Unravelling dust nucleation in astrophysical media

Developing a self-consistent non steady-state, non-equilibrium polymer nucleation model for AGB stellar winds

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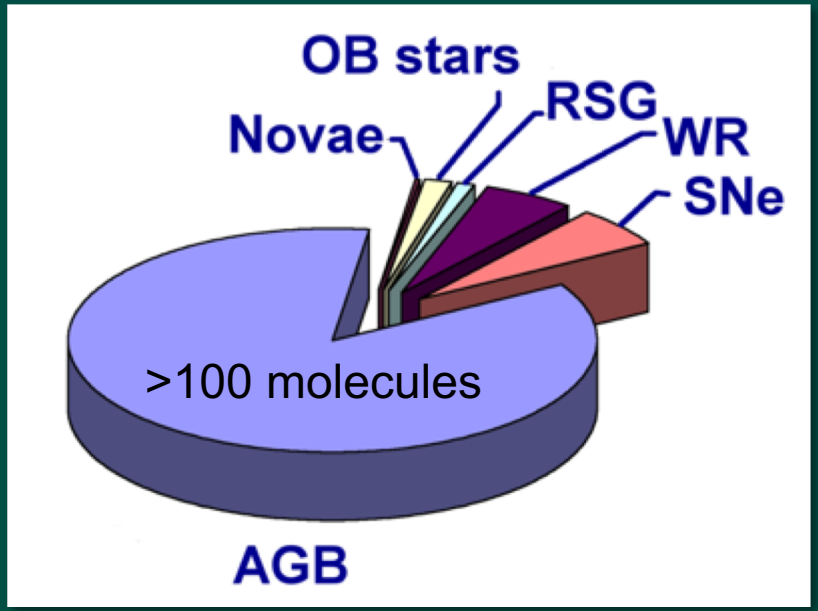
– University of Leeds – UK

