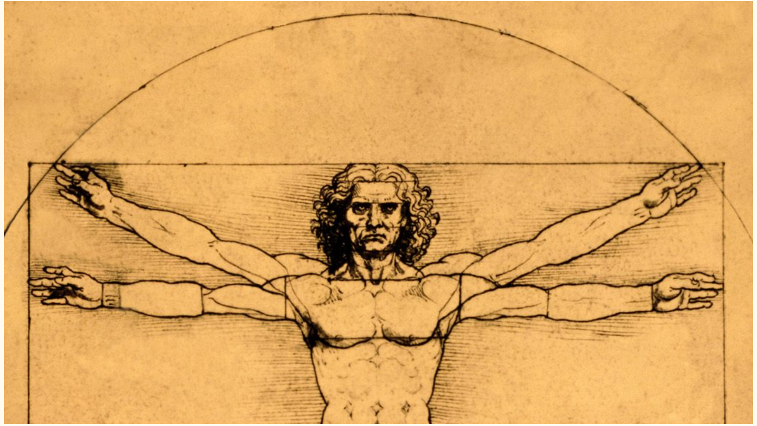
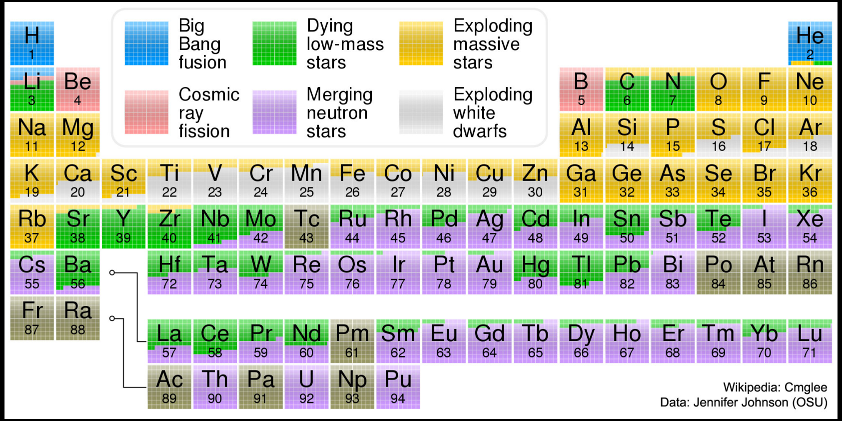


We are made of stardust

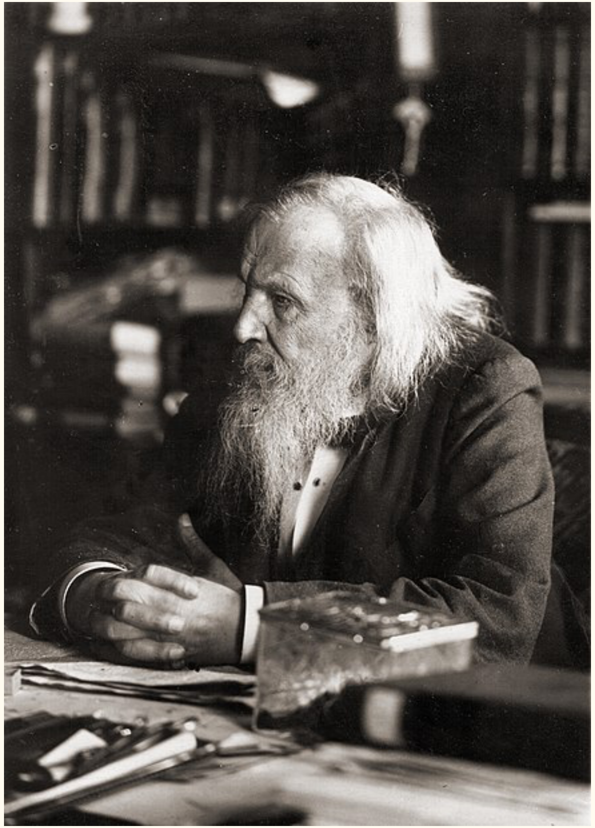


Evolved stars govern the periodic table of Mendeleev

Leen Decin – KU Leuven – Belgium
– University of Leeds – UK

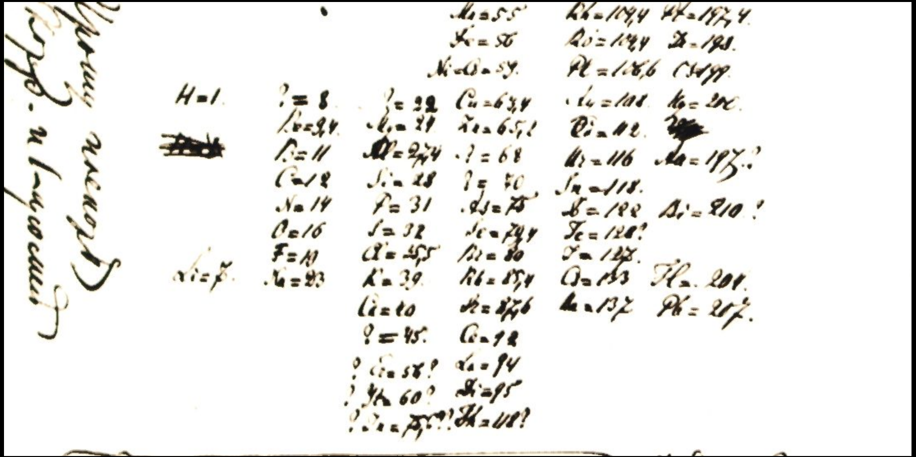
European Research Council

Dmitri Ivanovich Mendeleev

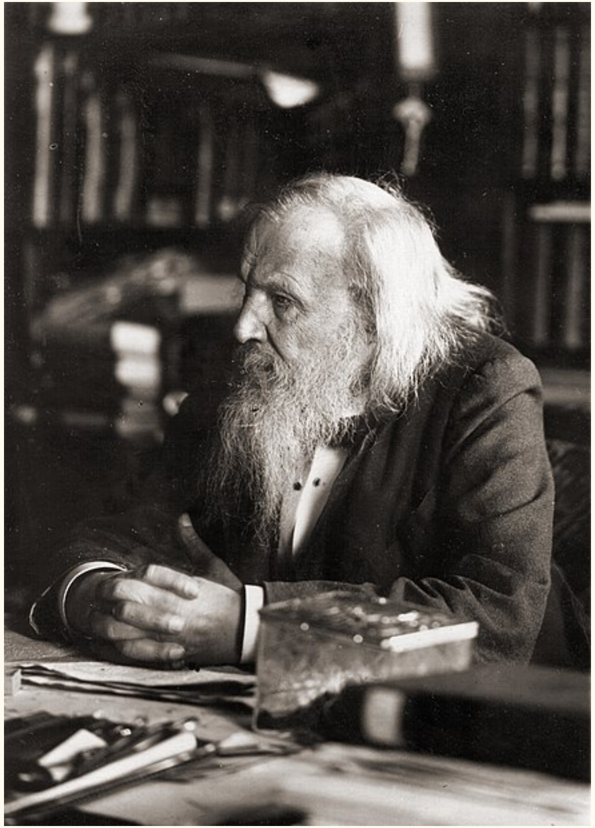


1834 - 1907

1869

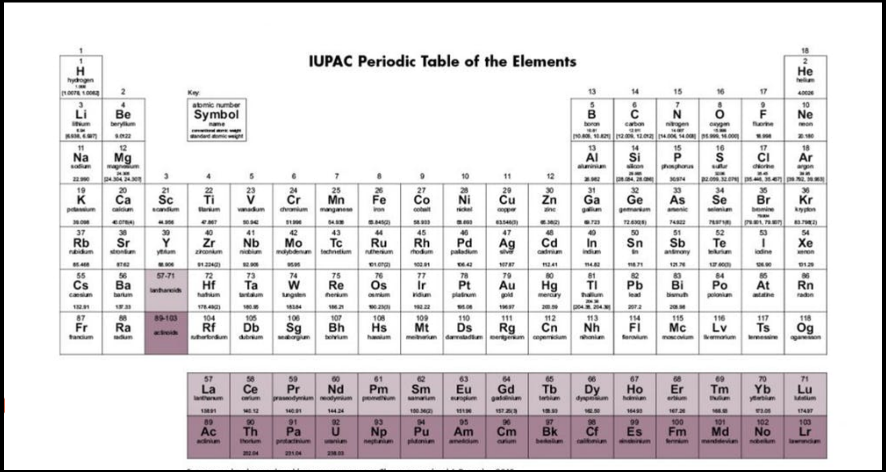


Dmitri Ivanovich Mendeleev



1834 - 1907

2019



Part 1 – The origin of the periodic elements

→ atomic mixture

› role nuclear reactions in evolved stars

Part 2 – From atoms to dust

→ atomic, molecular, dust composition

› role of stellar winds

Part 3 – Enrichment of the interstellar medium

→ atoms, (exited) molecules, (large) grains

› role of bow shocks

Part 4 – The quest for dust nucleation

› Why wonder about astrochemistry in old stars' winds?

Part I -
The cosmic origin of the periodic elements

Initial conditions - Standard Model physics

T<1 sec

$$n + e^{+} \rightleftharpoons \bar{\nu}_e + p$$
$$n + \nu_e \rightleftharpoons p + e^{-}$$

→ Freeze-out: n/p~1/6

Big Bang nucleosynthesis

10 sec < T < 20 min

Freeze-out: n/p~1/6

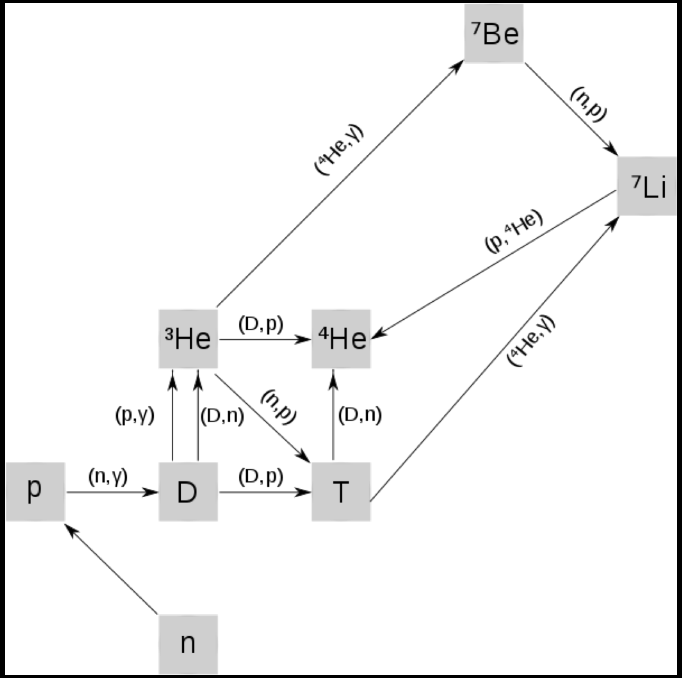
↓

n decay: n/p~1/7

n fused → ^{4}He

↓

~8% He (~25% in mass)



Big Bang nucleosynthesis

10 sec < T < 20 min

Freeze-out: n/p~1/6

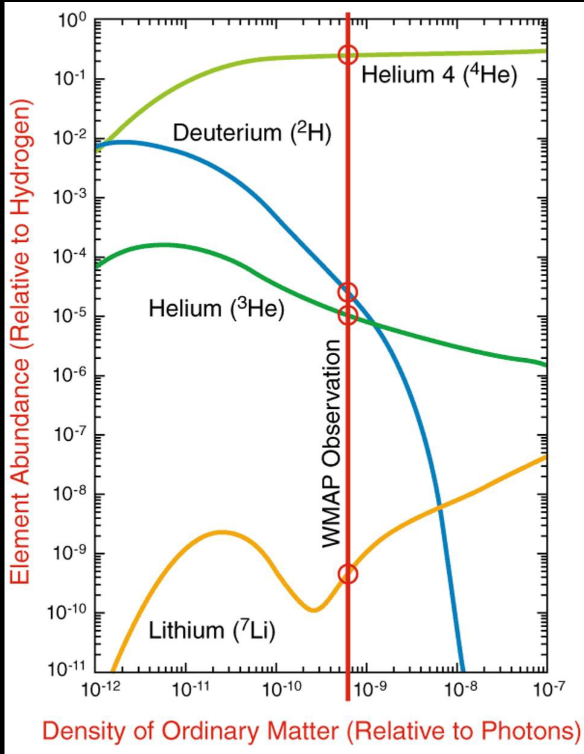
↓

n decay: n/p~1/7

n fused → ^{4}He

↓

~8% He (~25% in mass)

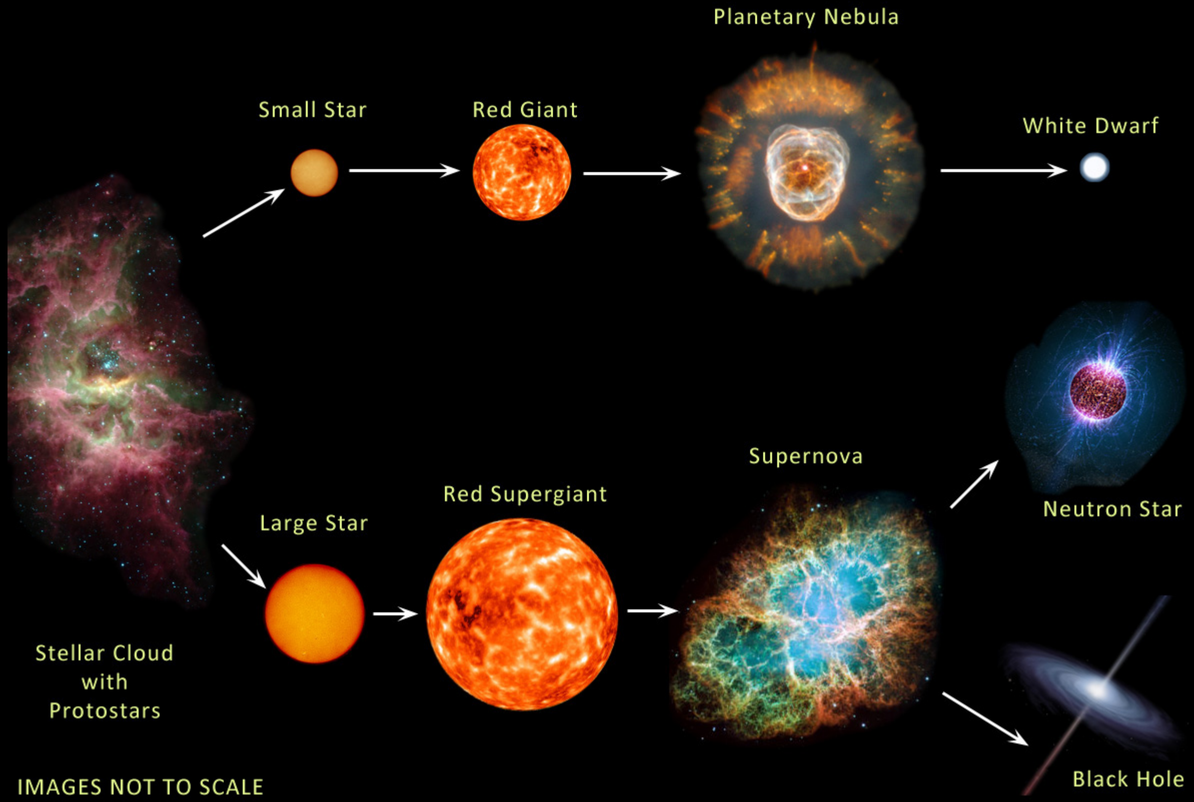


The periodic table through time

T ~ 15 min

Stellar nucleosynthesis

Stellar evolution

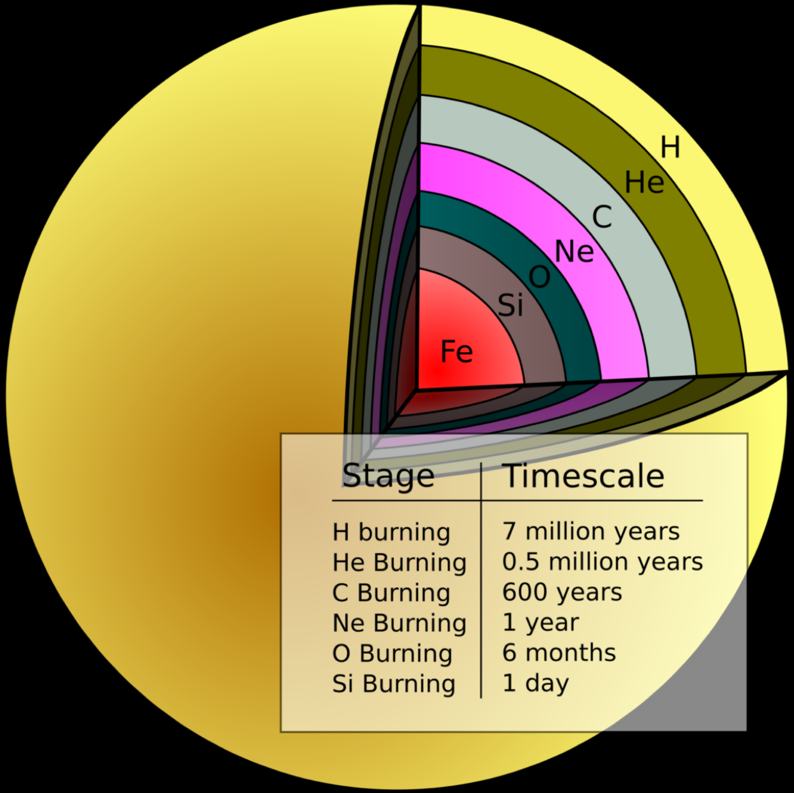


Stellar nucleosynthesis

Hydrogen fusion - Deuterium fusion - Proton-proton chain - CNO cycle	**Helium fusion** - Triple α-process - α -process

