due to Ehernfest, who classified phase transitions according to the analytic character of the free-energy across phase boundaries (the Ehernfest classification is incorrect)
- The *global* minimum of free-energy is separated from a region of a *local* minimum that is stable to small perturbations - a **metastable** state.
- Phase separation proceeds with sufficiently large fluctuations - **nucleation**.

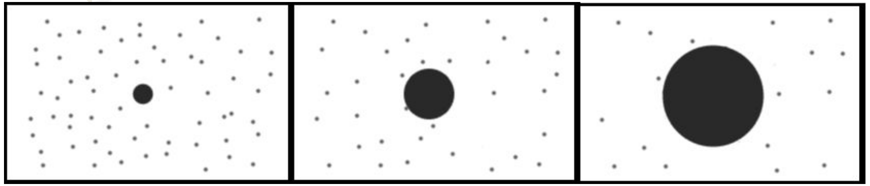
The **critical size** of the prescribes the kinetics of the phase transition

State I is most stable configuration on this free-energy surface

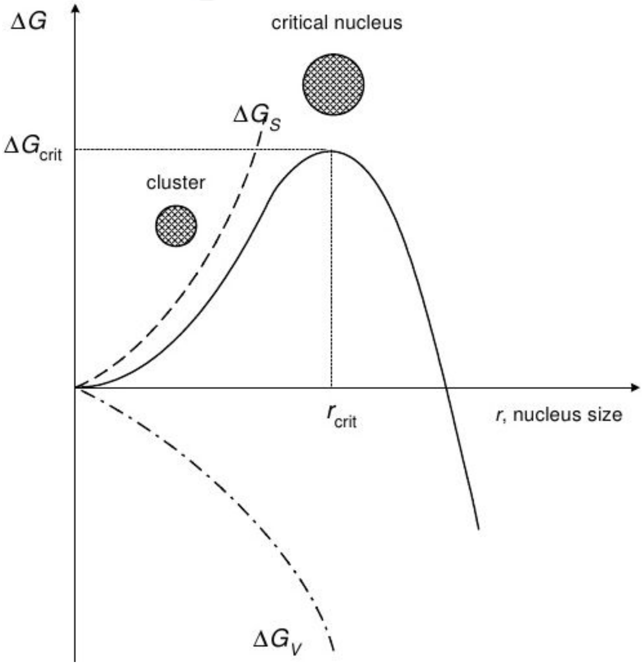


State IV is most stable configuration, *but energy barrier prevents spontaneous phase change* from State III

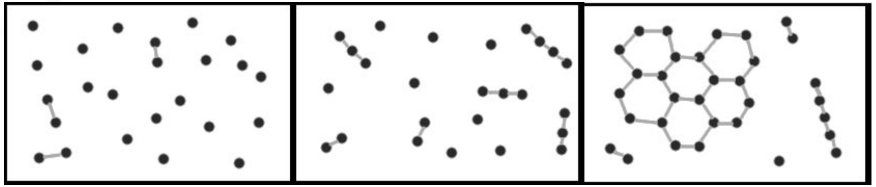
Classical Nucleation Theory (Droplet Model)