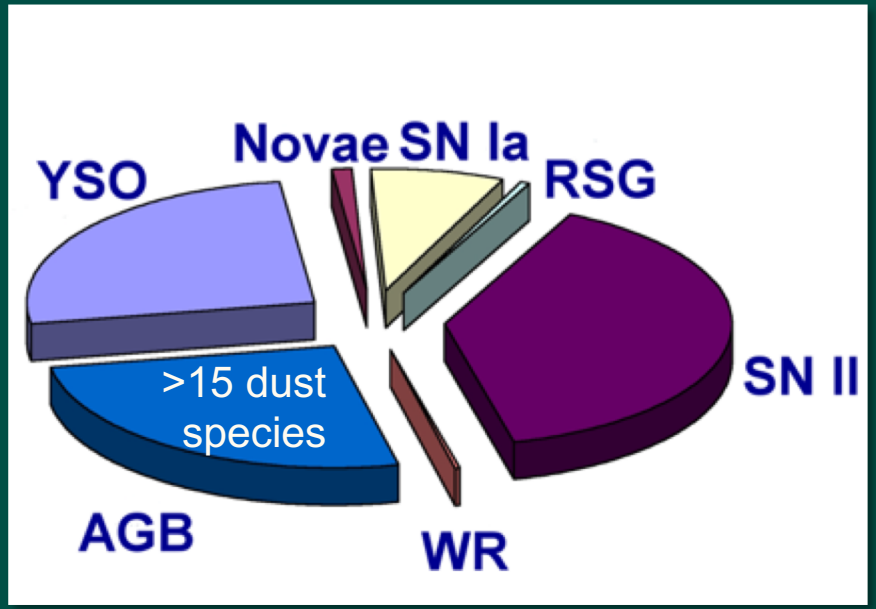
Justification

interstellar

gas

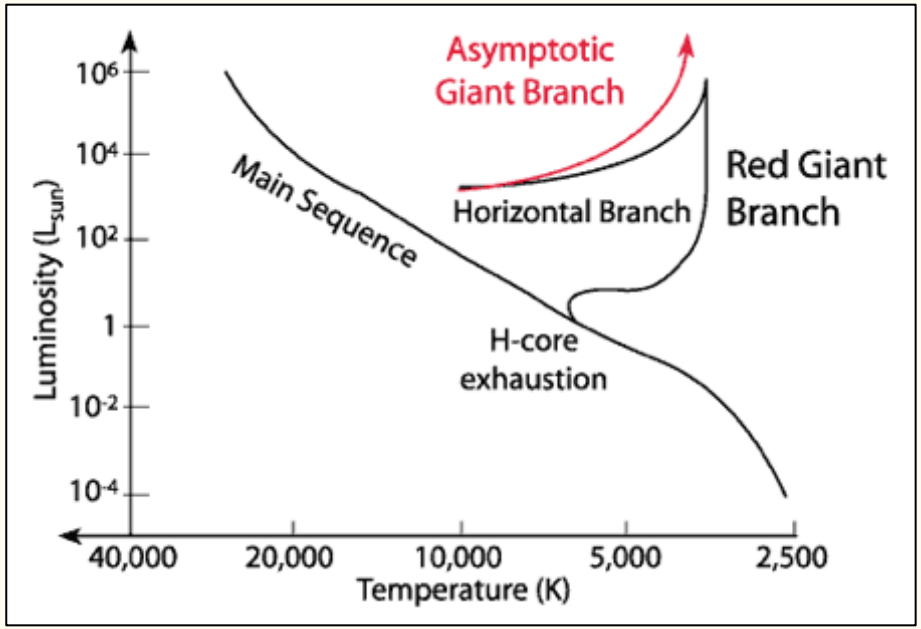


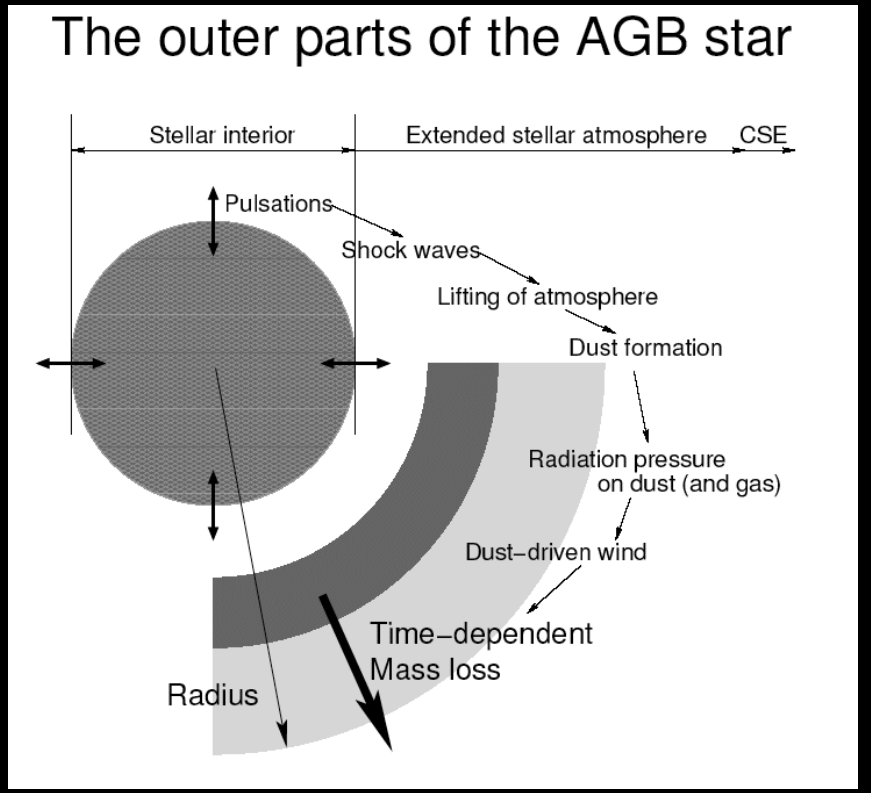
dust



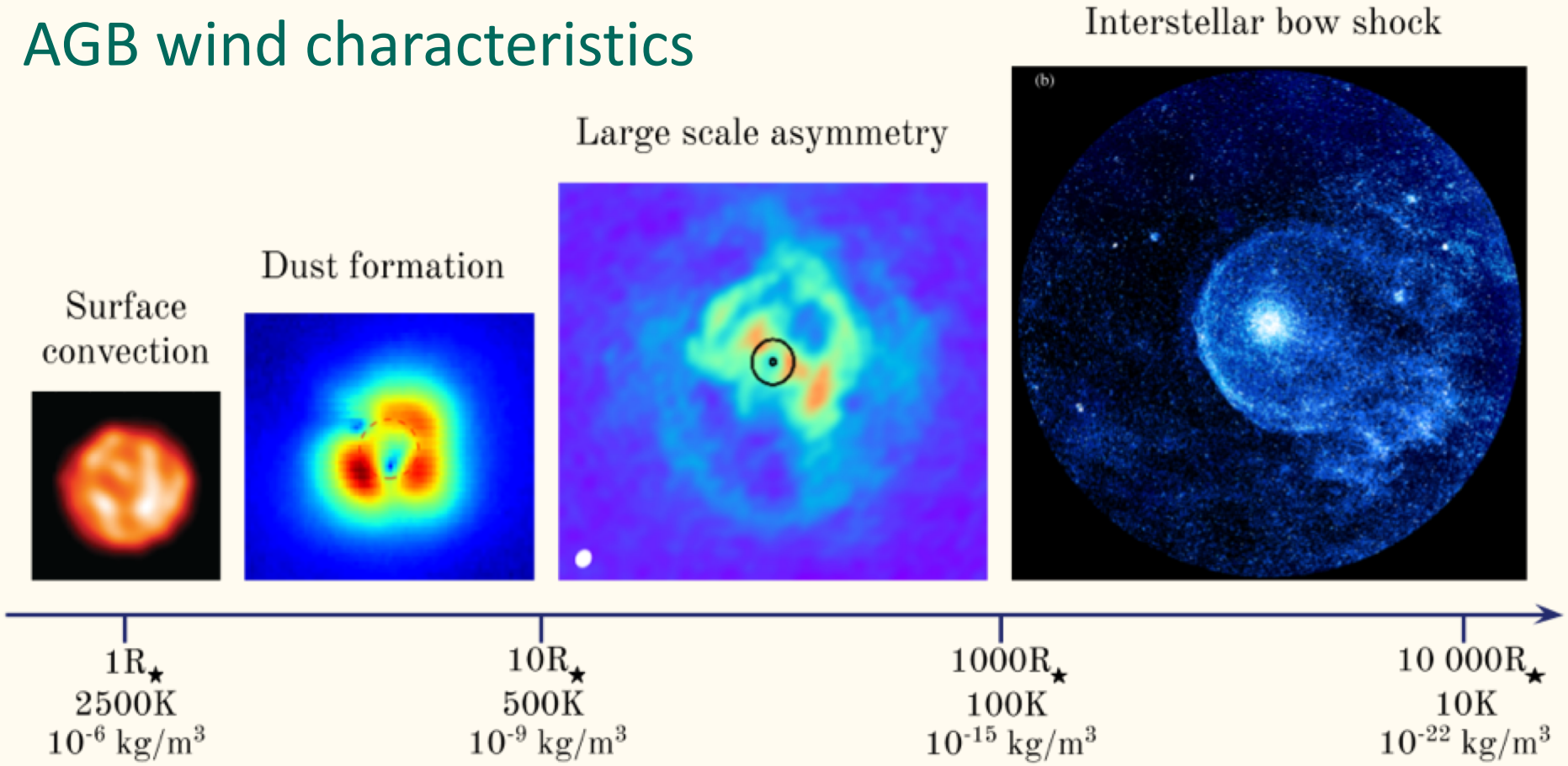
What is an AGB star?

M_{ini} ~0.8 – 8 $M_{\odot}$





AGB wind characteristics

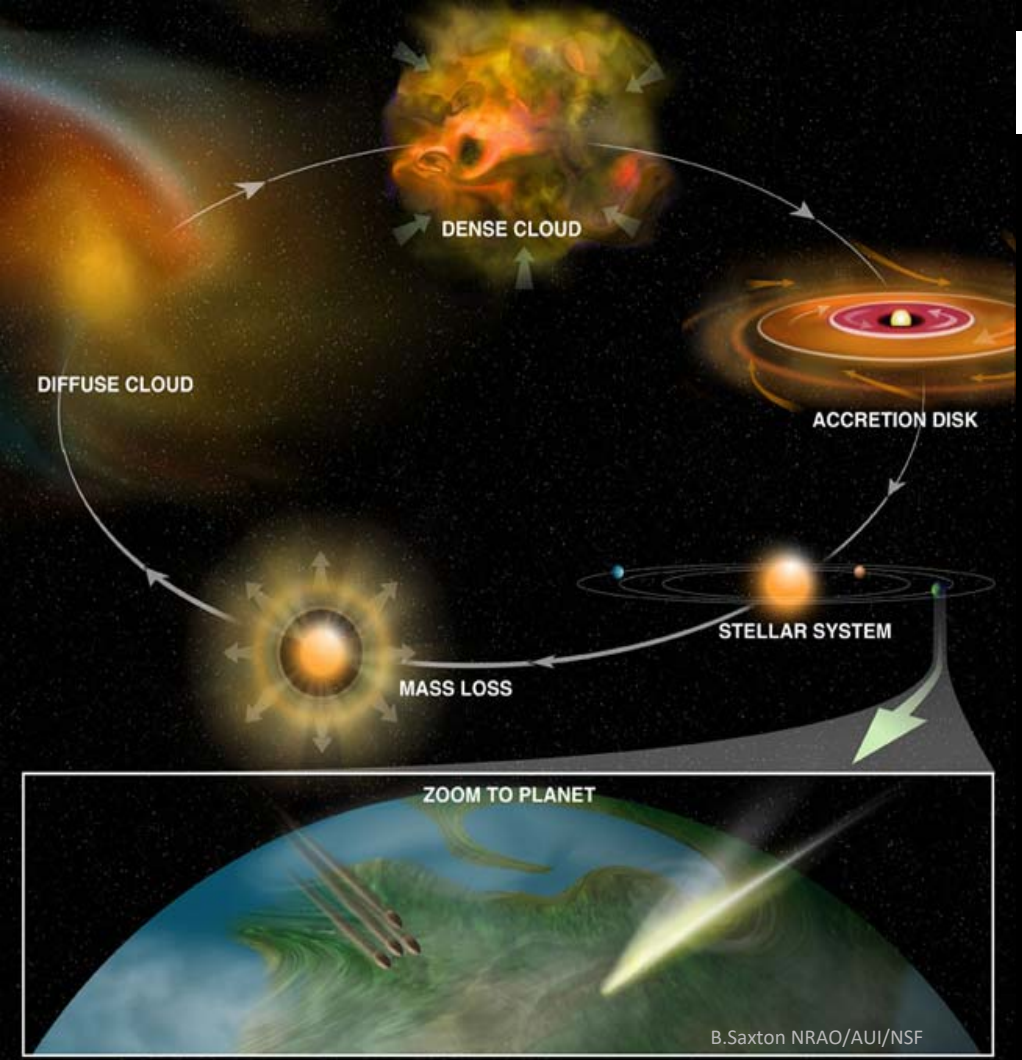


Interferometry at 1.625 µm (Paladini et al. 2018)

Polarised dust at 820 nm (Khouri et al. 2016)

HCN (J=4→3) ~845 µm (Decin et al. 2018)

Far ultraviolet ~134-179 nm (Sahai et al. 2010)