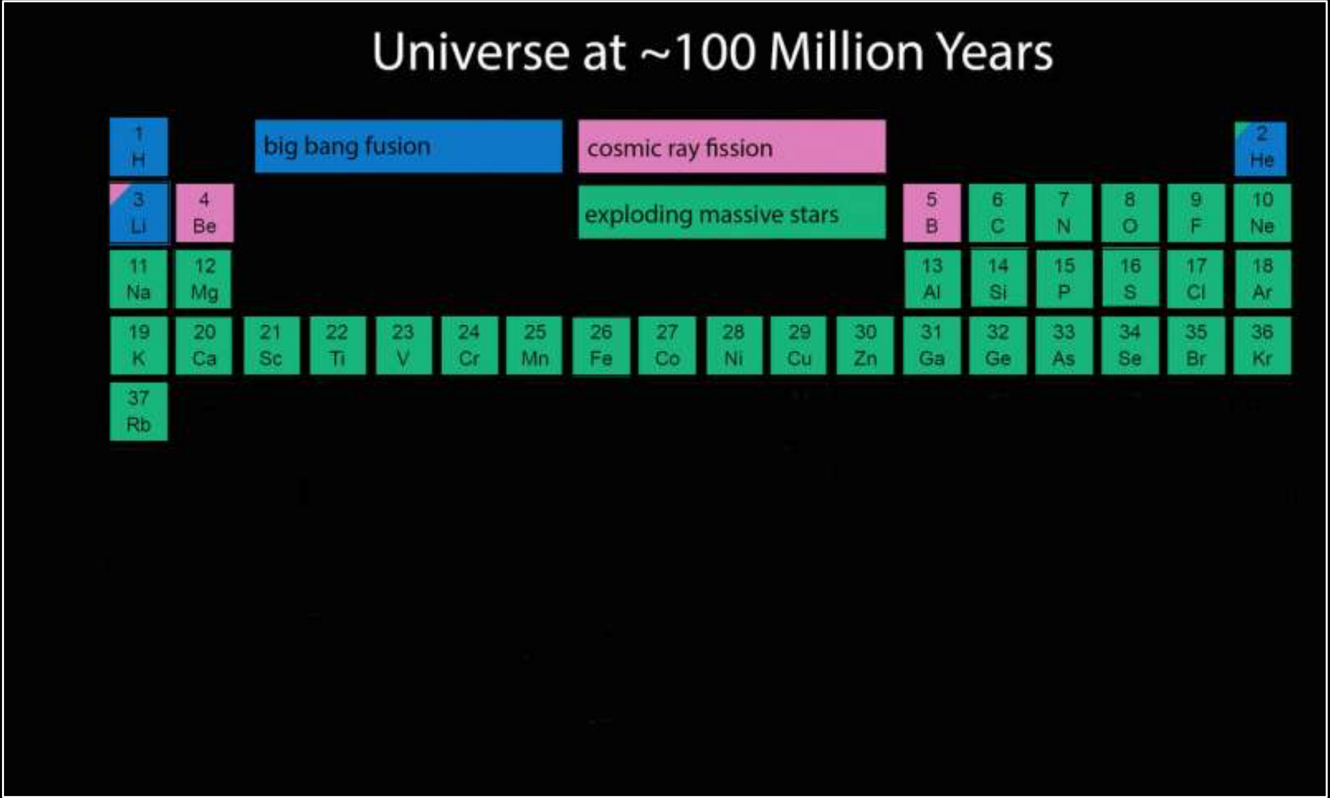
Fusion of heavier elements
- Li, C, Ne, O, Si-burning
	Production of elements > Fe
	- Neutron capture
	  - r-process
	  - s-process
	- Proton capture
	  - Rp-process
	  - P-process
	- Photo-disintegration

Stellar nucleosynthesis: massive stars

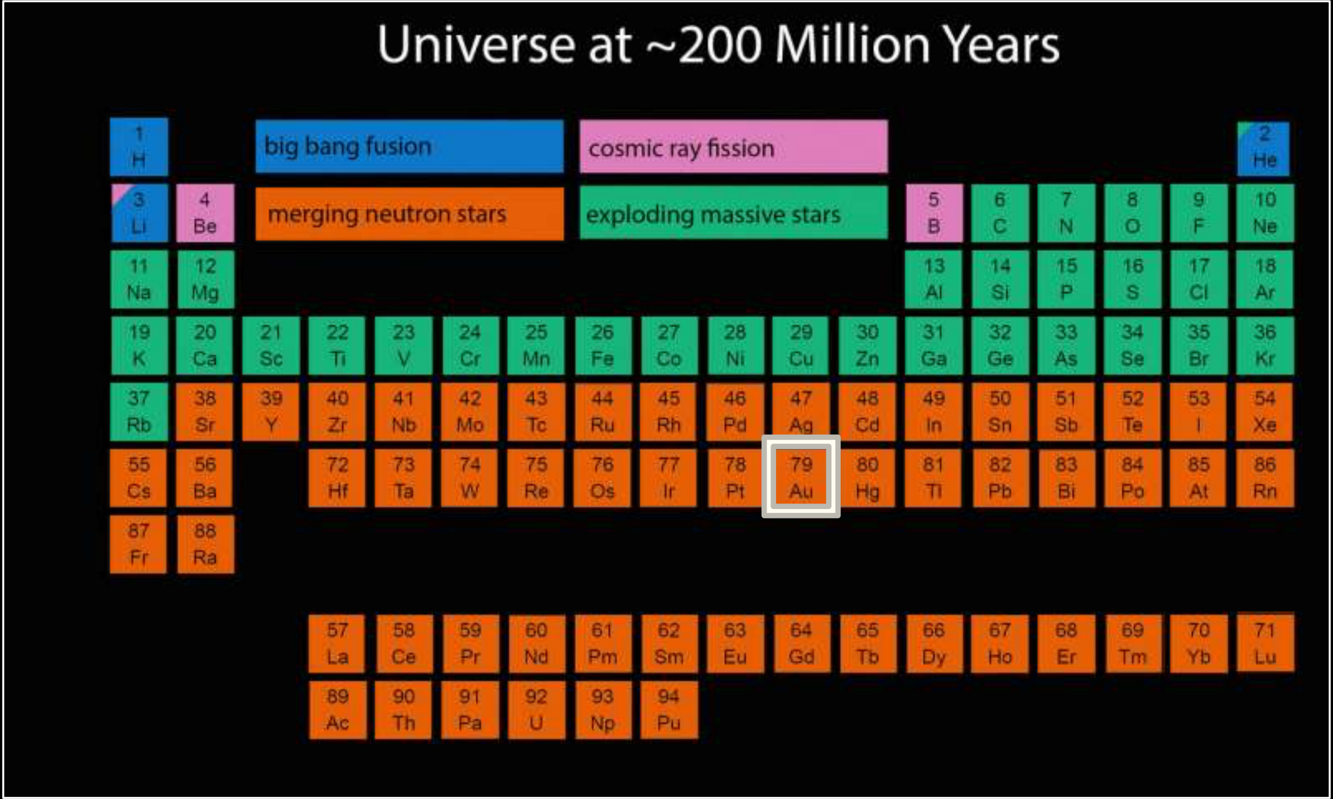


Stage	Timescale
H burning	7 million years
He Burning	0.5 million years
C Burning	600 years
Ne Burning	1 year
O Burning	6 months
Si Burning	1 day

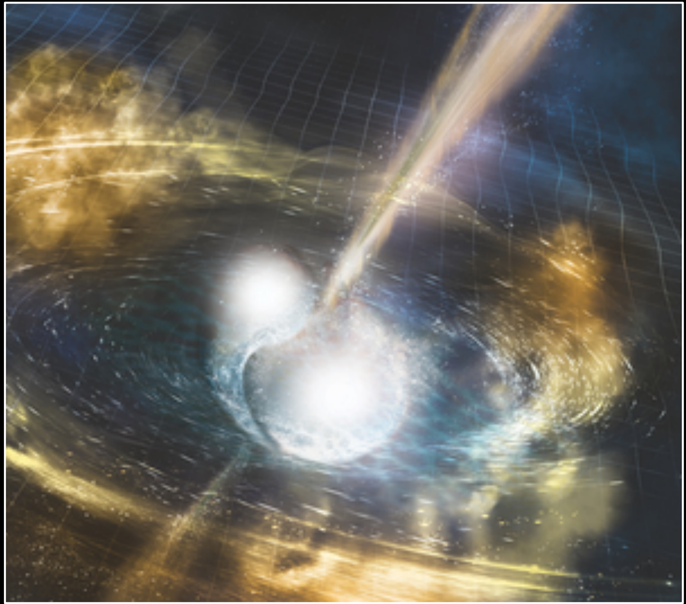
The periodic table through time



The periodic table through time

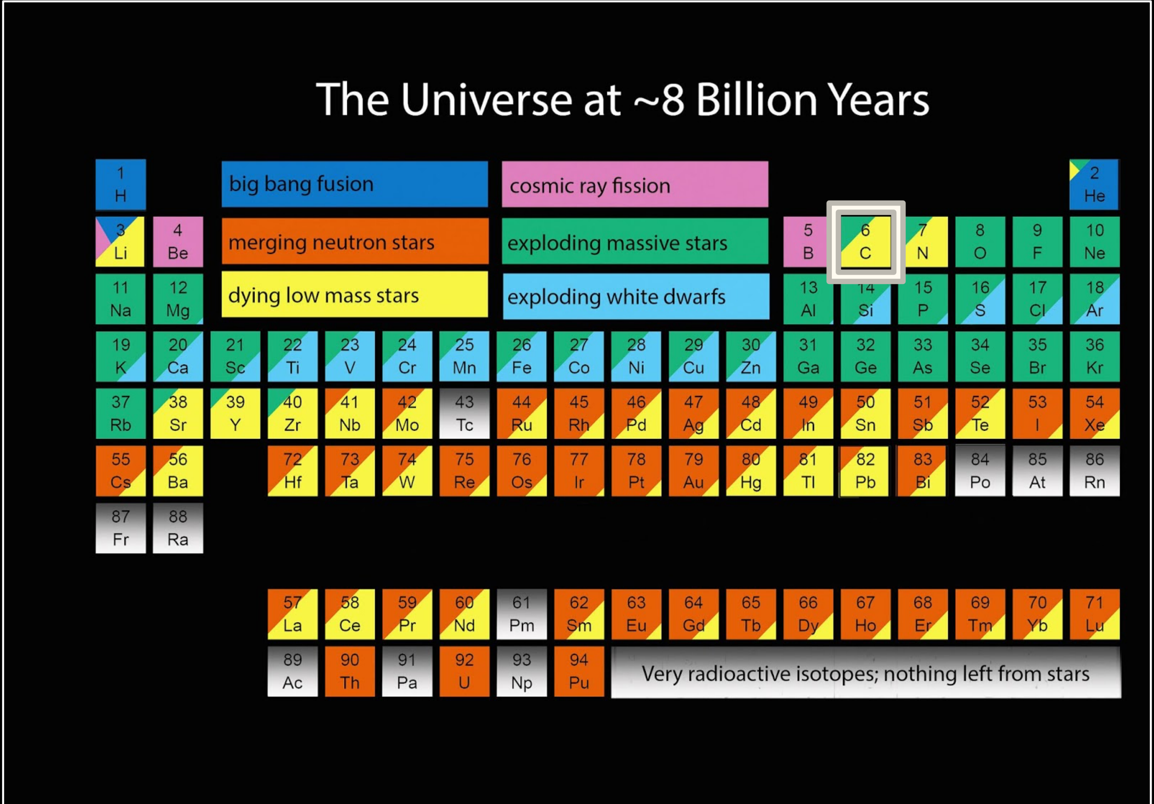


GW170817



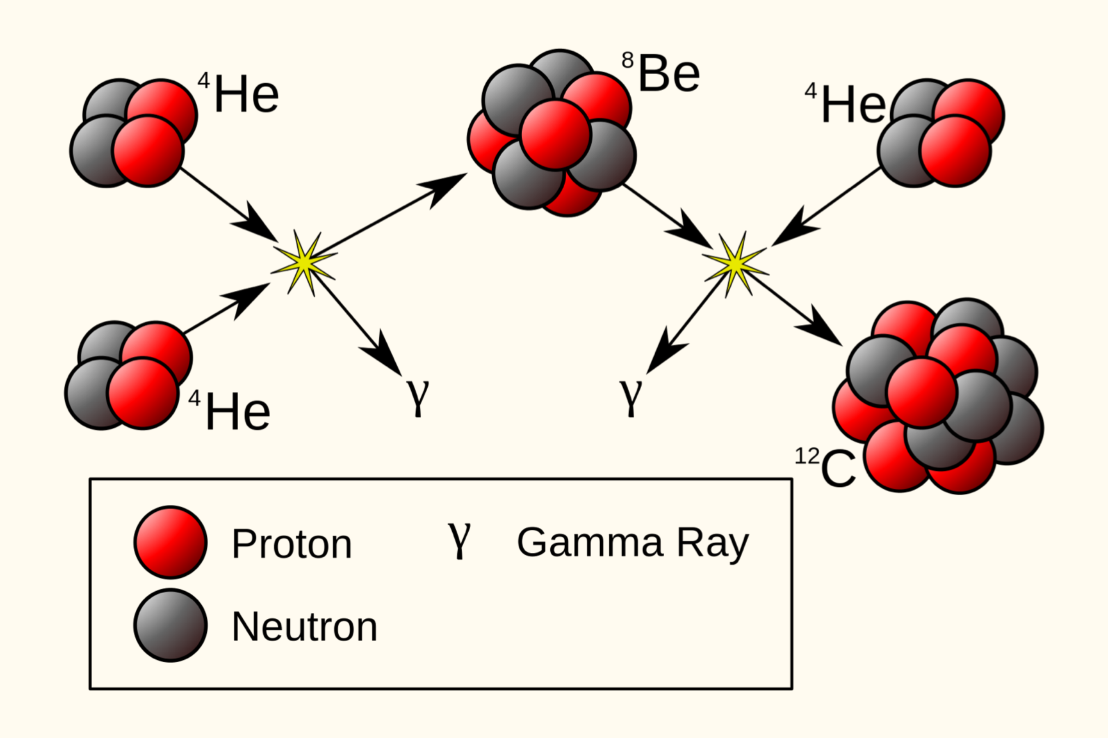
r-process: gold, platinum

The periodic table through time



Hoyle (1954): triple-α process
B^2FH (1957): s-process

Triple-α process



$${}^{4}_{2}He + {}^{4}_{2}He \rightarrow {}^{8}_{4}Be \quad (-0.0918\ MeV)$$

$${}^{8}_{4}Be + {}^{4}_{2}He \rightarrow {}^{12}_{6}C + 2\gamma \quad (+7.367\ MeV)$$