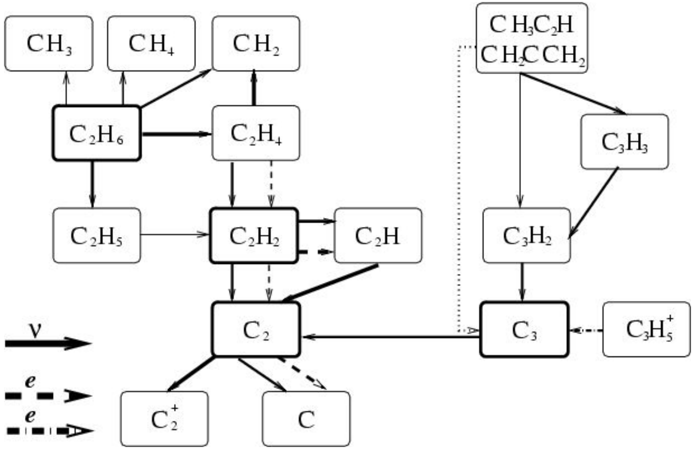


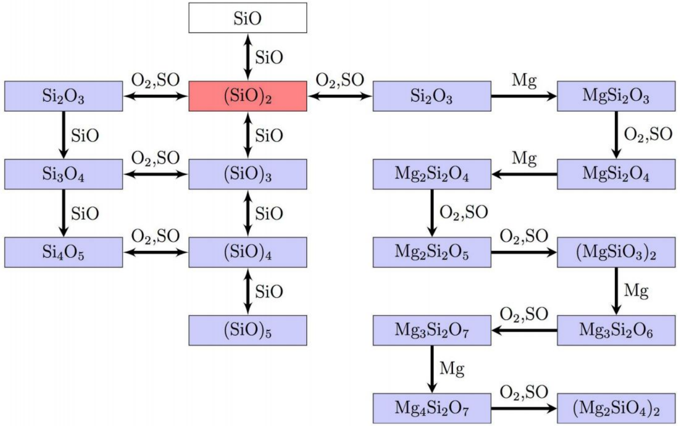
$$\Delta G_n = -n\Delta\mu + c\,(v_0 n)^{\frac{2}{3}}\,\sigma$$