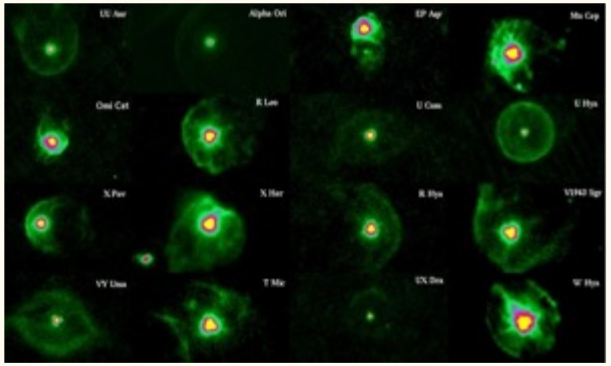


The chemical life cycle of gas and dust species

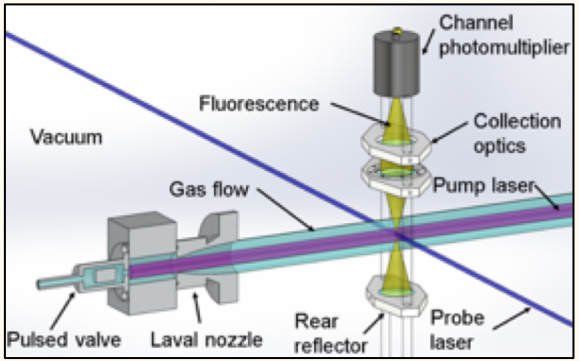
Understanding the onset of the AGB wind and its chemical composition

1. What kind of material?
2. How much material?
3. How fast is it being lost?

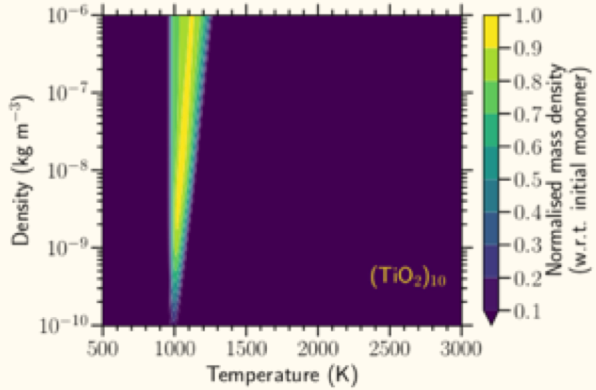
Observations



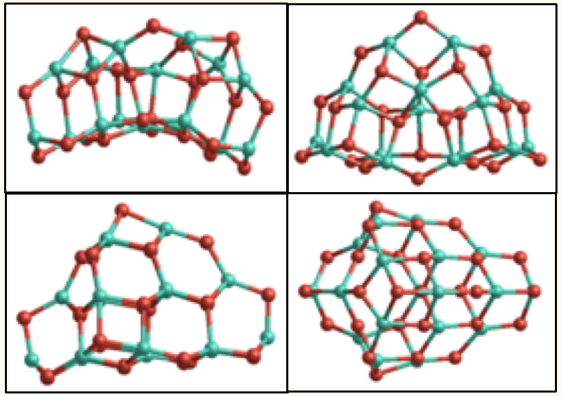
Laboratory



Simulations

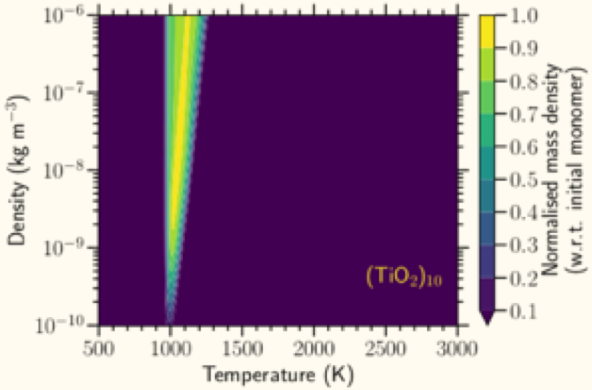


Theory

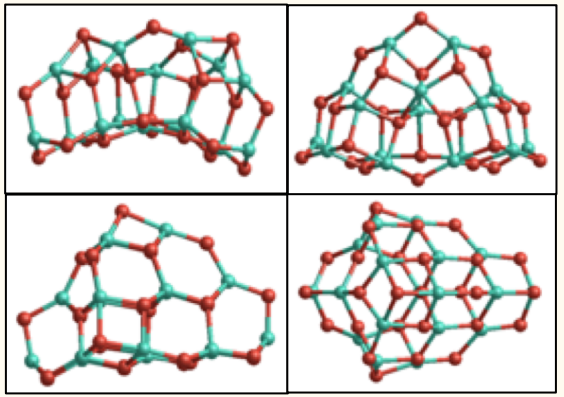


Observations

Laboratory



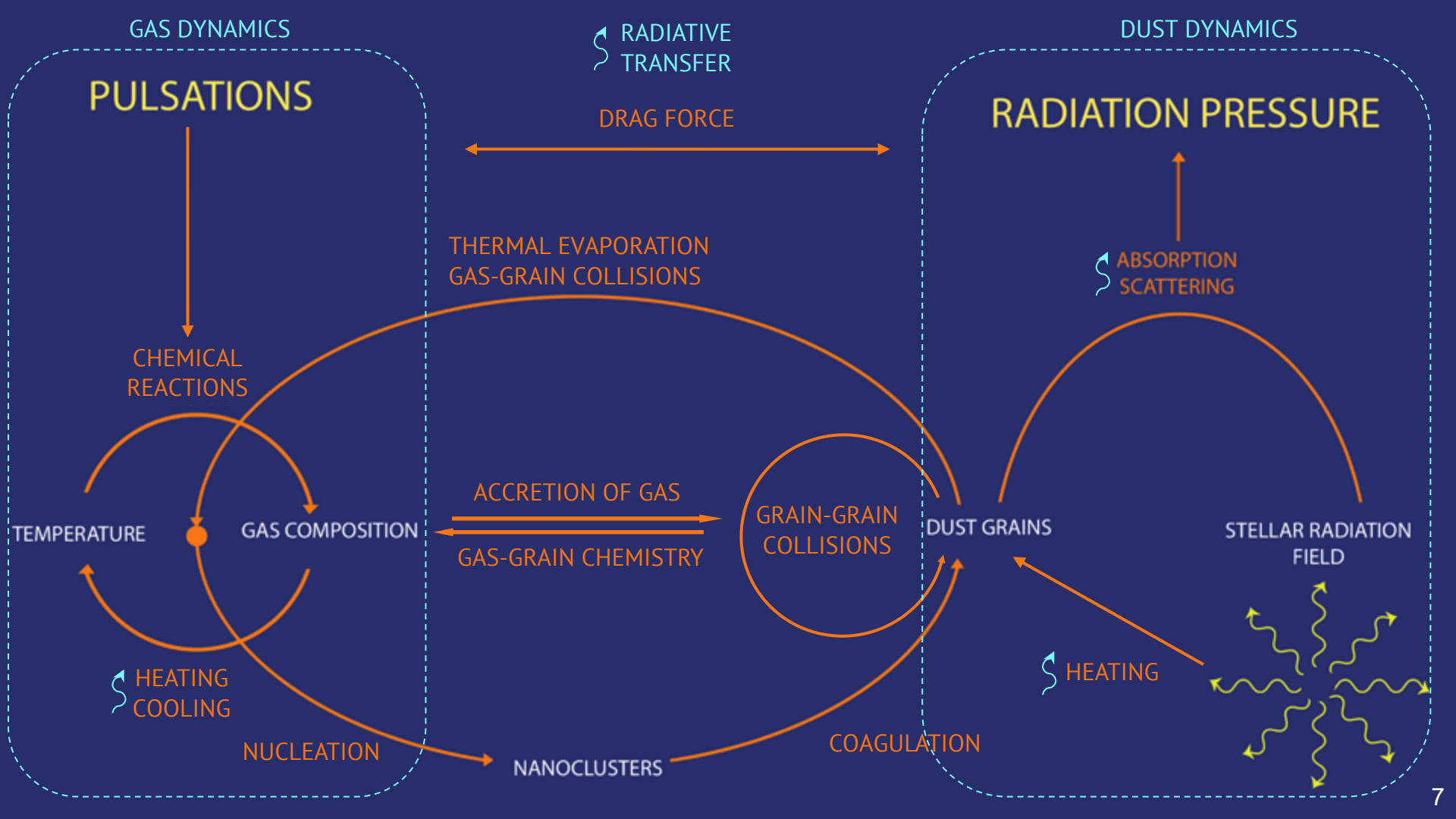
Simulations



Theory

Oxygen-rich winds

- Other astrophysical media
  - Novae, supernovae, protoplanetary nebulae, interstellar shocks, exoplanets, …
- ALMA
  - oxides & hydroxides as dust precursors