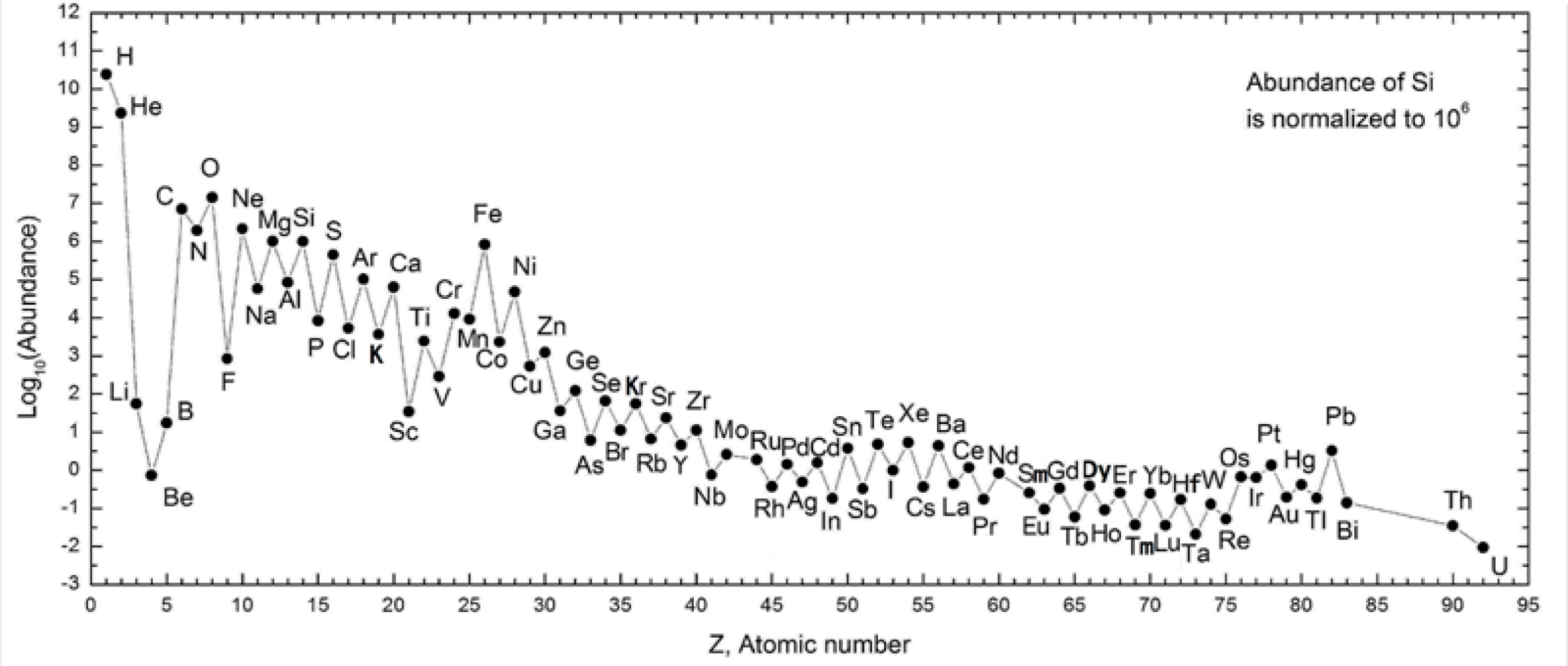
$${}^{12}_{6}C + {}^{4}_{2}He \rightarrow {}^{16}_{8}O + \gamma \quad (+7.162\ MeV)$$

We exist …

hence there must be a 7.68 MeV ^{12}C resonance

The cosmic chemical budget

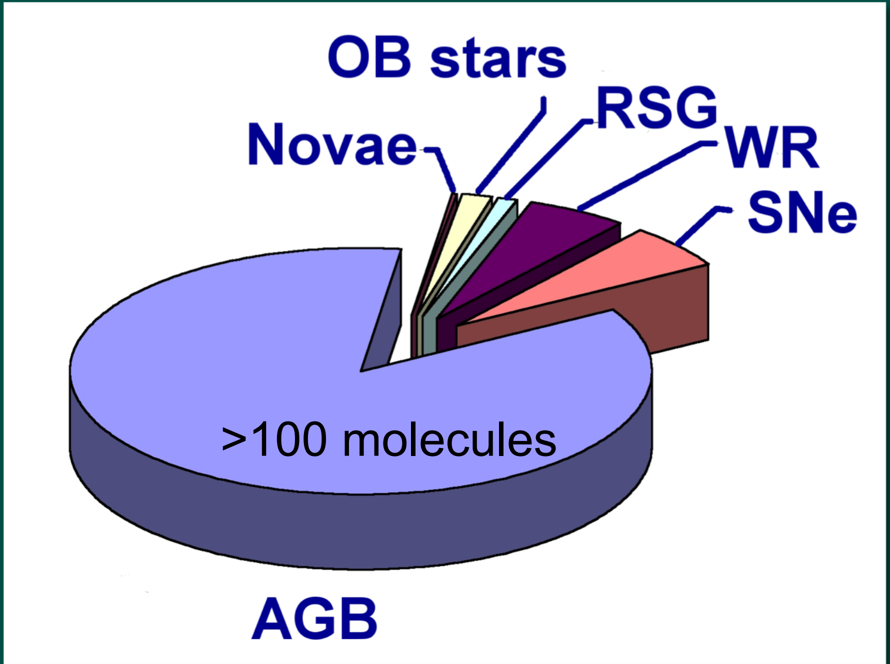
Suess & Urey (1956)



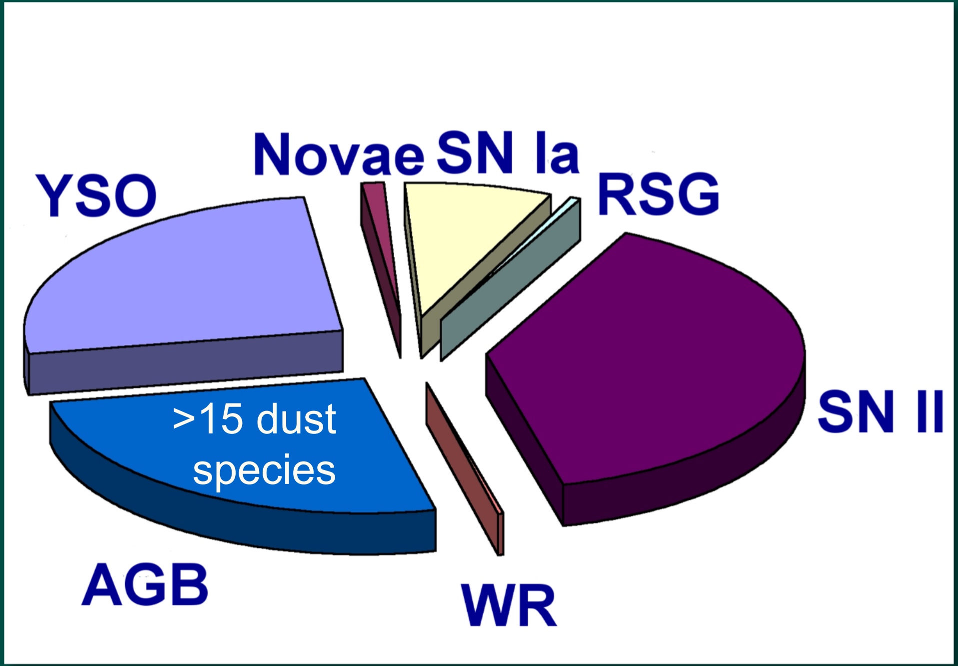
Part II -
From atoms to dust

Interstellar budget

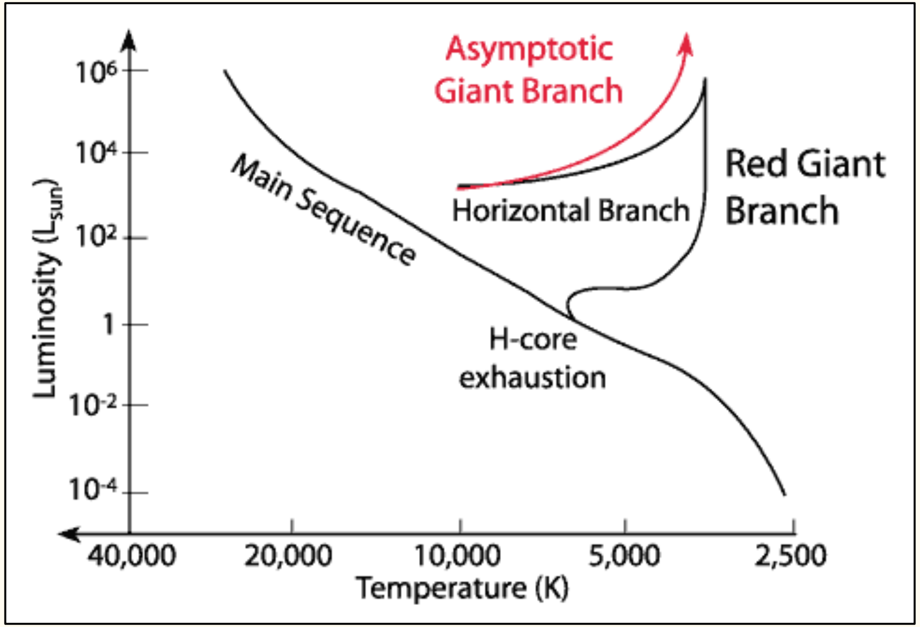
gas

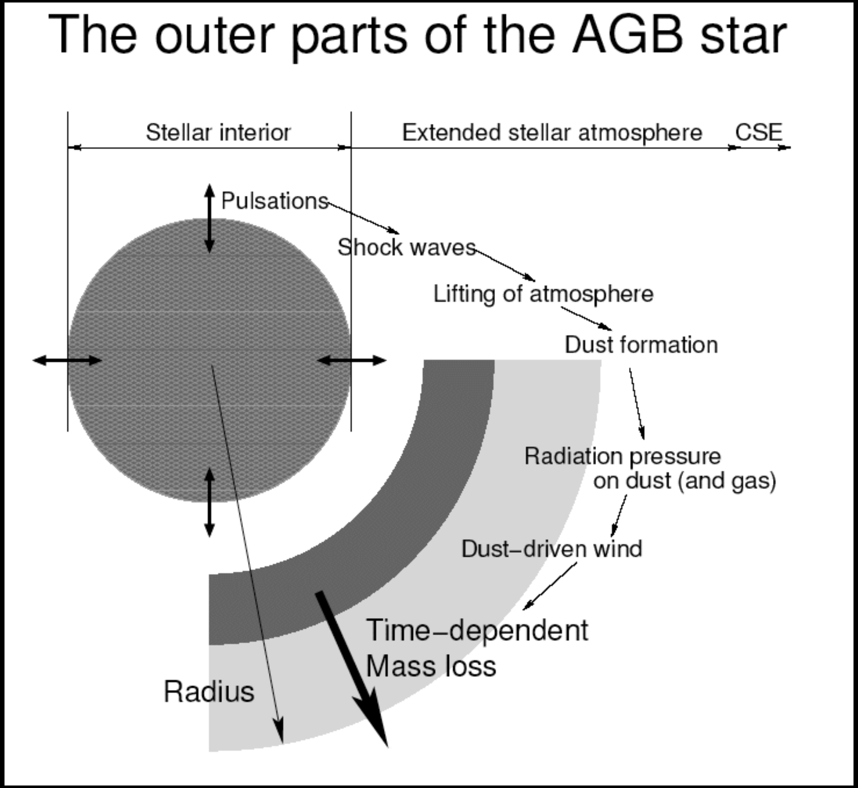


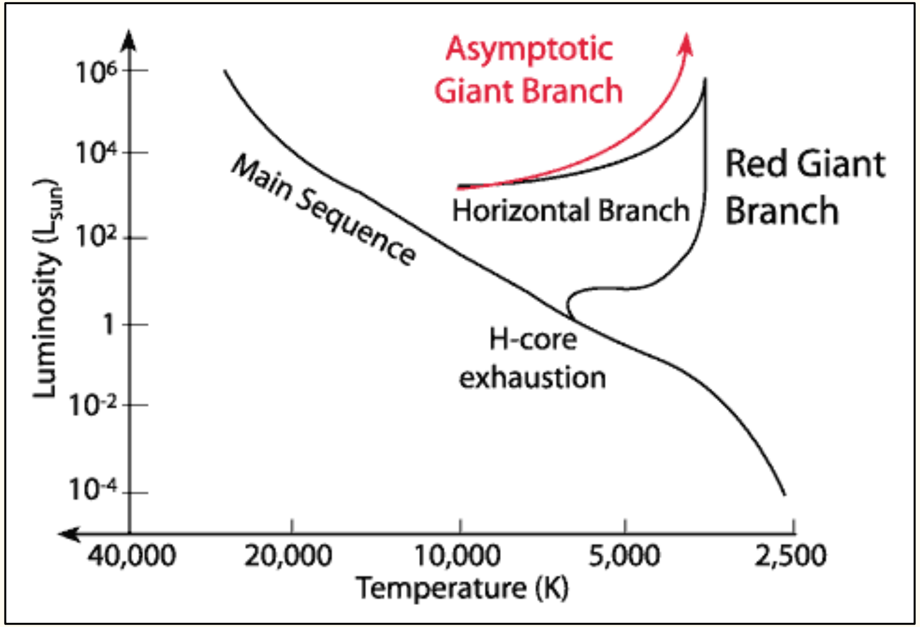
dust

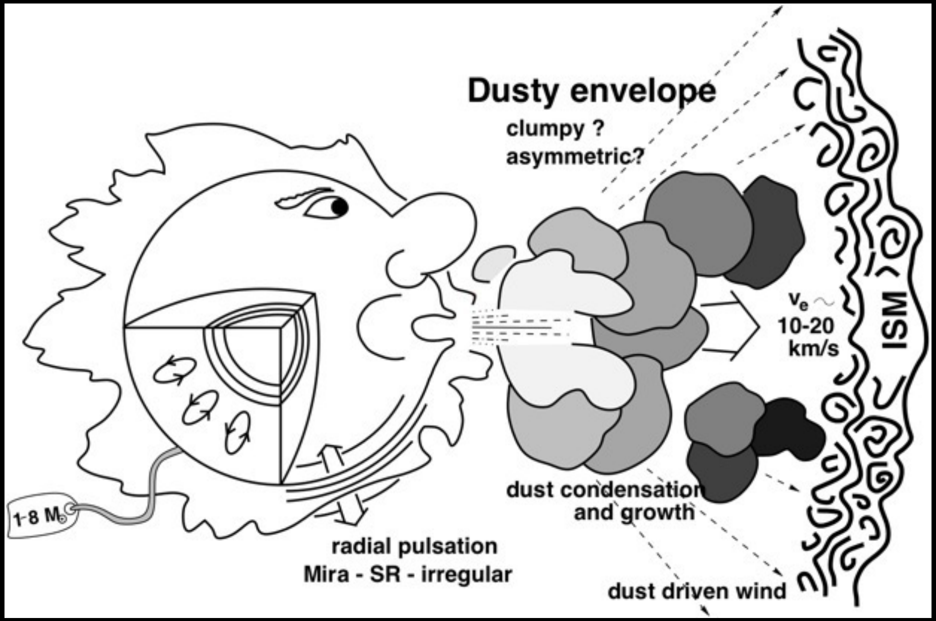


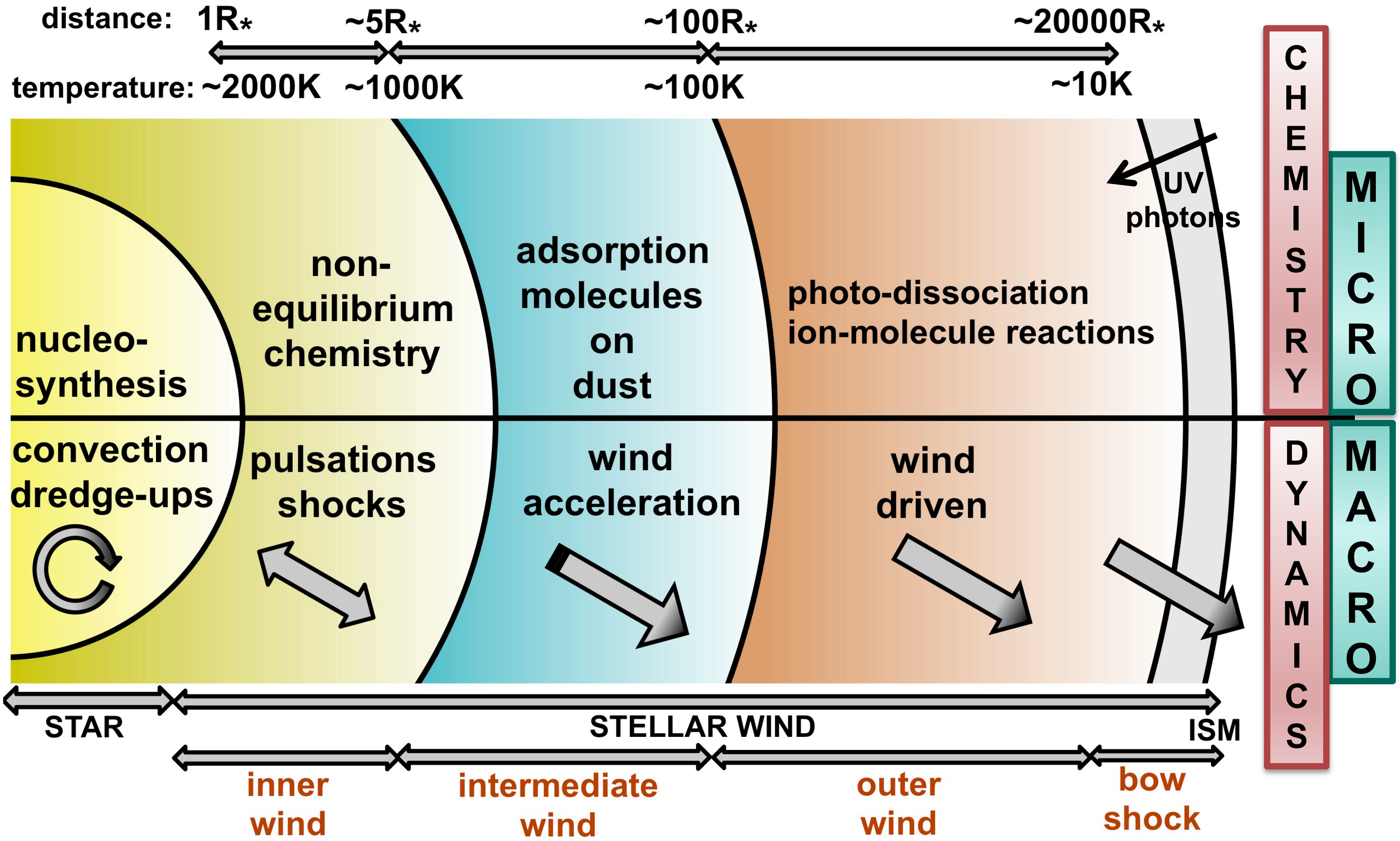
What is an AGB star?