Kinetics Nucleation

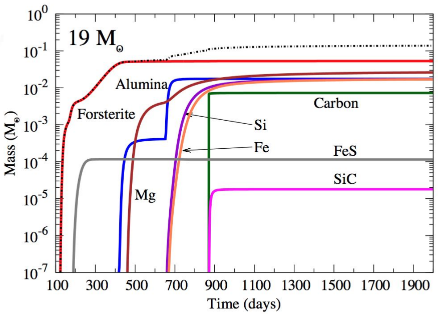






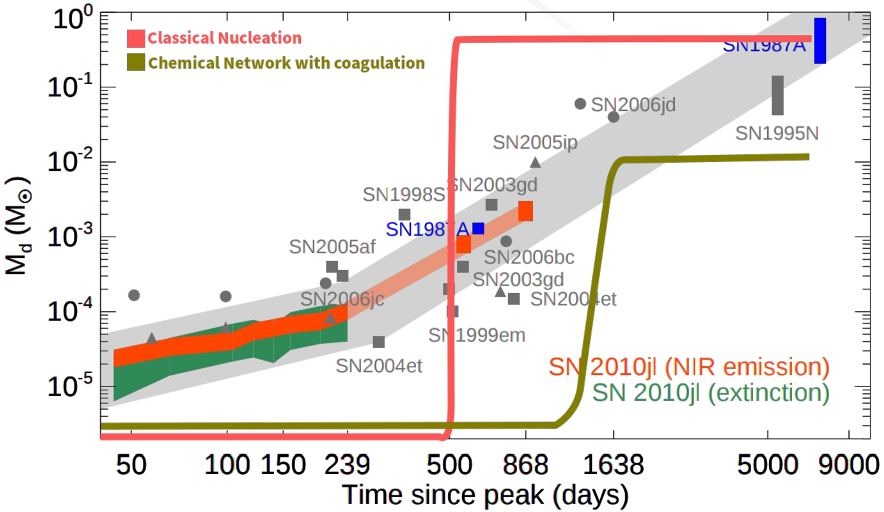
Goumans & Bromley 2012

Reconciling with Observation



Sarangi & Cherchneff 2014

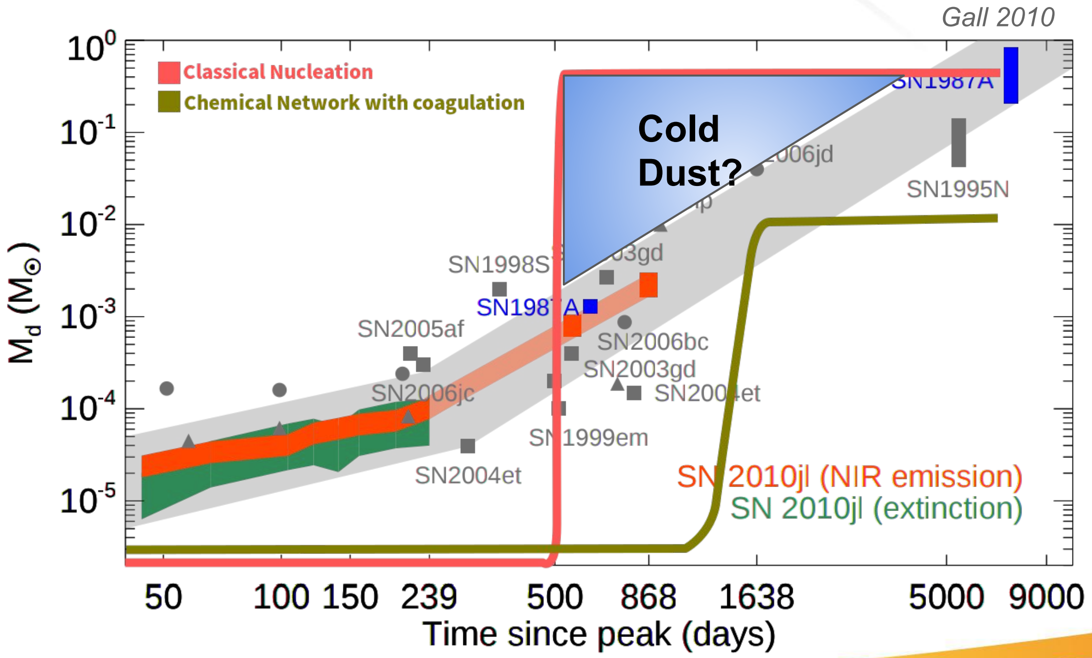
Gall 2010



Computational models have struggled to reproduce observed dust formation

Deficient data?

One possibility is that observational data is missing a large component of cold dust



A Mixed Approach

Atomistic Nucleation Theory:

- No spherical cows; discard the droplet model, consider real molecules.

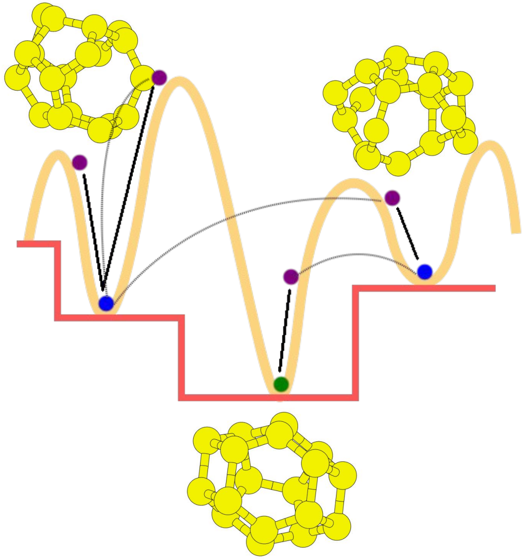
$$G_{n,ex} = c(v_0 n)^{2/3}\sigma \qquad G_{n,ex} = n\lambda - E_n$$

- Each n-cluster is the ground-state molecule with n monomers.

$$H|\Psi\rangle = E|\Psi\rangle$$

$$H = T + V + W$$
$$= \frac{\hbar}{2m_e}\sum_{i=1}^{N}\nabla^2 + \sum_{i=1}^{N} v_{ext} + \frac{e^2}{2}\sum_{i\neq j}^{N}\frac{1}{|\mathbf{r_i} - \mathbf{r_j}|}$$