GAS DYNAMICS
RADIATIVE TRANSFER
DUST DYNAMICS
PULSATIONS
DRAG FORCE
RADIATION PRESSURE
THERMAL EVAPORATION
GAS-GRAIN COLLISIONS
ABSORPTION
SCATTERING
CHEMICAL REACTIONS
ACCRETION OF GAS
GRAIN-GRAIN COLLISIONS
TEMPERATURE
GAS COMPOSITION
GAS-GRAIN CHEMISTRY
DUST GRAINS
STELLAR RADIATION FIELD
HEATING
COOLING
HEATING
NUCLEATION
NANOCLUSTERS
COAGULATION

Self-consistent AGB wind

Hydrochemistry

+

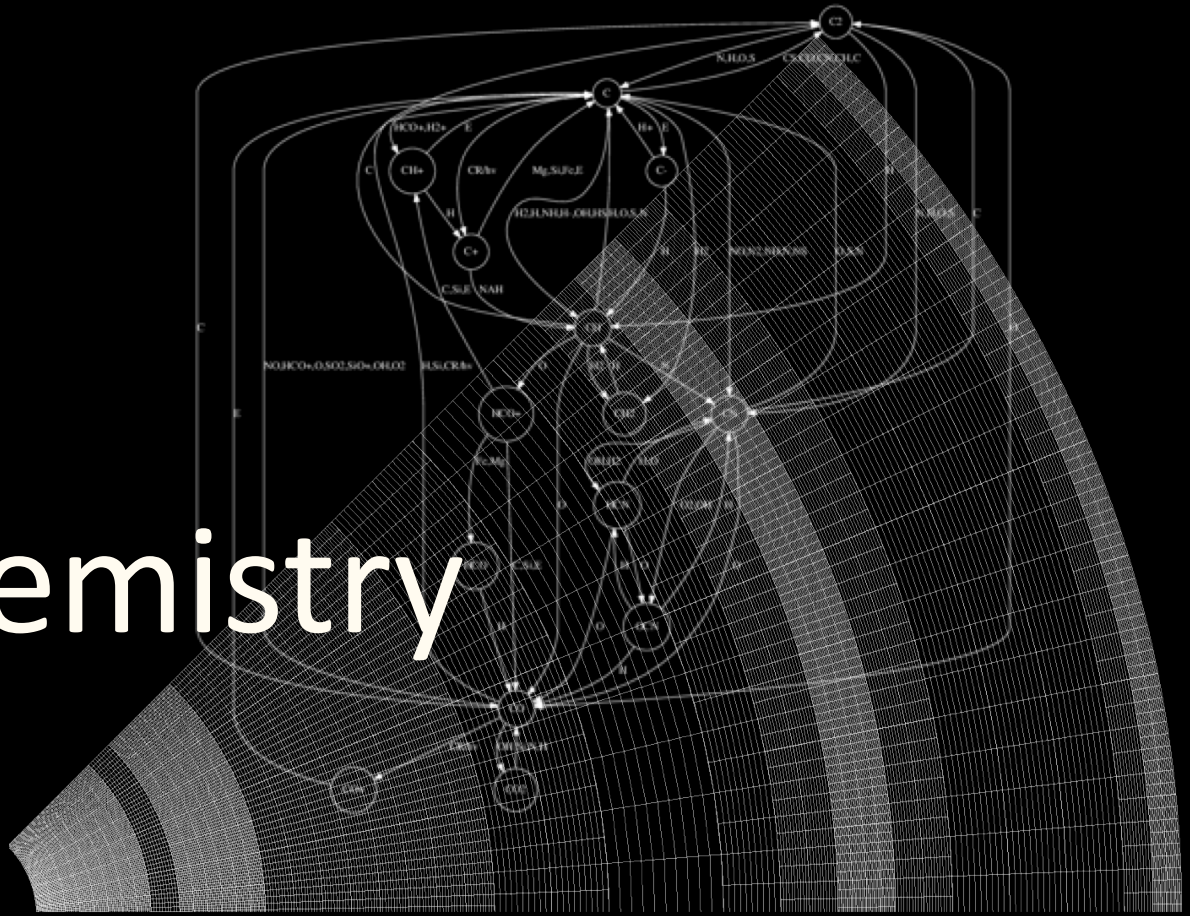
Nucleation theory

+

Dust evolution with radiation field

Boulangier 2019

Hydrochemistry



Current chemistry

Equilibrium

List of species

2 step improvement

Non-Equilibrium
Time dependent

Coupled to hydrodynamics

List of reactions

Reduced list of reactions

~1700 reactions
~160 species

~250 reactions
~70 species

Reduction algorithm

Speed-up factor ~20

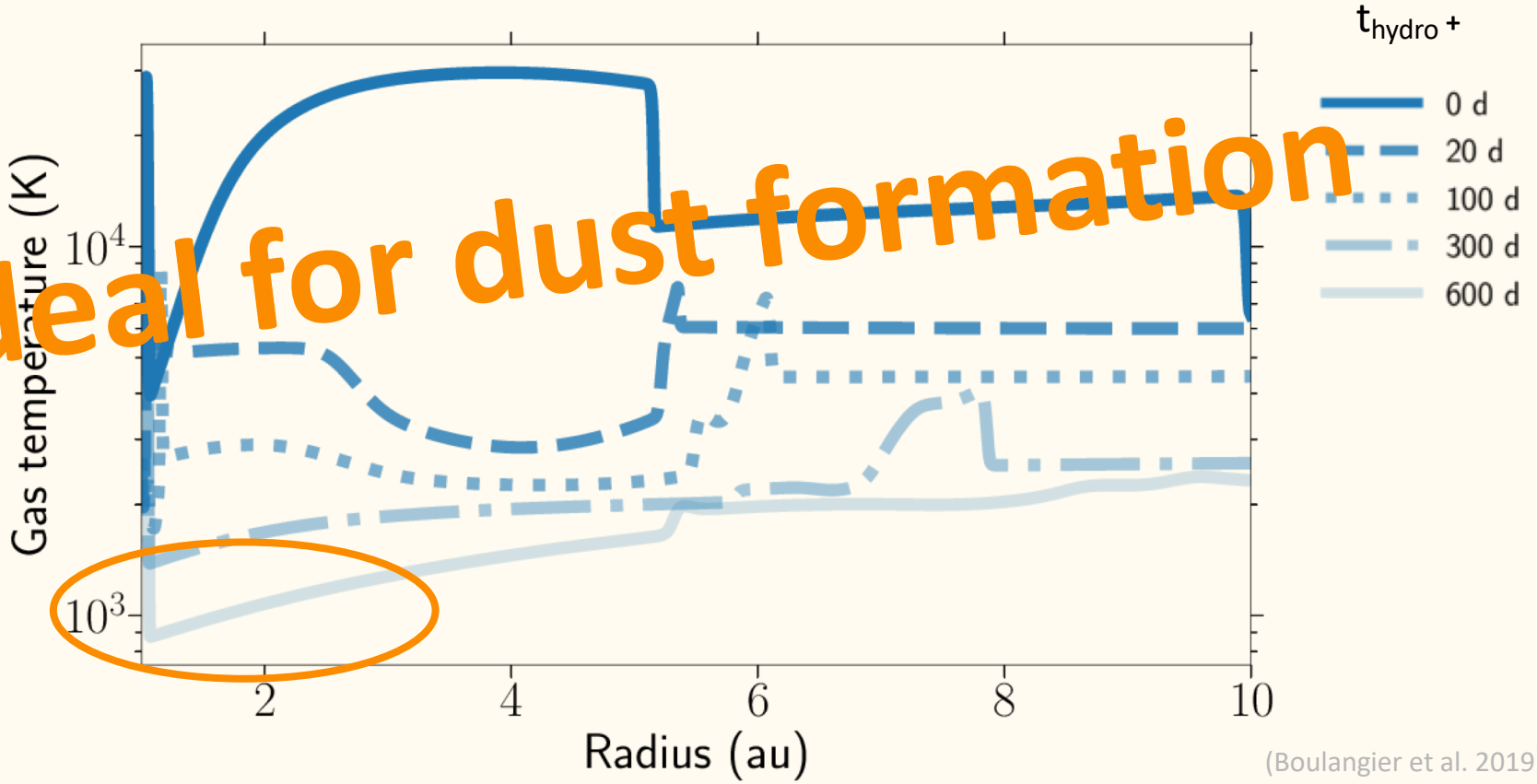
Microphysical heating and cooling processes