Asymptotic
Giant Branch
Red Giant
Branch
Horizontal Branch
Main Sequence
H-core
exhaustion
Luminosity (L_{sun})
10^6
10^4
10^2
1
10^{-2}
10^{-4}
40,000
20,000
10,000
5,000
2,500
Temperature (K)

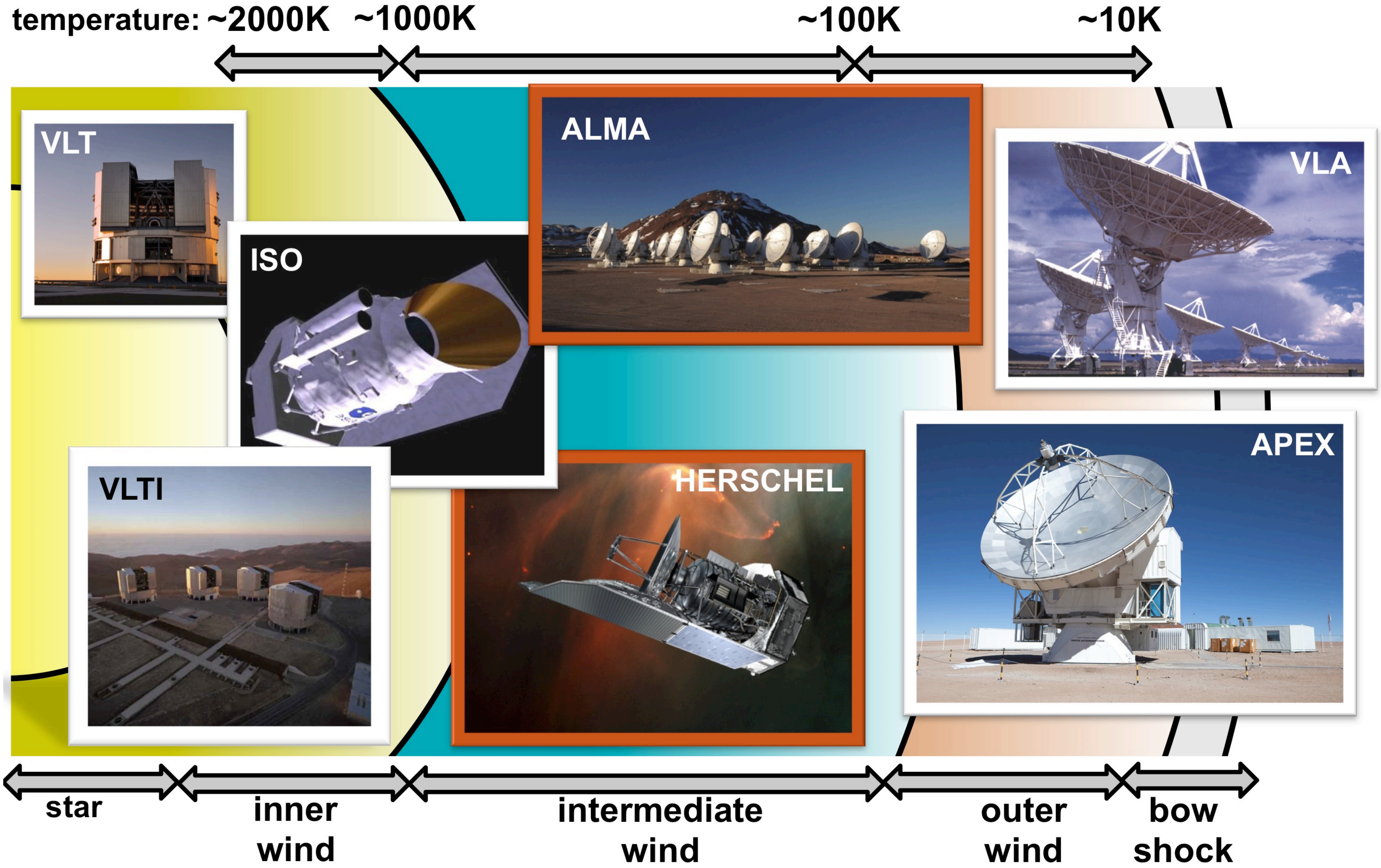

The outer parts of the AGB star
Stellar interior
Extended stellar atmosphere
CSE
Pulsations
Shock waves
Lifting of atmosphere
Dust formation
Radiation pressure
on dust (and gas)
Dust–driven wind
Time–dependent
Mass loss
Radius


Asymptotic
Giant Branch
Red Giant
Branch
Horizontal Branch
Main Sequence
H-core
exhaustion
Luminosity (L_{sun})
10^6
10^4
10^2
1
10^{-2}
10^{-4}
40,000
20,000
10,000
5,000
2,500
Temperature (K)

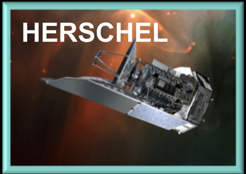

Dusty envelope
clumpy ?
asymmetric?
$v_e \sim$
10-20
km/s
ISM
dust condensation
and growth
radial pulsation
Mira - SR - irregular
dust driven wind
1-8 $M_\odot$


distance: 1R* ~5R* ~100R* ~20000R*
temperature: ~2000K ~1000K ~100K ~10K
nucleo-synthesis
non-equilibrium chemistry
adsorption molecules on dust
photo-dissociation ion-molecule reactions
UV photons
convection dredge-ups
pulsations shocks
wind acceleration
wind driven
STAR
STELLAR WIND
ISM
inner wind
intermediate wind
outer wind
bow shock
CHEMISTRY
DYNAMICS
MICRO
MACRO

Observing stellar winds

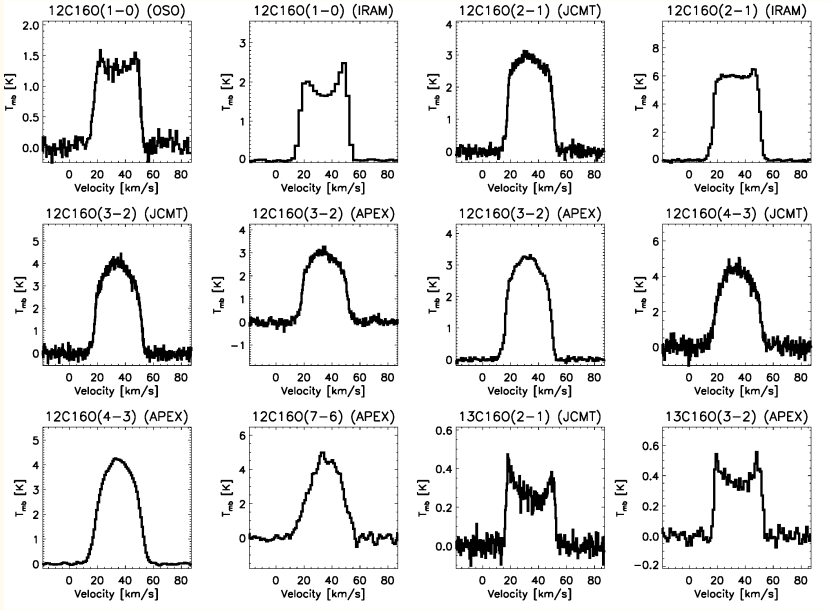

temperature: ~2000K ~1000K ~100K ~10K
VLT
ISO
ALMA
VLA
VLTI
HERSCHEL
APEX
star
inner wind
intermediate wind
outer wind
bow shock

Crucial role of Herschel



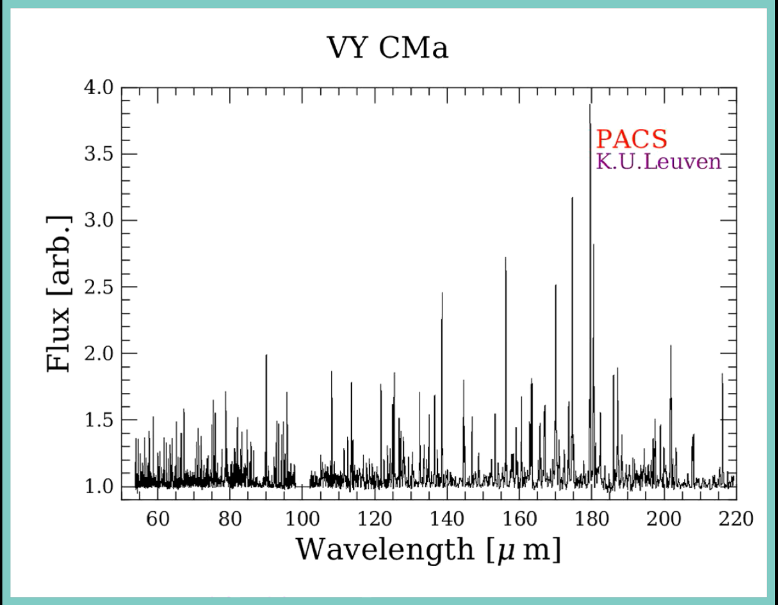
2009-2013

→ 12 molecular line transitions: ~40hr



Decin 2010

→ 930 molecular line transitions: 2hr

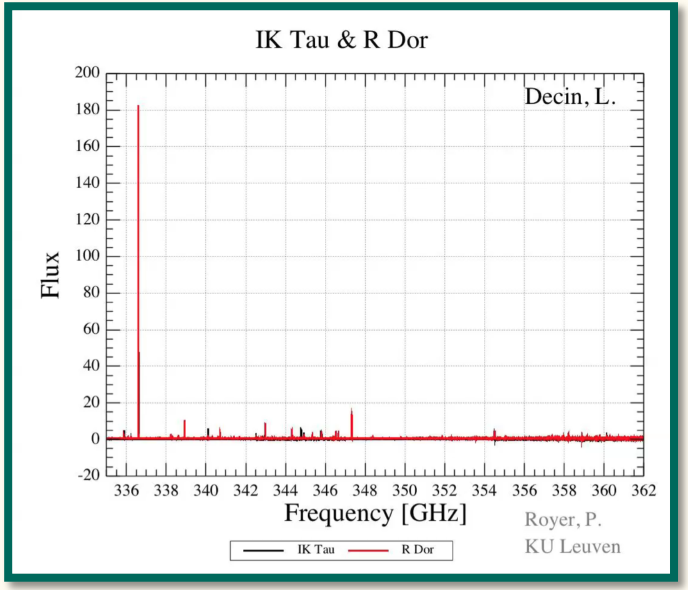


>50 targets

Royer 2010

Crucial role of ALMA

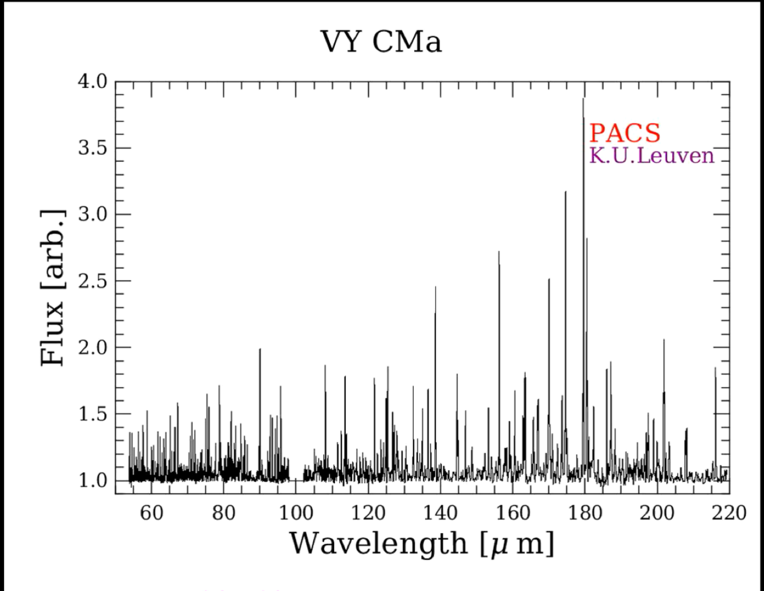
→ 100s molecular line transitions: 2Tb
spectrally resolved + channel maps