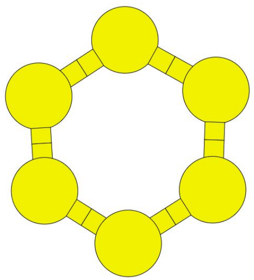
Ground-state Cluster Search

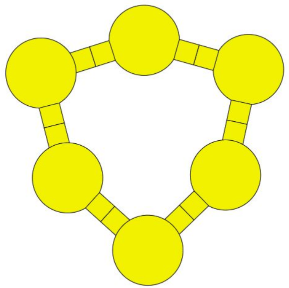


- The ground state cluster configuration is necessary
- A **particularly hard** computational problem
- Commonly done with “approximate” fast potential energy functions
- Precursor of “modern” ML techniques

Using Quantum Chemistry

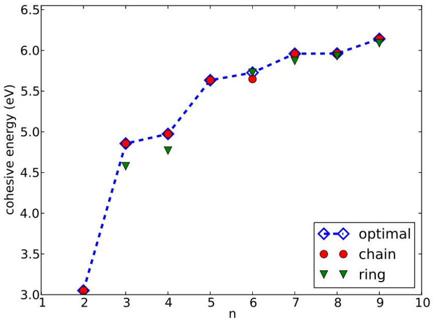
Ground-state searches generate candidate clusters, and these are then used in relaxations with QM codes.

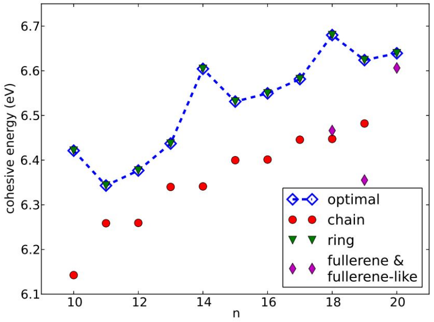


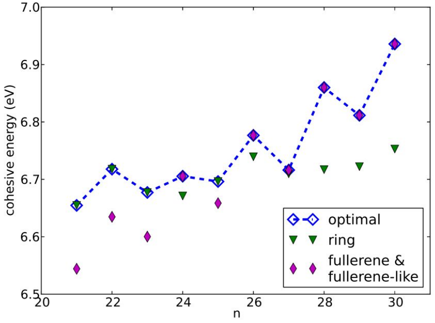


Application to Carbon Nucleation

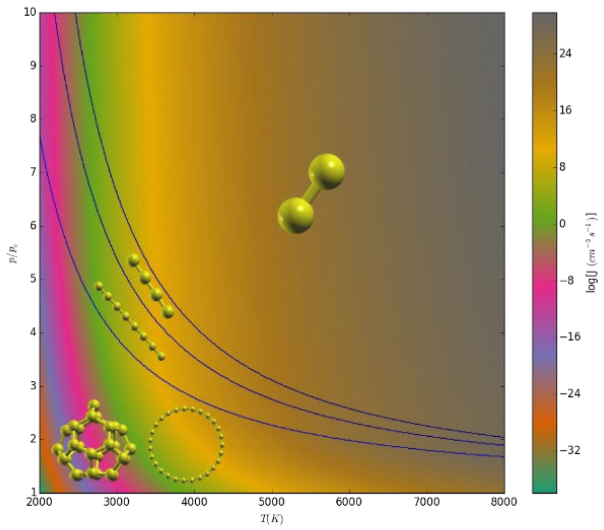
An example of candidate generation and QM binding energy evaluation