Process
H and He line cooling
H, He, He^+ collisional ionization by e^-
H^+ and He^+ recombination
He dielectric recombination
H (all levels) collisional excitation by e^-
He ($n = 2, 3, 4$ triplets) collisional excitation by e^-
He^+ ($n = 2$) collisional excitation by e^-
H_2 rovibrational lines cooling
Low density: collision by H, H^+, H_2, He, e^-
High density: LTE

Process
H_2 chemical cooling
H_2 chemical heating
CO rotational lines
Collisions by H and H_2
CIE cooling
H_2–H_2 and H_2–He pairs
Metal fine-structure line cooling
Cosmic ray heating

(Boulangier et al. 2019)

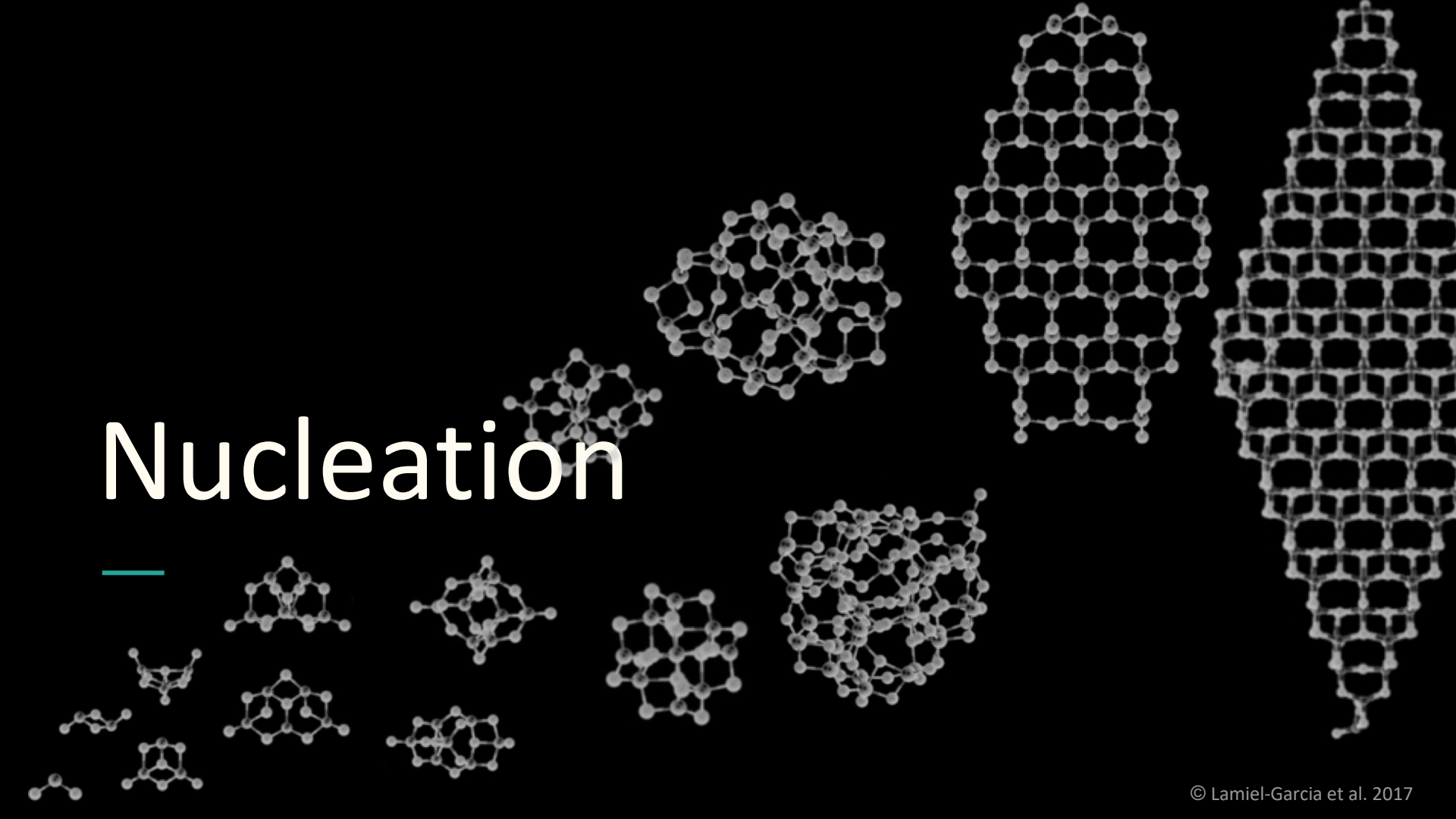
Cooling is very efficient



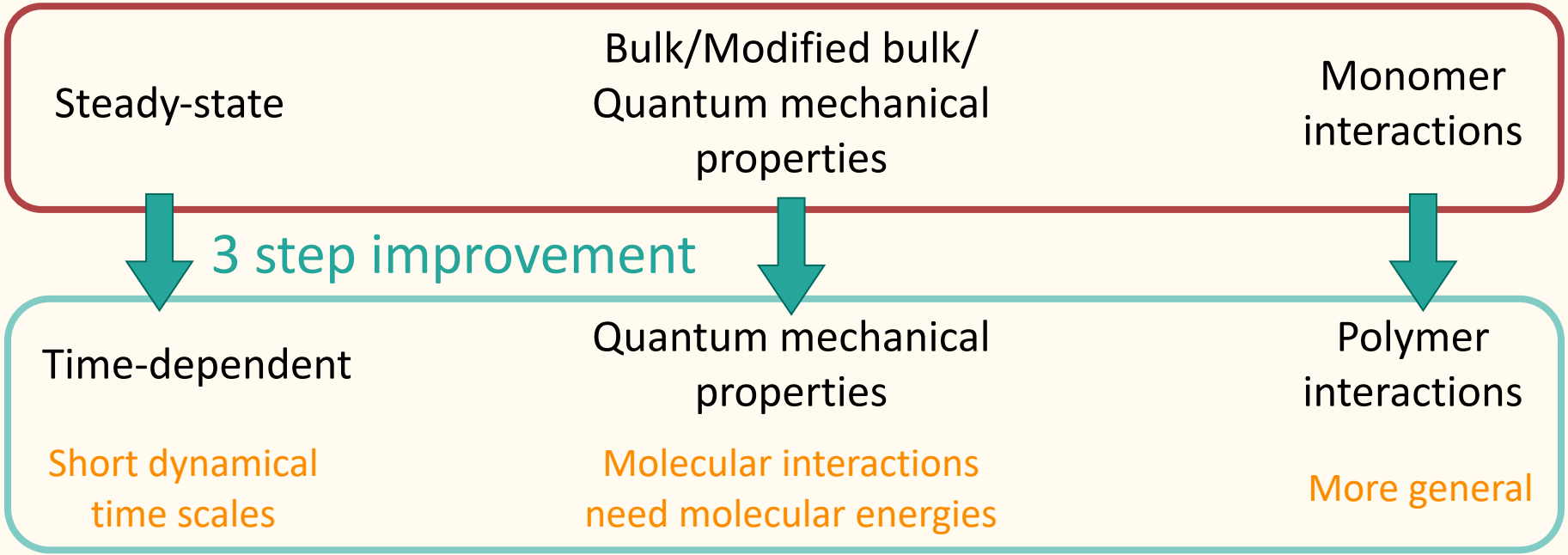
Ideal for dust formation

(Boulangier et al. 2019)