27 GHz

2009-2013

→ 930 molecular line transitions: 2hr

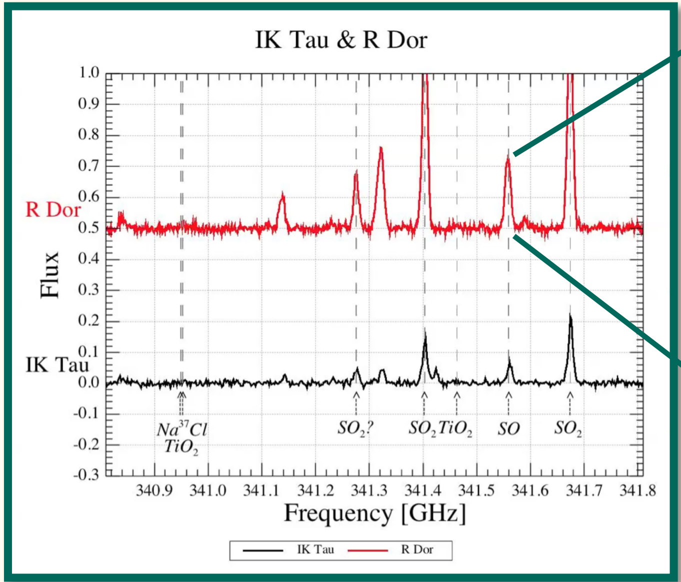


Royer 2010

>50 targets

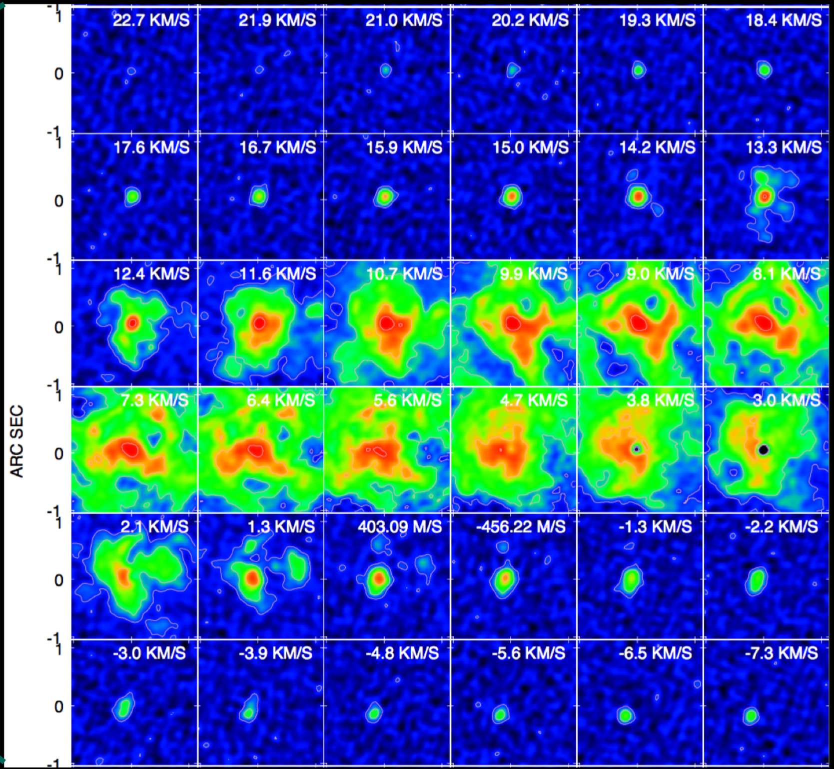
Crucial role of ALMA

→ 100s molecular line transitions: 2Tb
spectrally resolved + channel maps



27 GHz

120 x 150 mas



Decin 2017, 2018

Stellar wind: molecules

2-atoms:	AlCl	CP	NaCl	SiO
	AlF	CS	OH	SiS
	C_2	ClH	PN	SO
	CO	FH	SiC	
	CN	KCl	SiN	
3-atoms:	AlNC	FeCN	HNC	SiC_2
	C_3	HCN	KCN	SiCN
	C_2H	HCP	MgCN	SiCSi
	C_2S	H_2O	MgNC	SiNC
	CO_2	H_2S	NaCN	SO_2
4-atoms:	ℓ-C_3H	C_2H_2	HMgNC	PH_3
	C_3N	HC_2N	MgC_2H (?)	SiC_3
	C_3O	H_2CO	NC_2P (?)	
	C_3S	H_2CS	NH_3	
5-atoms:	C_5	c-C_3H_2	CH_2NH	H_2C_3
	C_4H	CH_2CN	HC_3N	HNC_3
	C_4Si	CH_4	HC_2NC	SiH_4
6-atoms:	C_5H	C_5S	CH_3CN	H_2C_4
	C_5N	C_2H_4	HC_4N	SiH_3CN (?)
≥7-atoms:	C_6H	CH_2CHCN	HC_7N	
	C_7H	CH_3CCH	HC_9N	
	C_8H	HC_5N	H_2C_6	
Ions:	C_4H^-	C_6H^-	C_8H^-	HCO^+
	CN^-	C_3N^-	C_5N^-	