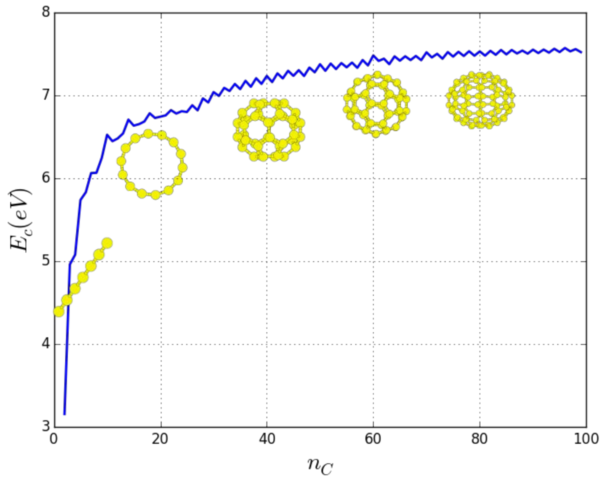






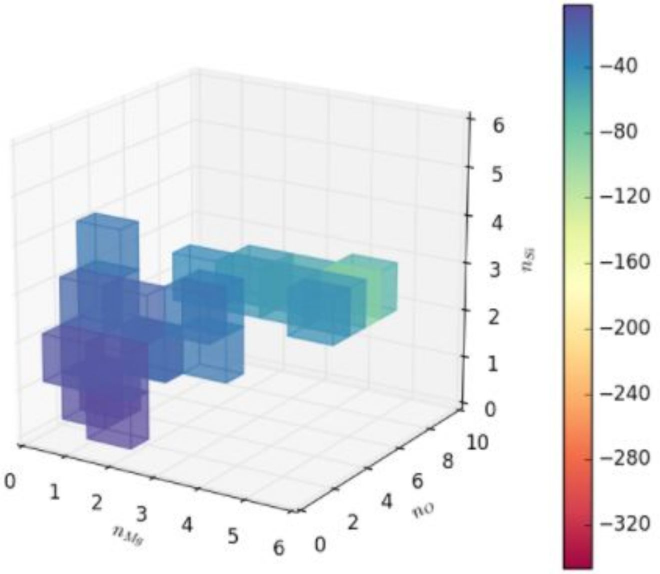
Application to Carbon



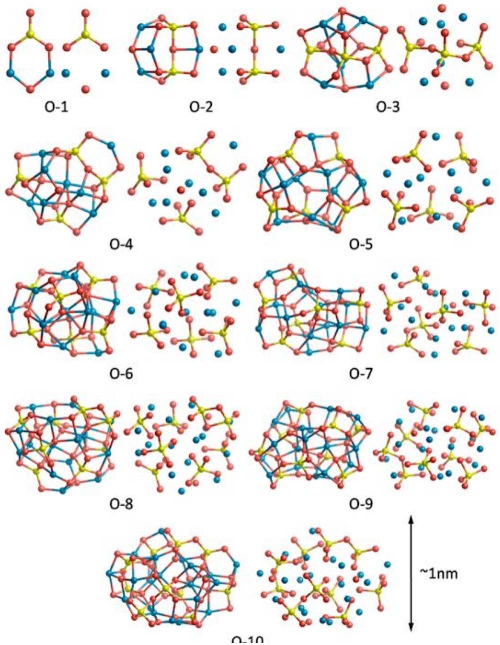


Multicomponent Nucleation

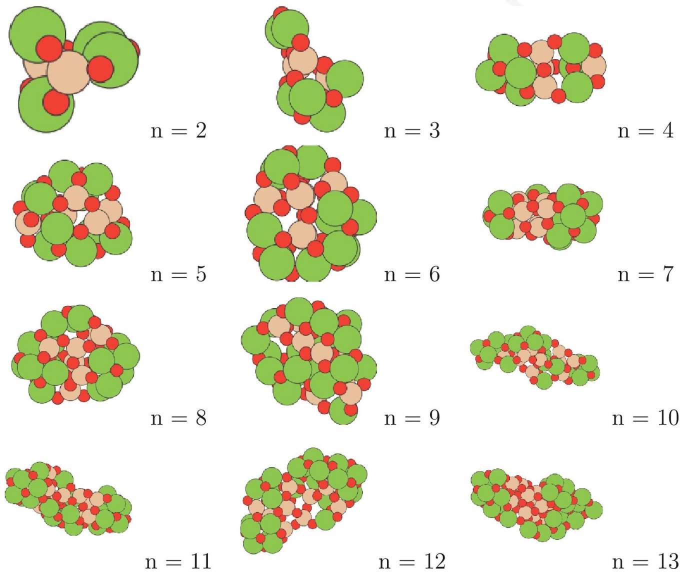
Moving to ground state cluster searches with multicomponent clusters posses new challenges, both to the identification of ground-state configurations and to the theoretical modelling of nucleation