Nucleation



Current nucleation



Current nucleation

Steady-state

Bulk/Modified bulk/ Quantum mechanical properties

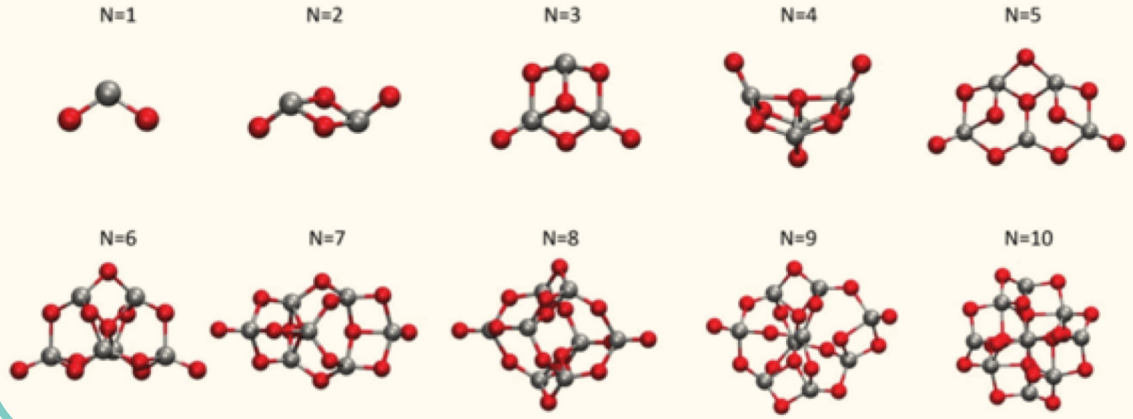
Monomer interactions

3 step improvement

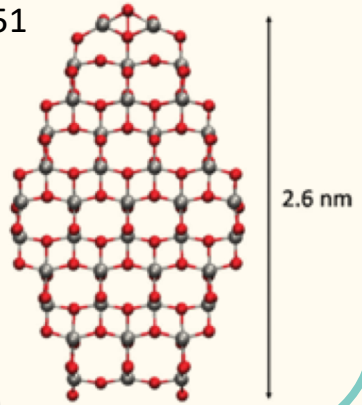
Time-dependent

Quantum mechanical properties

Polymer interactions



$(TiO_2)_N$ N=151 ≠



(Lamiel-Garcia et al. 2017)

Current nucleation

Steady-state

Bulk/Modified bulk/
Quantum mechanical
properties

Monomer
interactions

3 step improvement

Time-dependent

Short dynamical
time scales

Quantum mechanical
properties

Molecular interactions
need molecular energies

Polymer
interactions

More general

Coupled to large chemical network

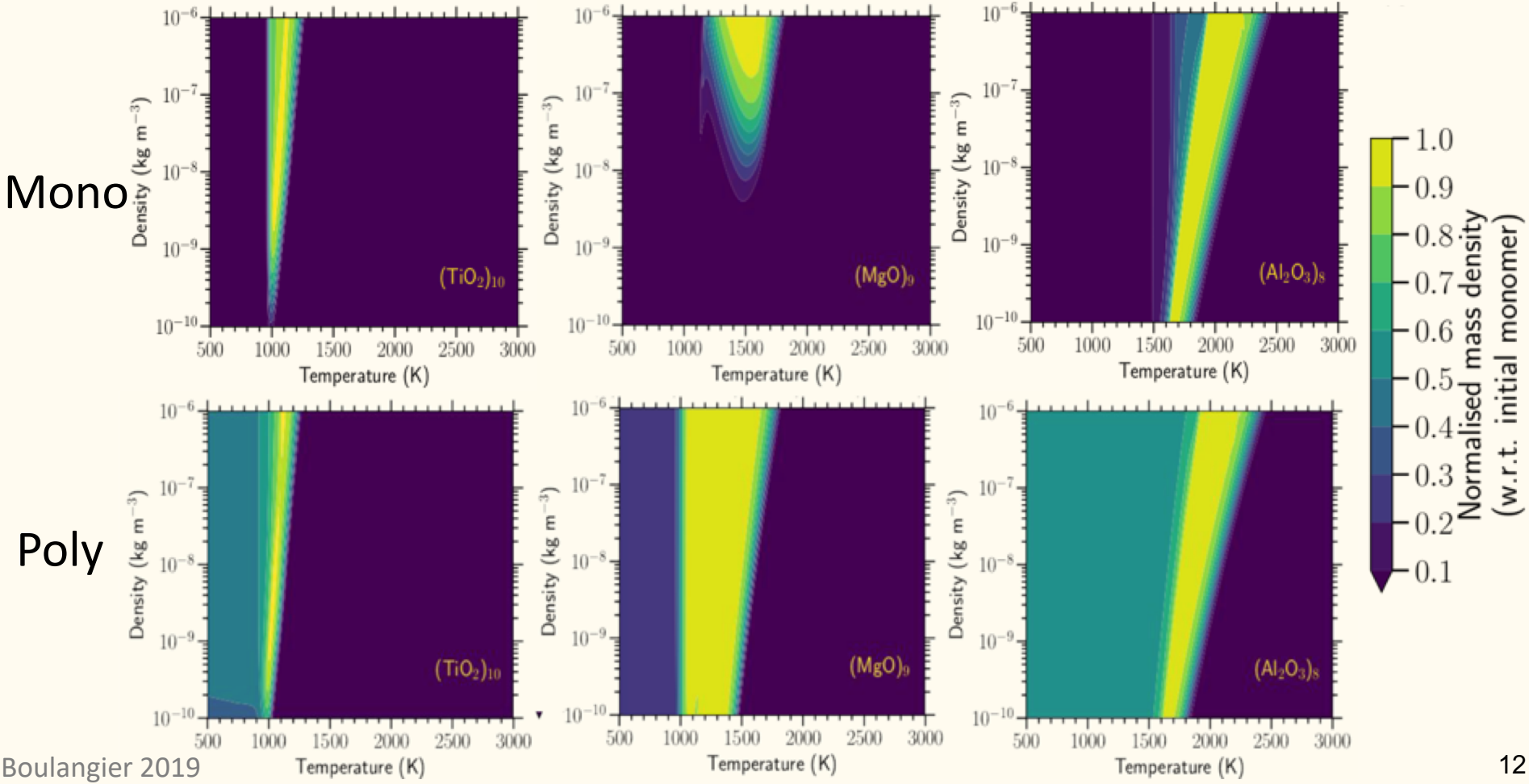
Competition for chemical “resources” ✚ No assumption of monomer existence

Nucleation candidates choice based on

Presolar grains + High bond energies + Atomic abundances

	$(TiO_2)_N$	$(SiO)_N$	$(MgO)_N$	$(Al_2O_3)_N$
N_{max}	10	10	10	8
Quantum mechanical properties	DFT: lowest energy isomer → Gibbs free energy → reversed reaction rate			
Extra reactions	**~20**	**1**	**~50**	**~100**

$(SiO)_{10} < (TiO_2)_{10} < (MgO)_9 < (Al_2O_3)_8$



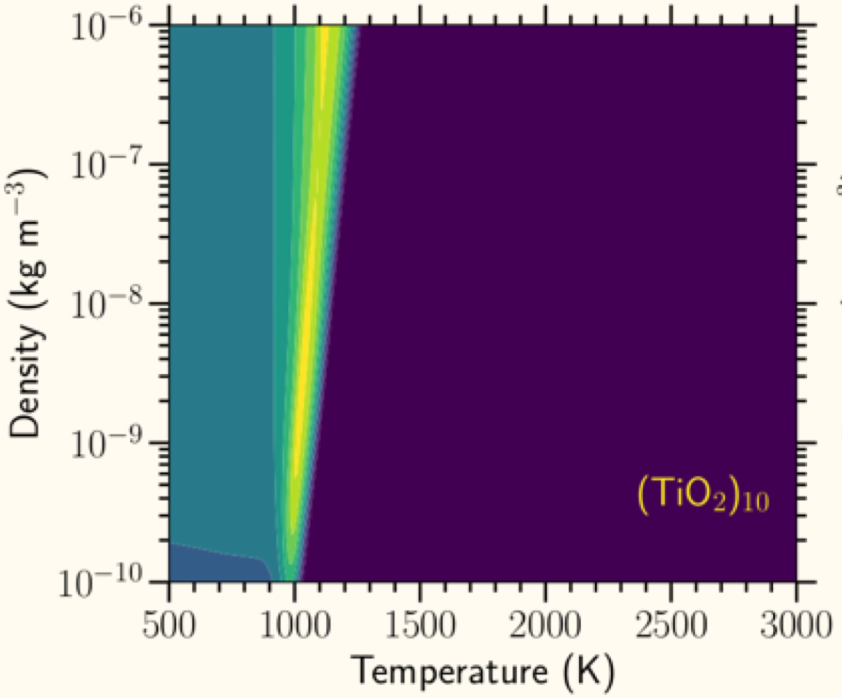
Boulangier 2019

What if combined with network?