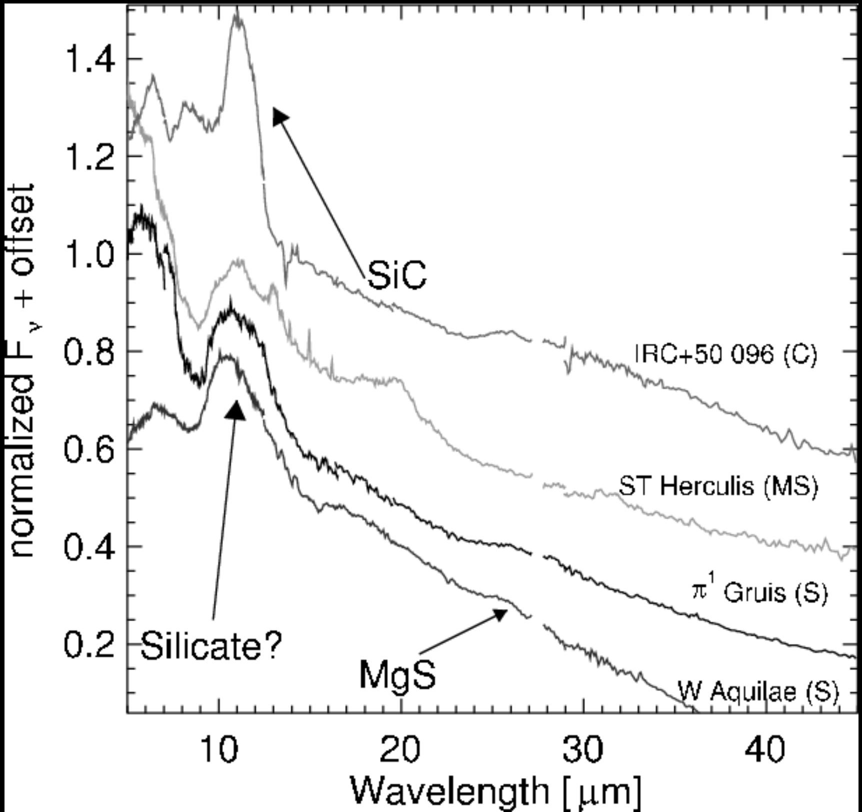
88 (>100) molecules

↓

70 –C–

Olofsson

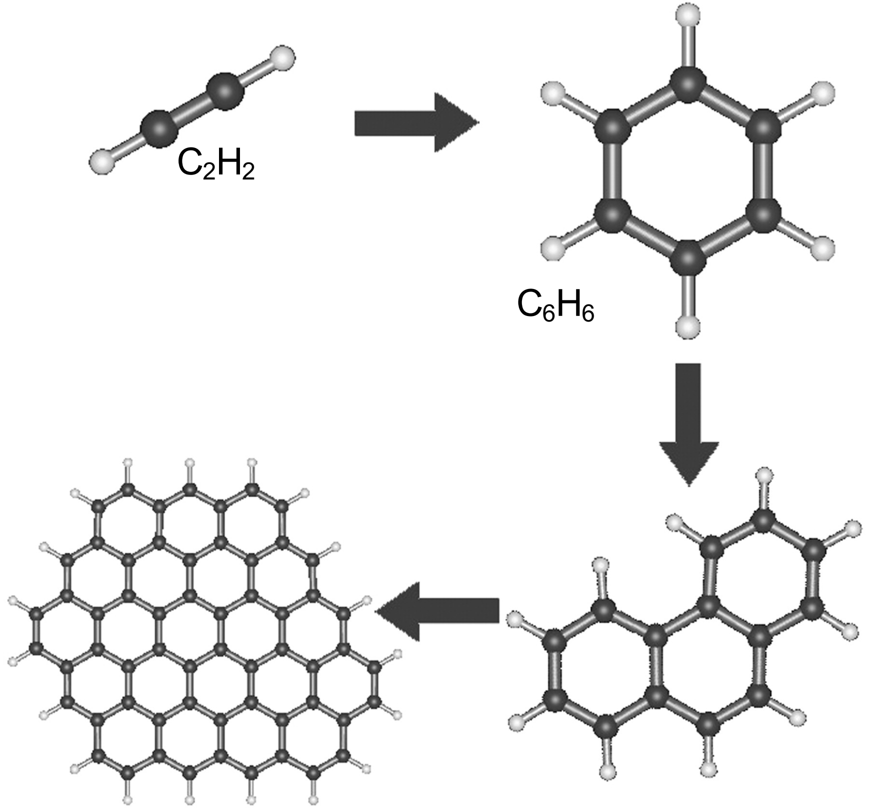
Stellar wind: dust



Hony 2009

Carbon-rich grains

C/O>1



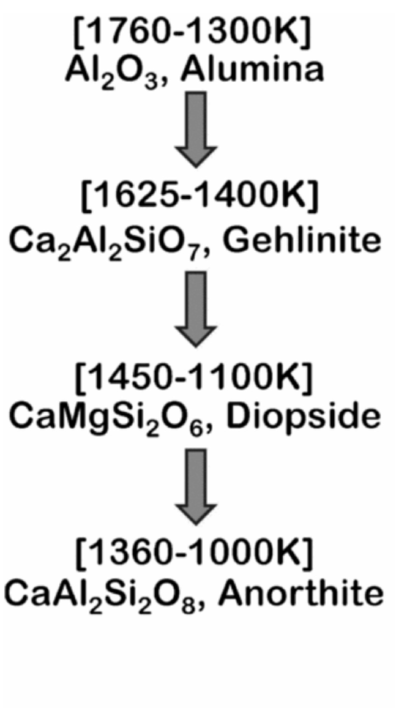
Cherchneff 2010
Ehrenfreund 2011

O-rich grains: 2 condensation sequences

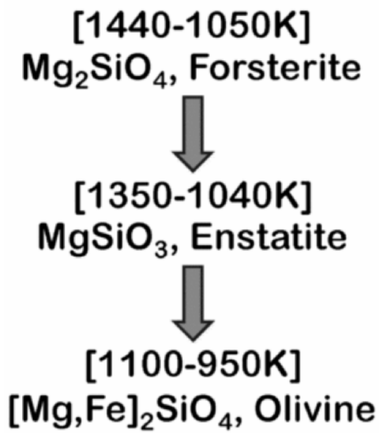
C/O<1

Tielens 1998

Al-oxides

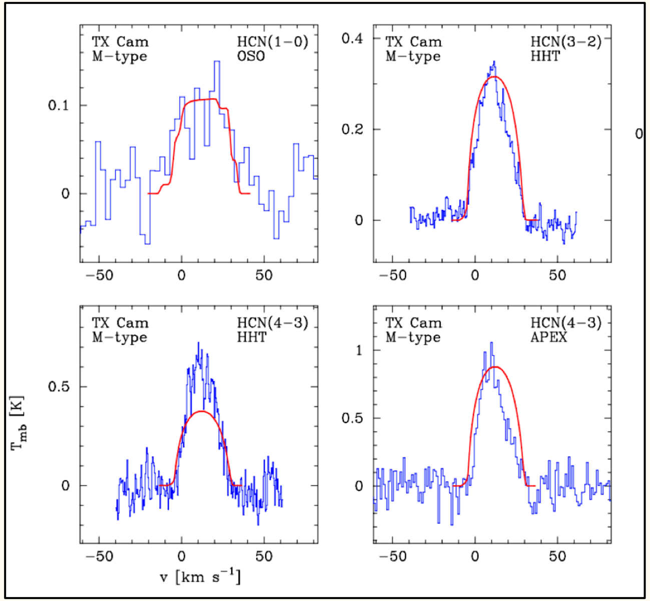


silicates



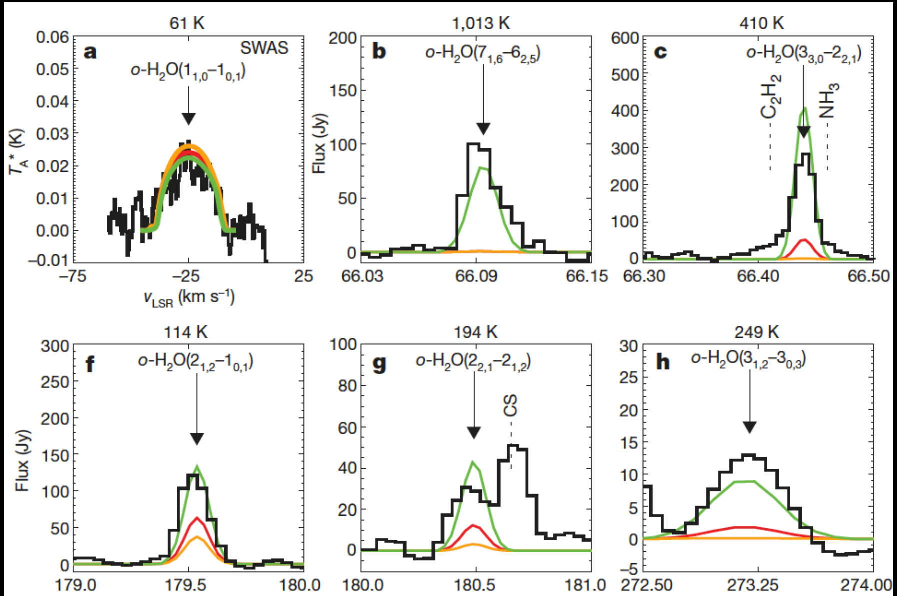
Chemical surprises

HCN@O-rich



Schöier 2013

H_2O@C-rich

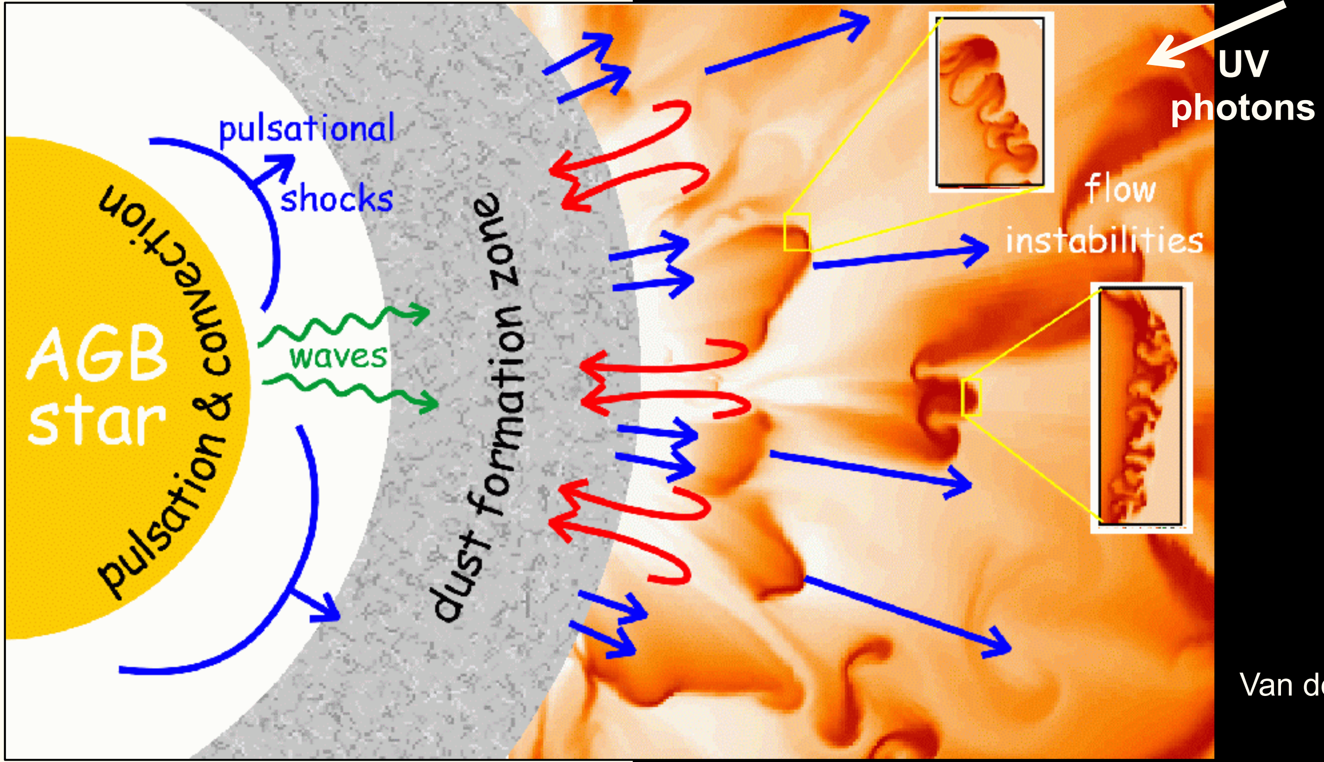


Decin 2010

Chemical surprises

Non-equilibrium chemistry due to pulsation-induced shocks

Photochemistry in a clumpy medium



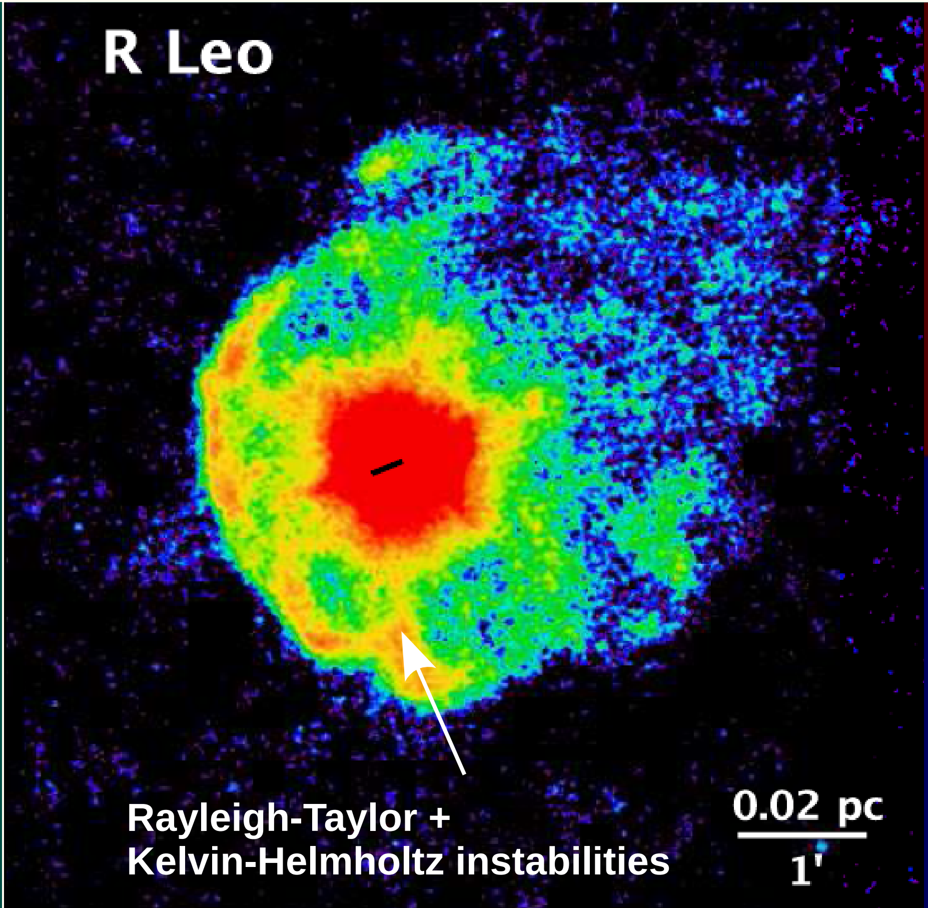
Cherchneff, Gobrecht

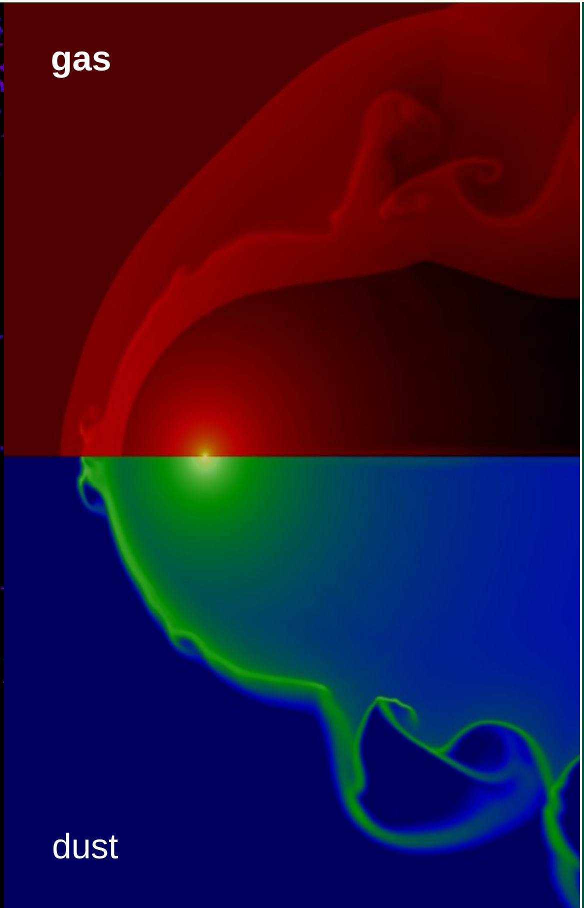
Van de Sande, Agúndez

Part III - Enrichment of the interstellar medium

Bow shocks

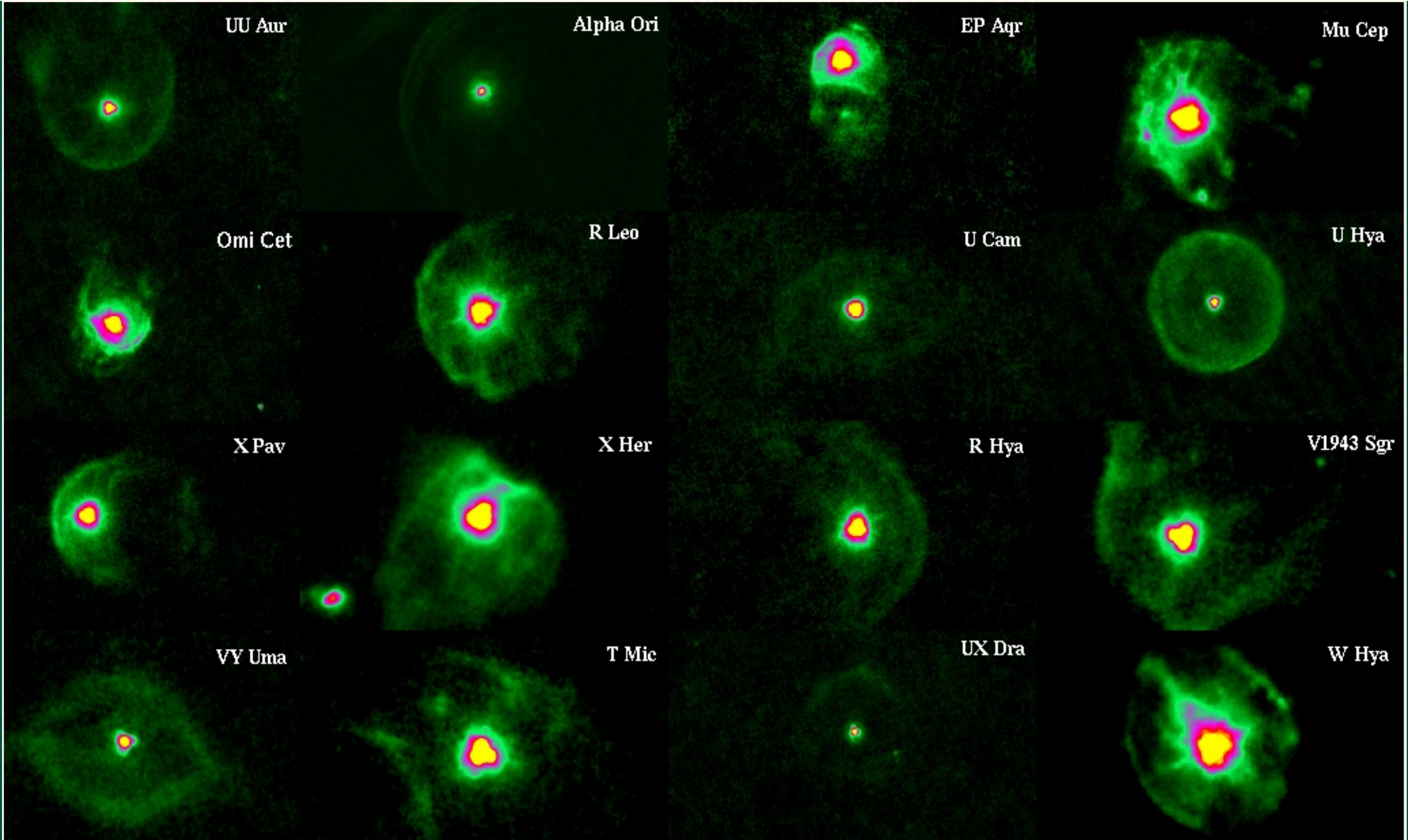
Bow shocks: interaction wind - ISM





Cox 2012

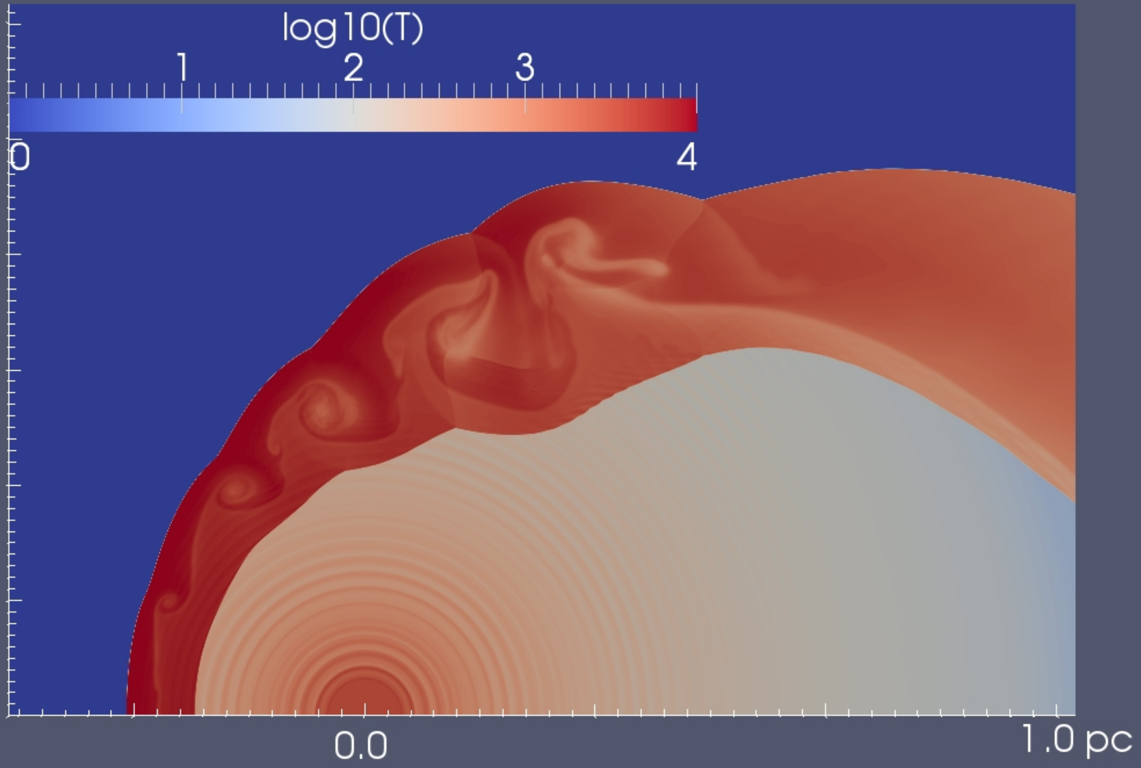
Bow shocks: interaction wind - ISM



Cox 2012

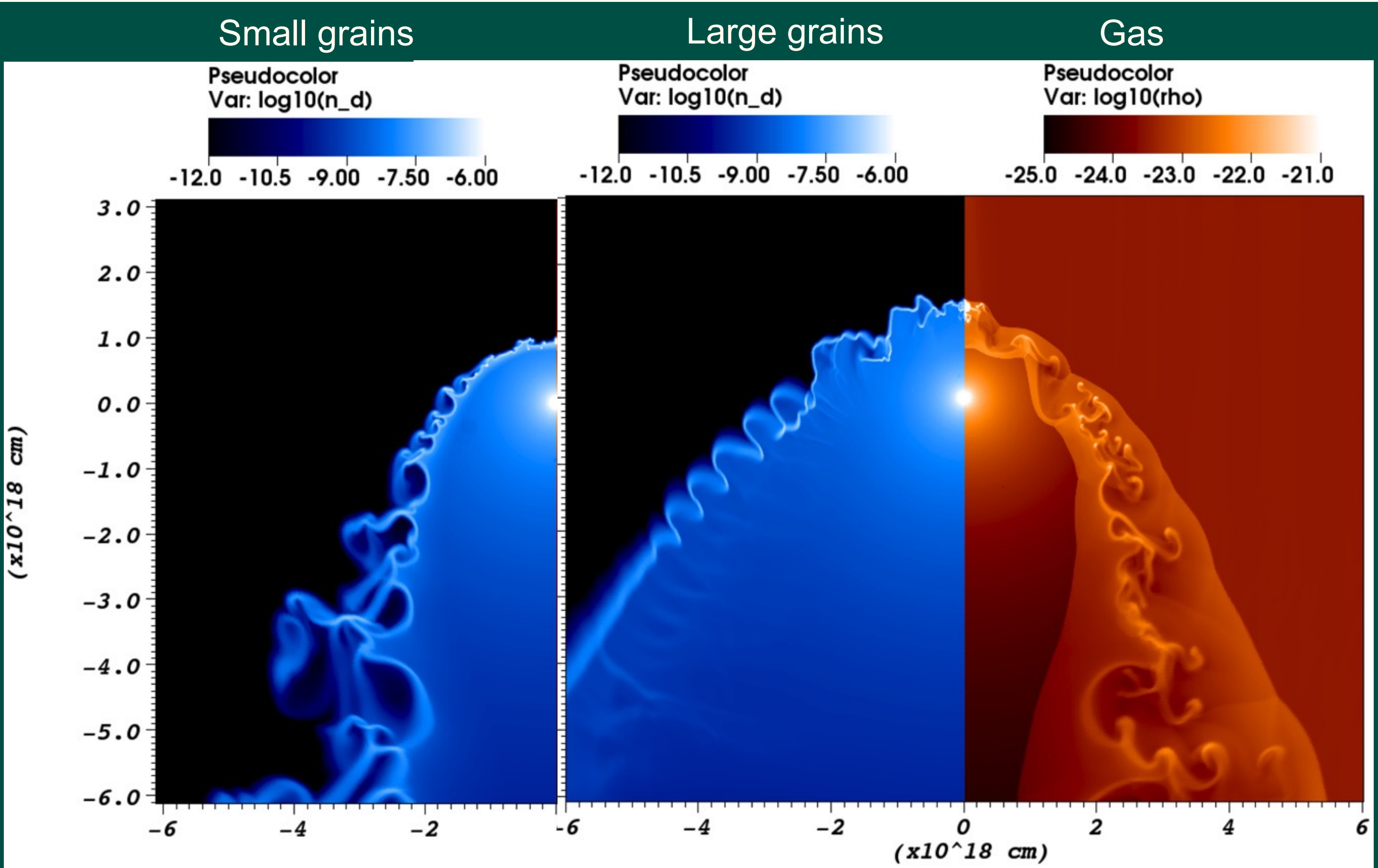
Bow shocks: interaction wind - ISM

gas temperature



Van Marle, 2012

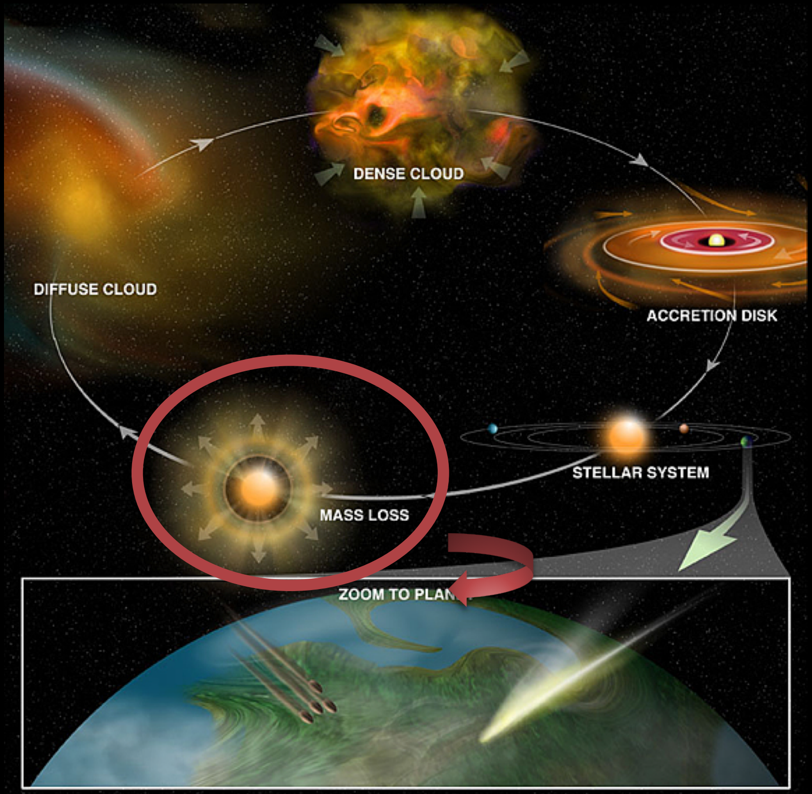
Bow shocks: interaction wind - ISM



Van Marle, 2012

Interstellar budget

Our life: thanks to old stars



STELLAR WIND

- ✓water (H, O)
- ✓muscles (C)
- ✓sand (Si)
- ✓atmosphere (N,O)