Multicomponent Nucleation



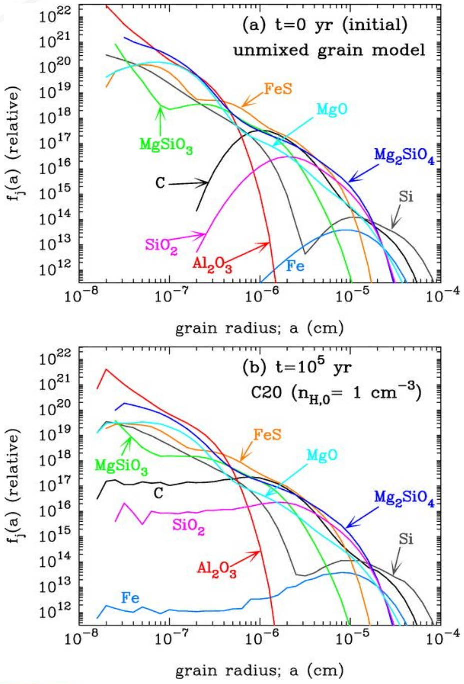
Escatllar 2019



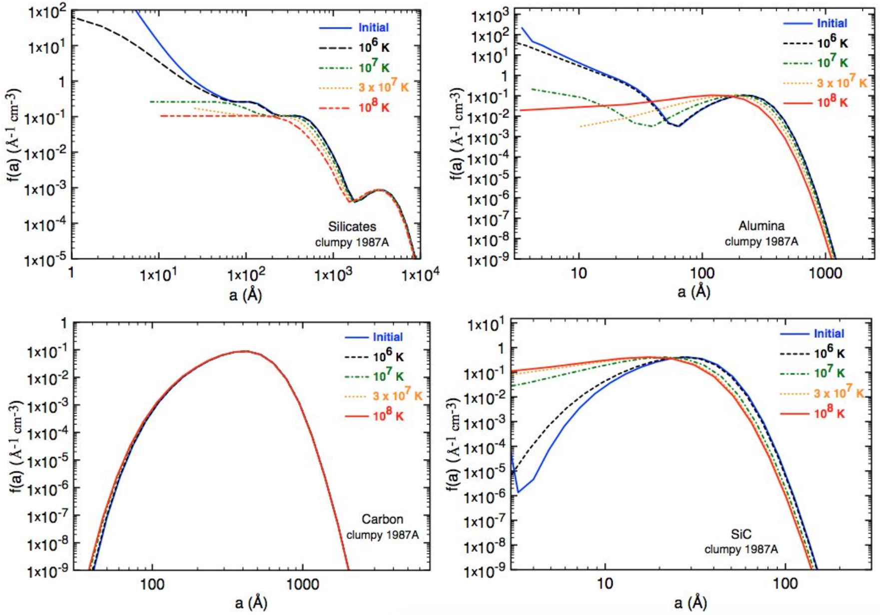
Mauney 2018

Destruction

Nozawa & Kozasa 2006

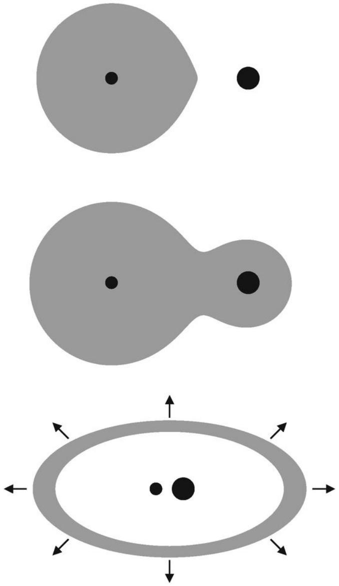


Biscaro & Cherchneff 2016



Dust Formation in Common Envelope Ejecta

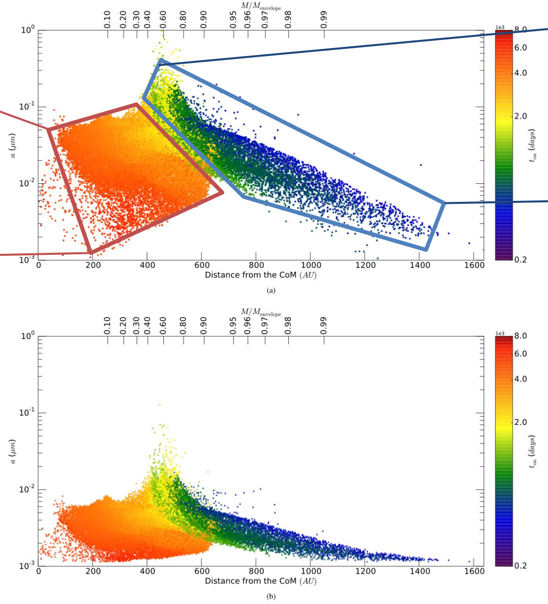
Dust From Common Envelopes



CE ejecta may be chemically diverse, and can produce novel dust species

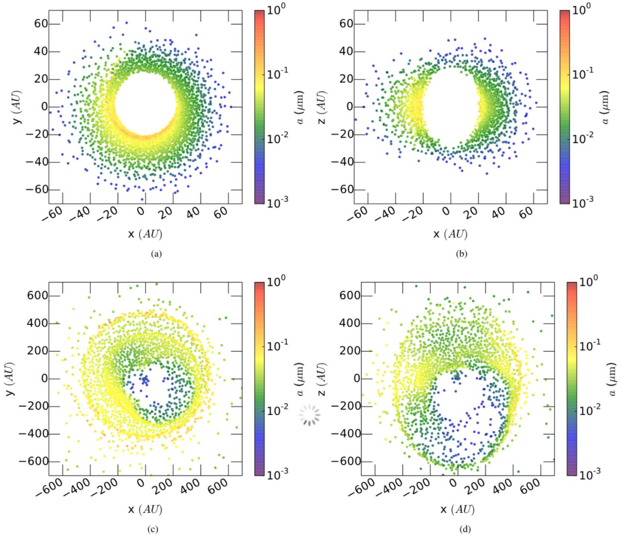
CE Dust Study: SPH
Iaconi et al. 2020

Inner Population
- 900~5000d
- Multiple grain sizes
- Inner layers of primary, self-interacting



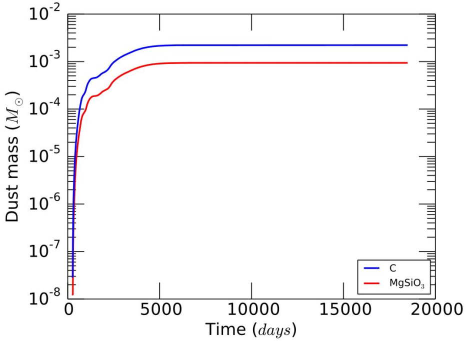
Outer Population
- 300~900d
- Small grains at large distances first, larger grains later/closer
- Outer layers of primary

CE Dust Study: SPH
Iaconi et al. 2020



Early compression of the ejecta prompts large grain formation

Equatorially concentrated dust formation



Dust from CE may contribute 1-2 10^{-4} $M_\odot$/yr