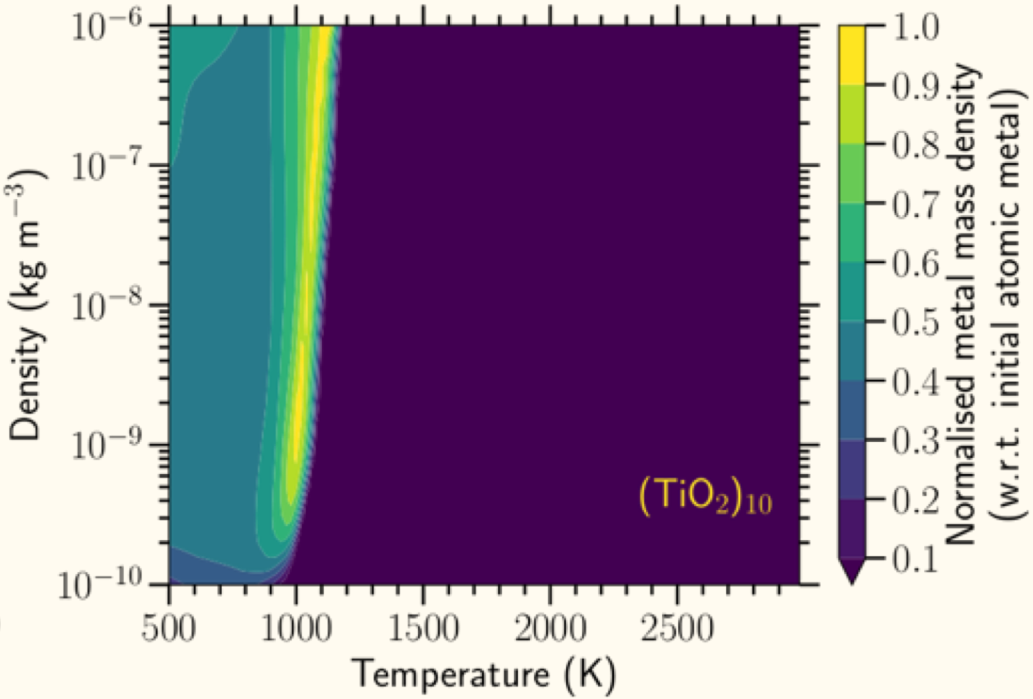
1. No Al_2O_3 → No Al_2O_3-clusters
2. No MgO → No MgO-clusters
3. SiO-clusters equally inefficient
4. TiO_2-clusters equally efficient