- ✓molecules
- ✓dust

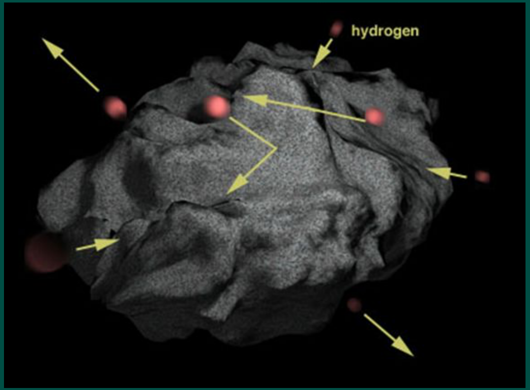
→ **unique E.T. chemical labs**

Interstellar budget: H_2

A + B → AB (+M)

$H + H \rightarrow H_2$

surface of dust grains



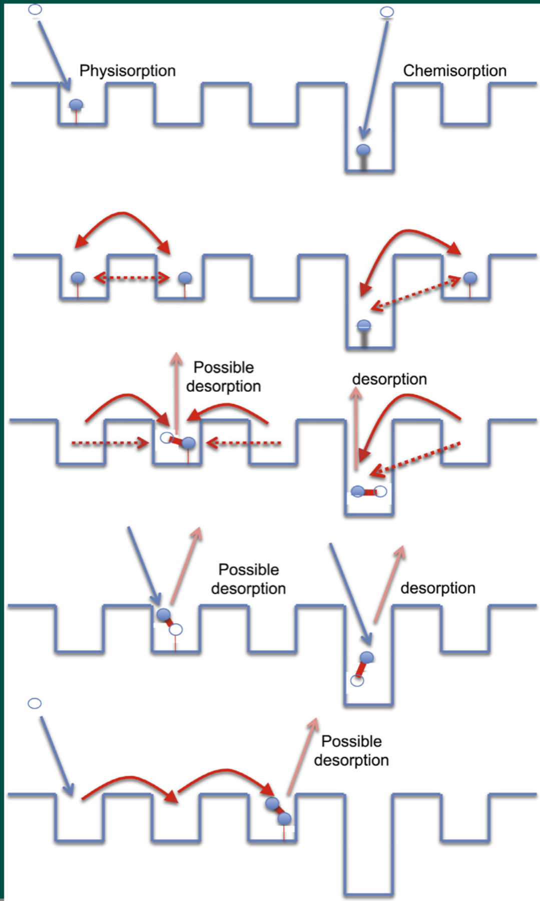
sticking

diffusion

Langmuir-Hinshelwood mechanism

Eley-Rideal mechanism

‘hot atom’ mechanism



Wakelam 2017

Part IV -
The quest of dust nucleation

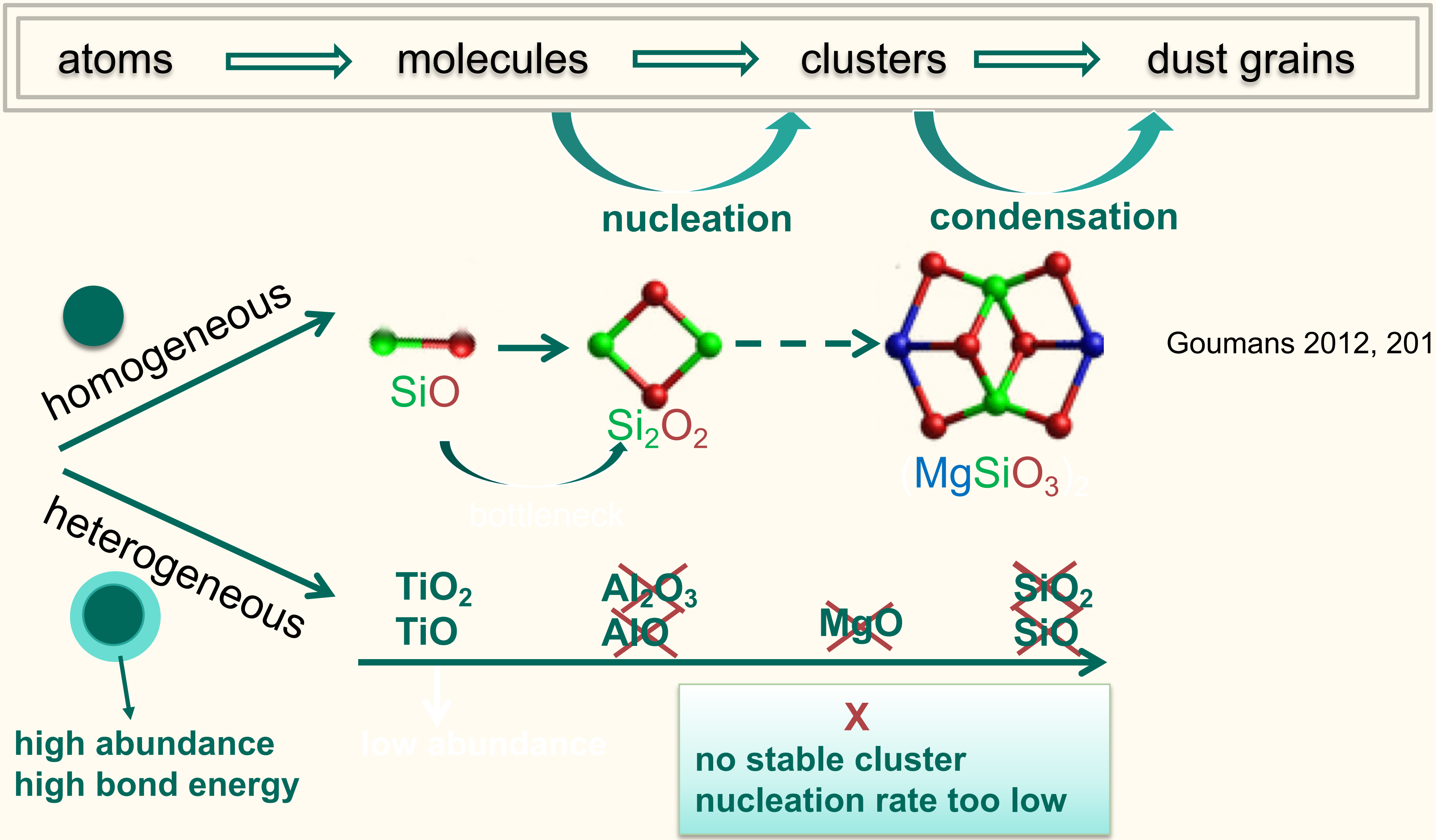
Oxygen-rich winds

Why?