TiO_2-clusters are the best candidate

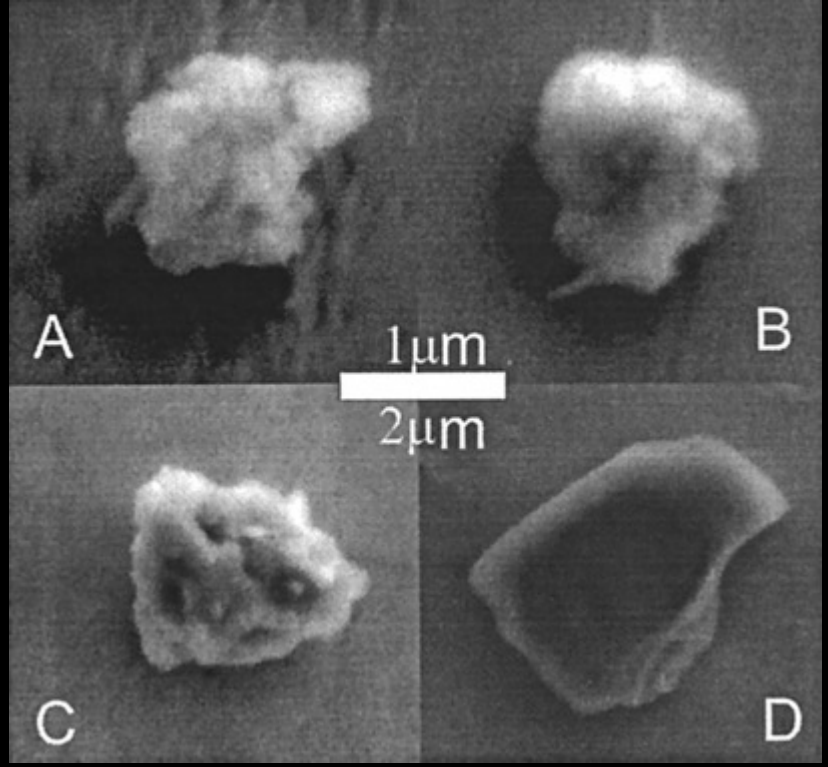
A priori TiO_2 existence



Combined in large network

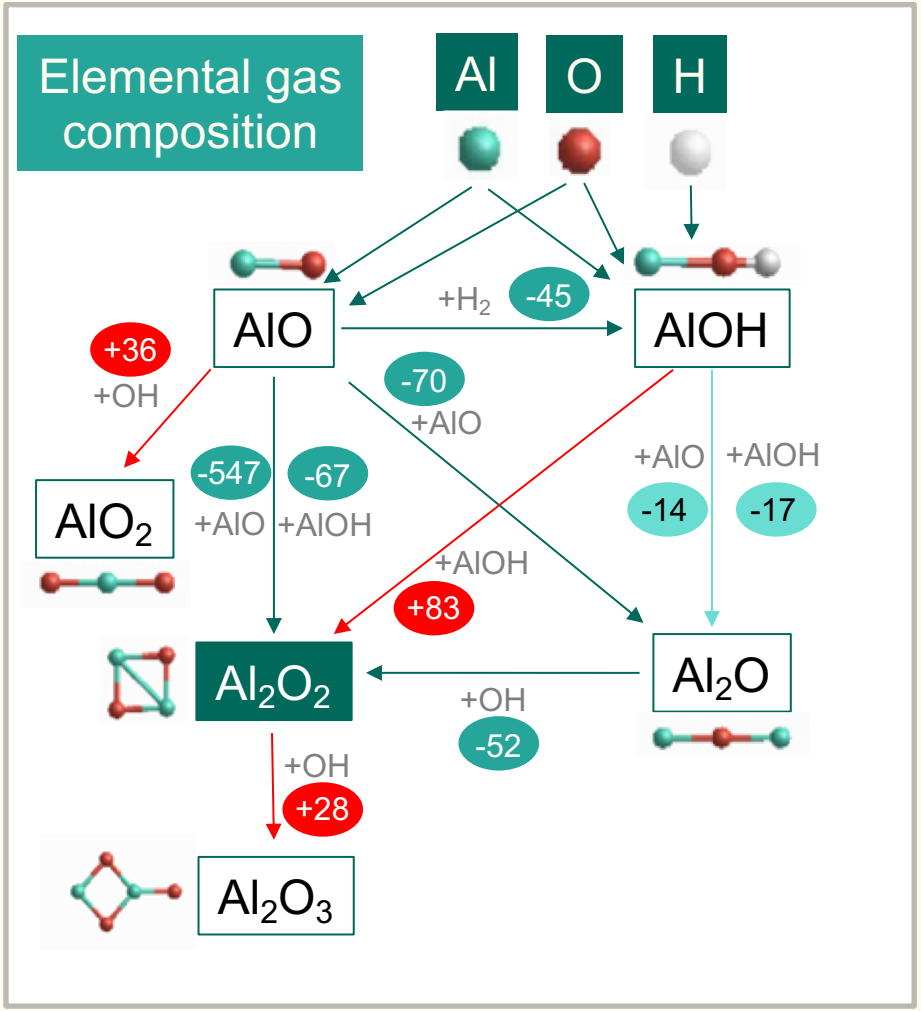


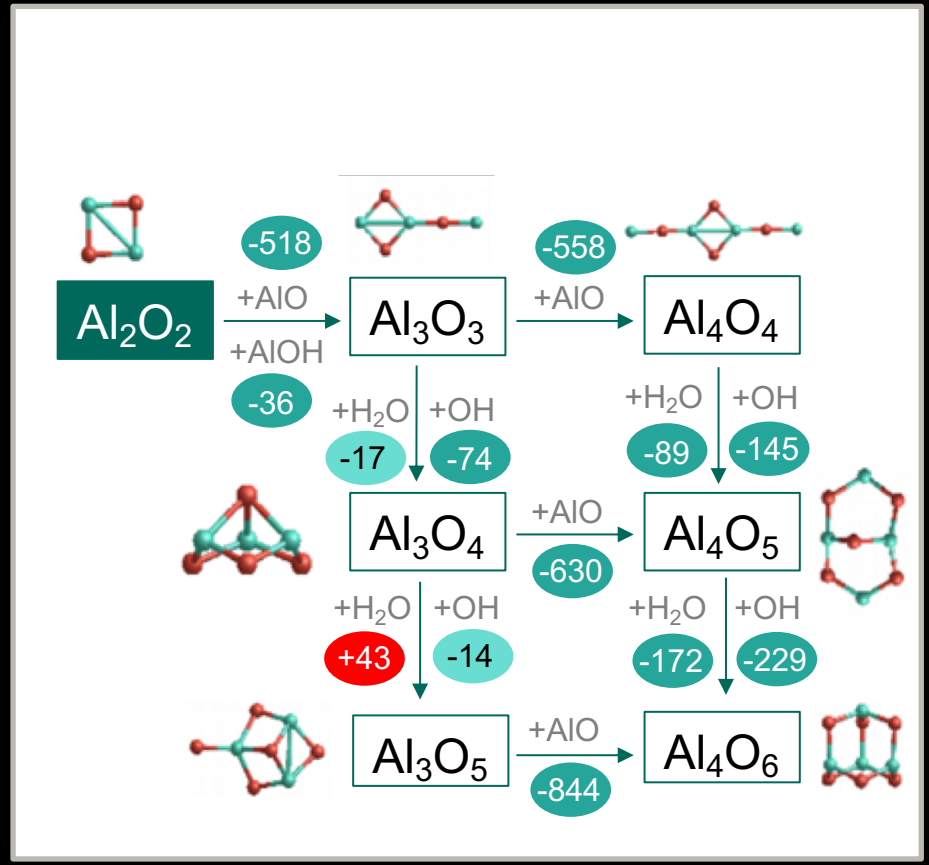
Planet Earth – Meteorites



Al_2O_3-clusters are best candidate

- Abundant in presolar grains (much more than Ti-oxides)
- Dust observed close to the star (at high temperature)
  Only feasible for Al_2O_3
- Need for revision of Al-reactions or bypass $(Al_2O_3)_{n=1}$

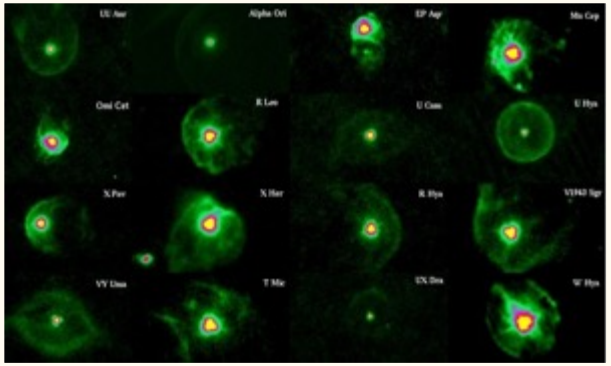




Gobrecht et al. (in prep)

Future

Observations



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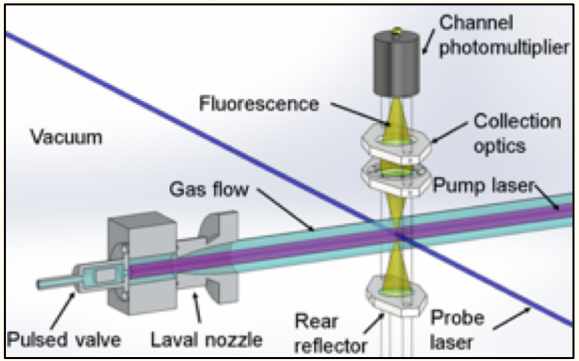
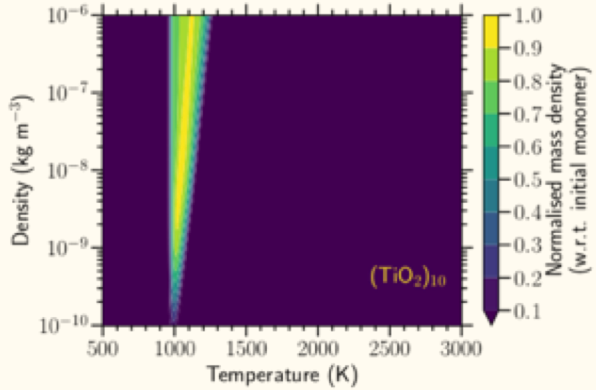
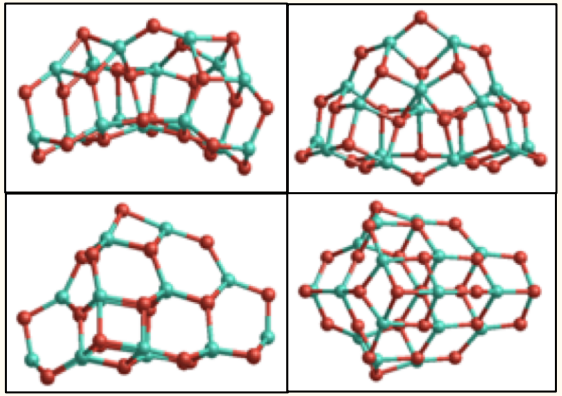


Simulations

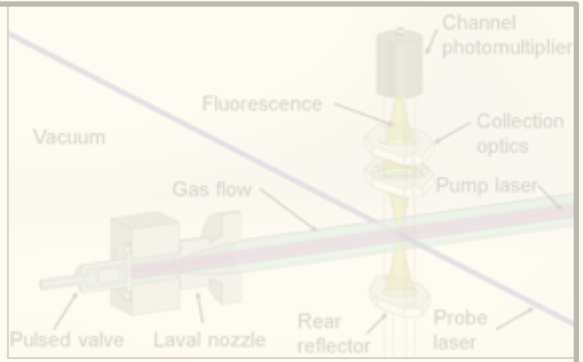


Theory



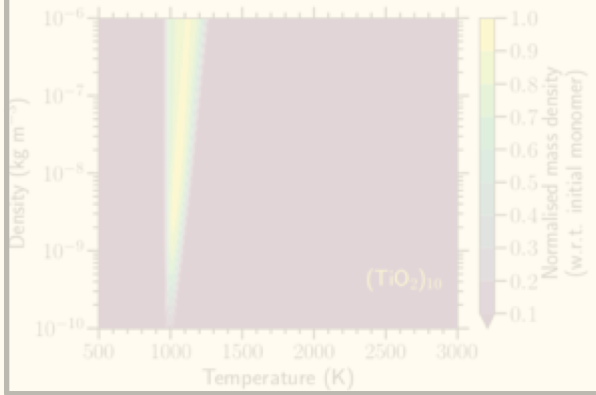
Observations

Laboratory



THANKS!

XT



Simulations

Theory

You have to look within for value, but beyond for perspective.

- Denis Waitley -