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

ATOMIUM

Corundum – Conundrum
Setting the stage

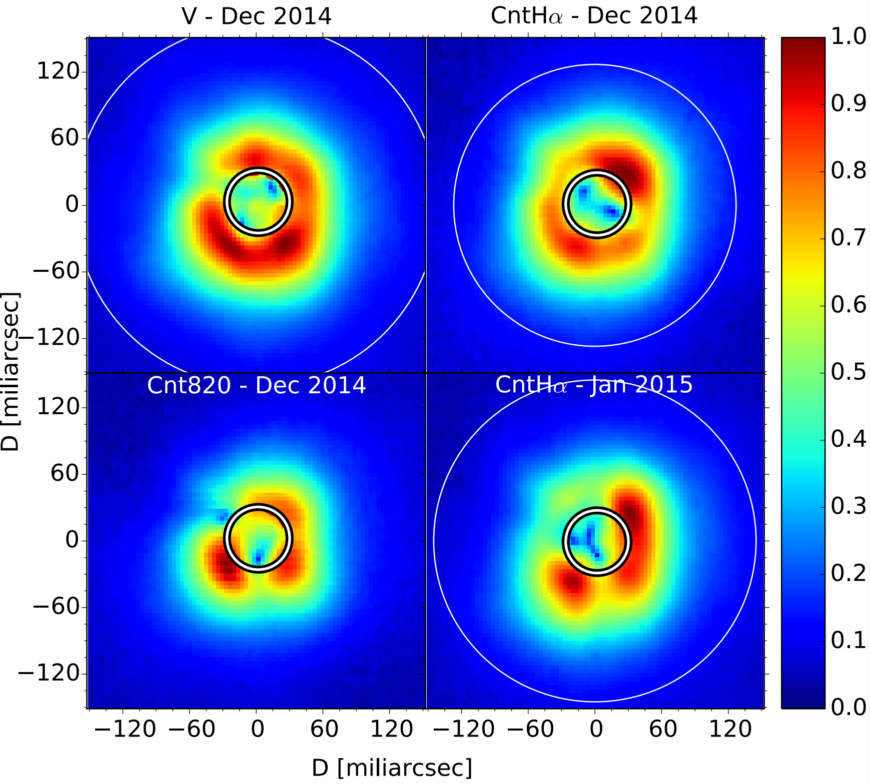


Goumans 2012, 2013

Corundum – Conundrum Observations

Dust grains in R Dor

Norris 2012, Khouri 2016



→ Large (300 nm) grains at 0.5 R_*

- Composition?
  Fe-free silicates or Al_2O_3

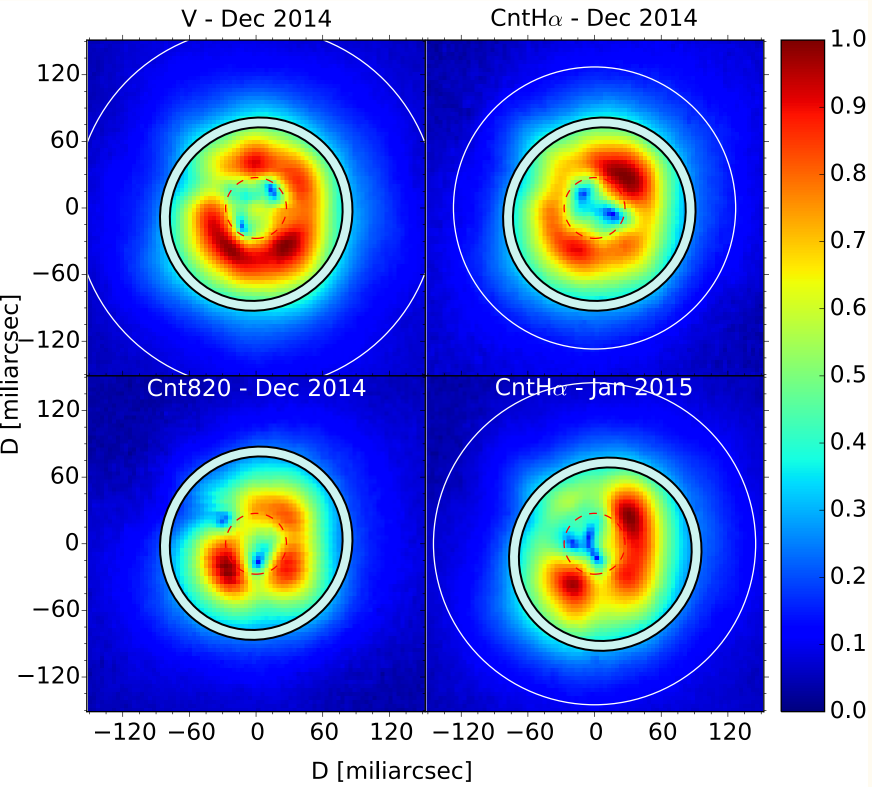
◯ = stellar surface

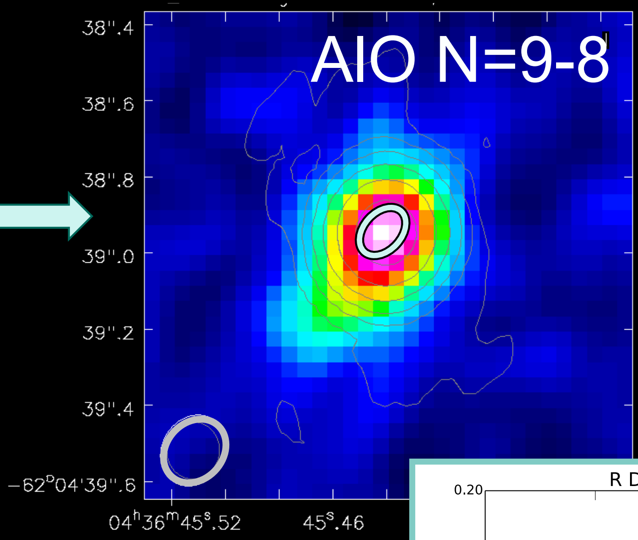
Dust grains

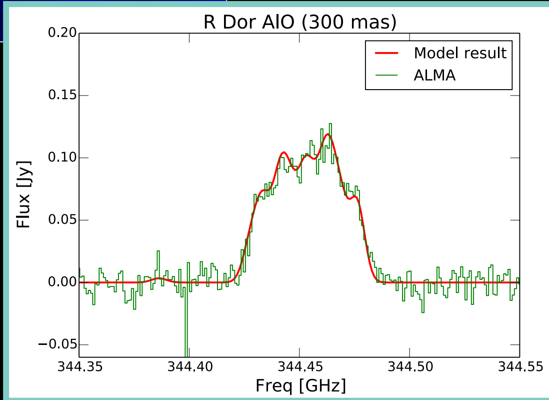
Al-bearing molecules

AlO, (AlOH), AlCl

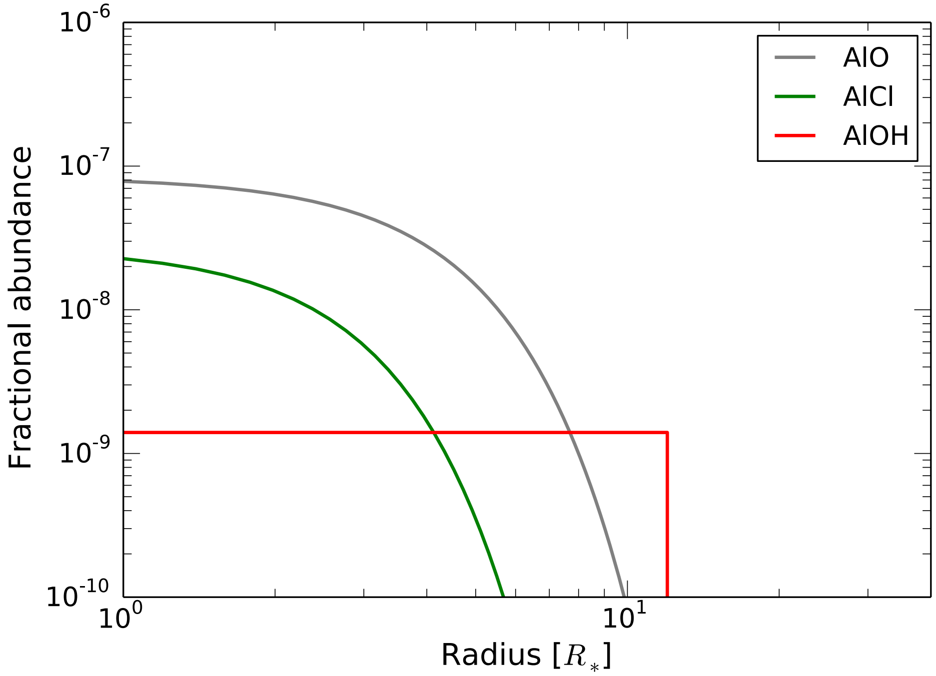
Norris 2012, Khouri 2016







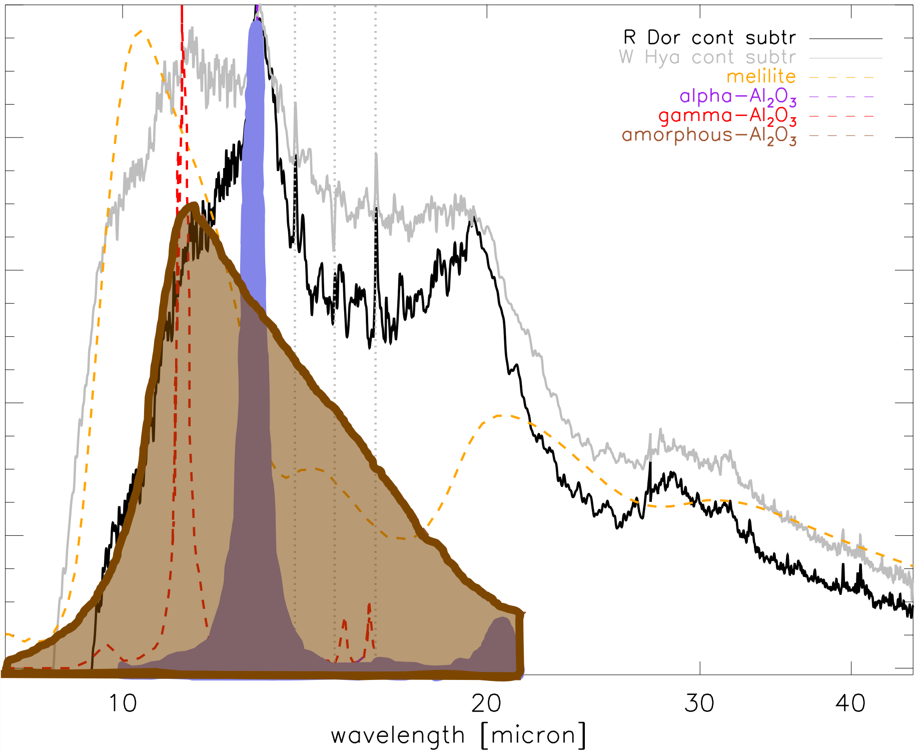
Al-bearing molecules



→ **$\lesssim$2% Al**

- Room for Al-bearing grains

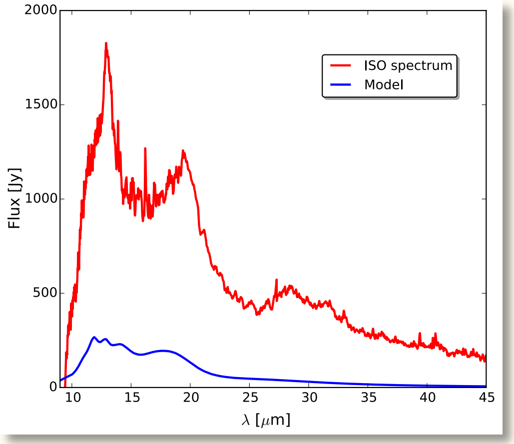
Spectral energy distribution



- Al_2O_3 grains
  - crystalline (α-Al_2O_3) + amorphous

Al_2O_3 dust grains in R Dor

Al_2O_3 emission from outflow

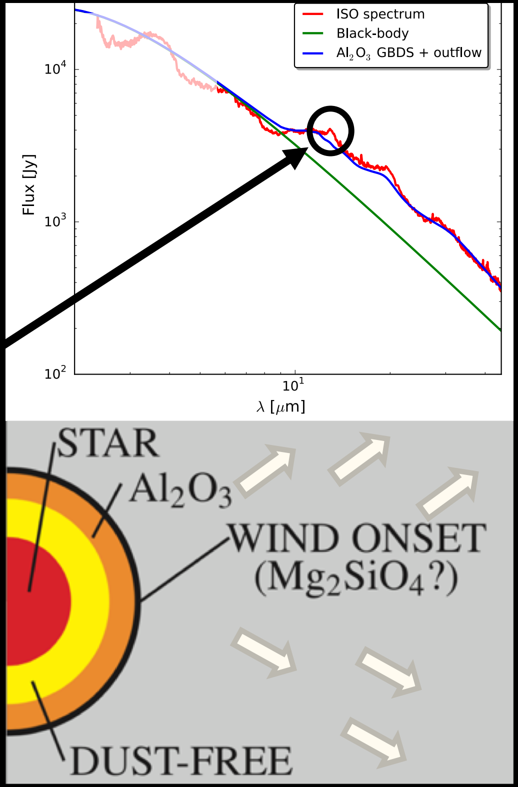


T(Al_2O_3) ~1200 – 1600K

crystalline!

11 micron feature?

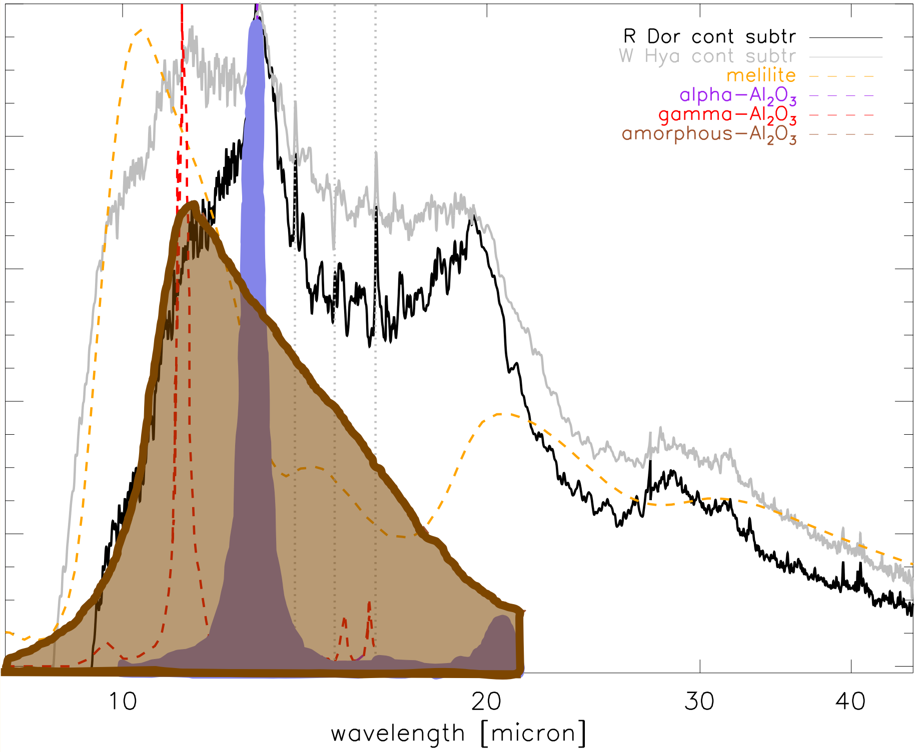
Al_2O_3 emission from GBDS+outflow

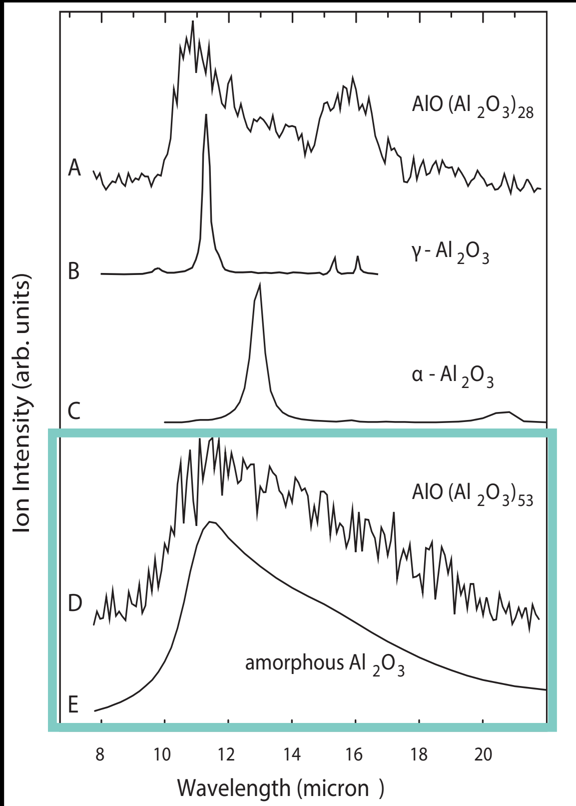


Khouri 2015

Conjecture

large clusters $(Al_2O_3)_n$ ($n \geq 34$)

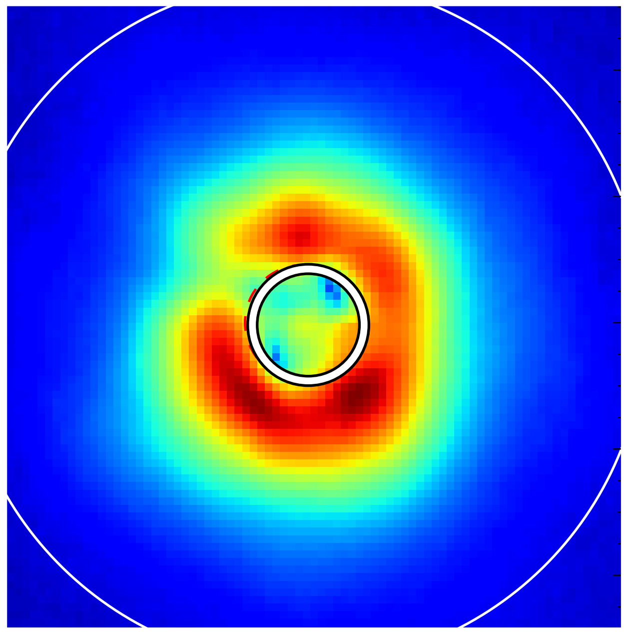




van Heijnsbergen 2003, Demyk 2004, Decin 2017

Conundrum…

Norris 2012, Khouri 2016

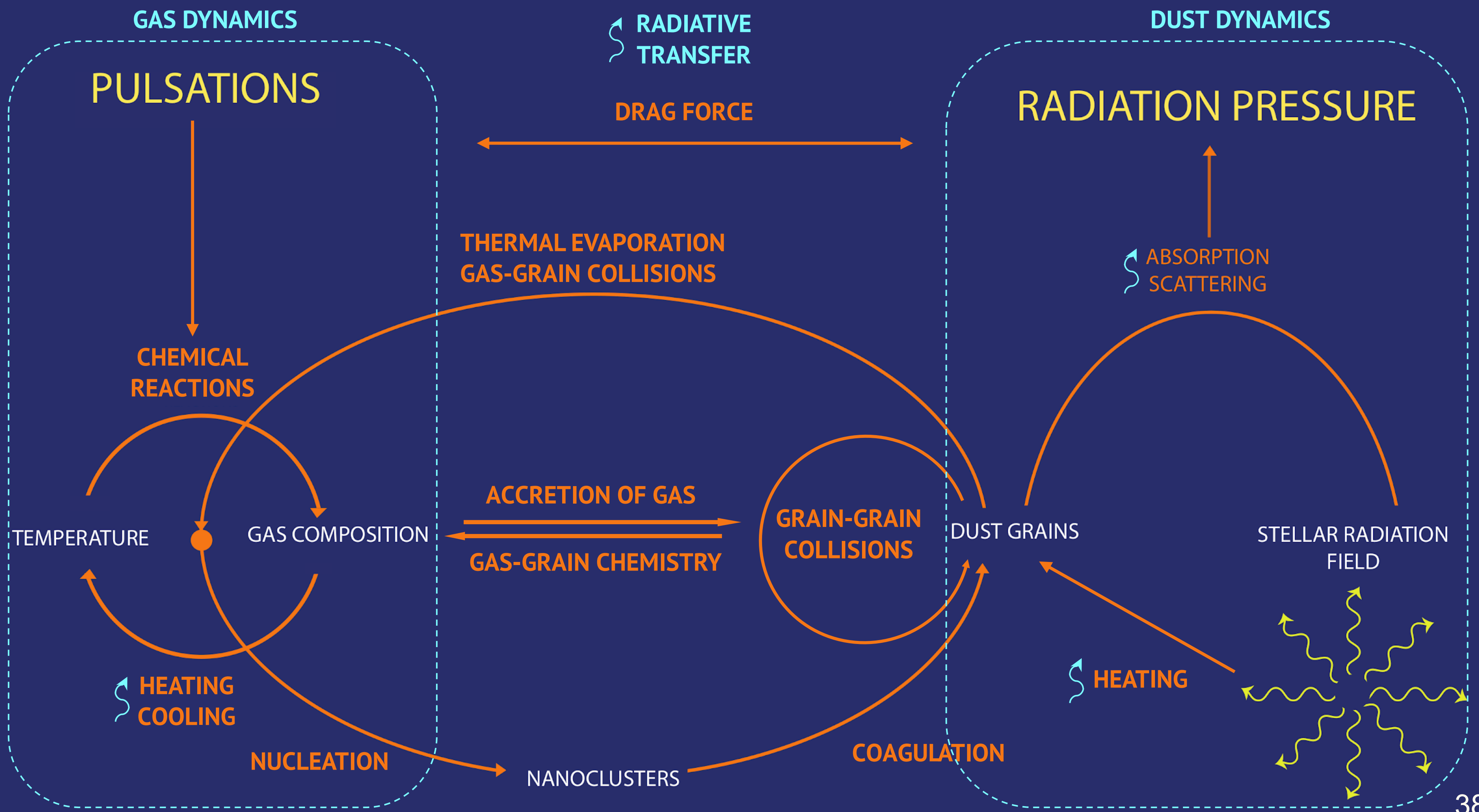


◯ = stellar surface

?

- → Large (300 nm) grains at 0.5 R_*
- → Composition: Fe-free silicates or α-Al_2O_3?
- → First condensation seeds?

Corundum – Conundrum: Theory


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
DUST GRAINS
STELLAR RADIATION FIELD
GAS-GRAIN CHEMISTRY
HEATING
COOLING
HEATING
NUCLEATION
COAGULATION
NANOCLUSTERS

Self-consistent AGB wind

Hydrochemistry

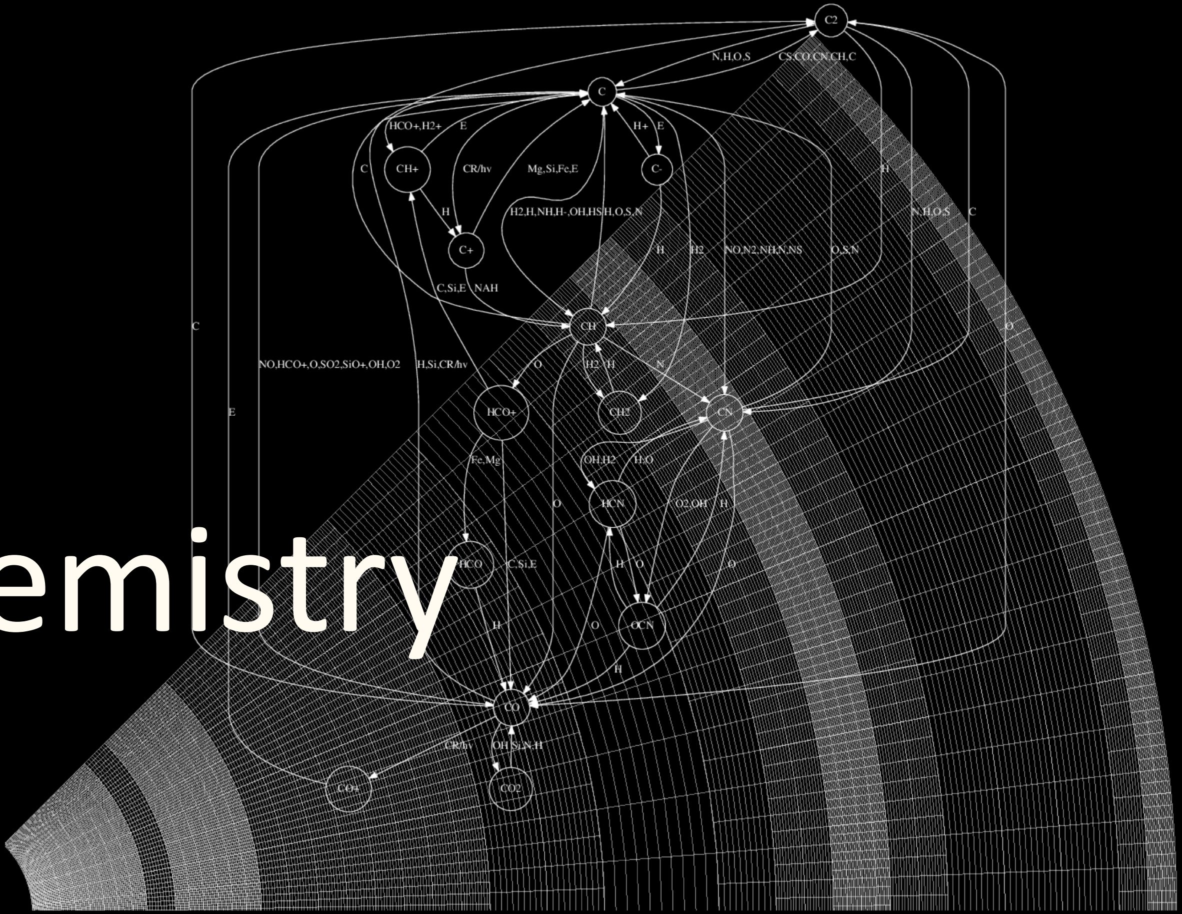
+

Nucleation theory

+

Dust evolution with radiation field

Hydrochemistry



Current chemistry

2 step improvement

Equilibrium → Non-Equilibrium Time dependent → Coupled to hydrodynamics

List of species → List of reactions → Reduced list of reactions

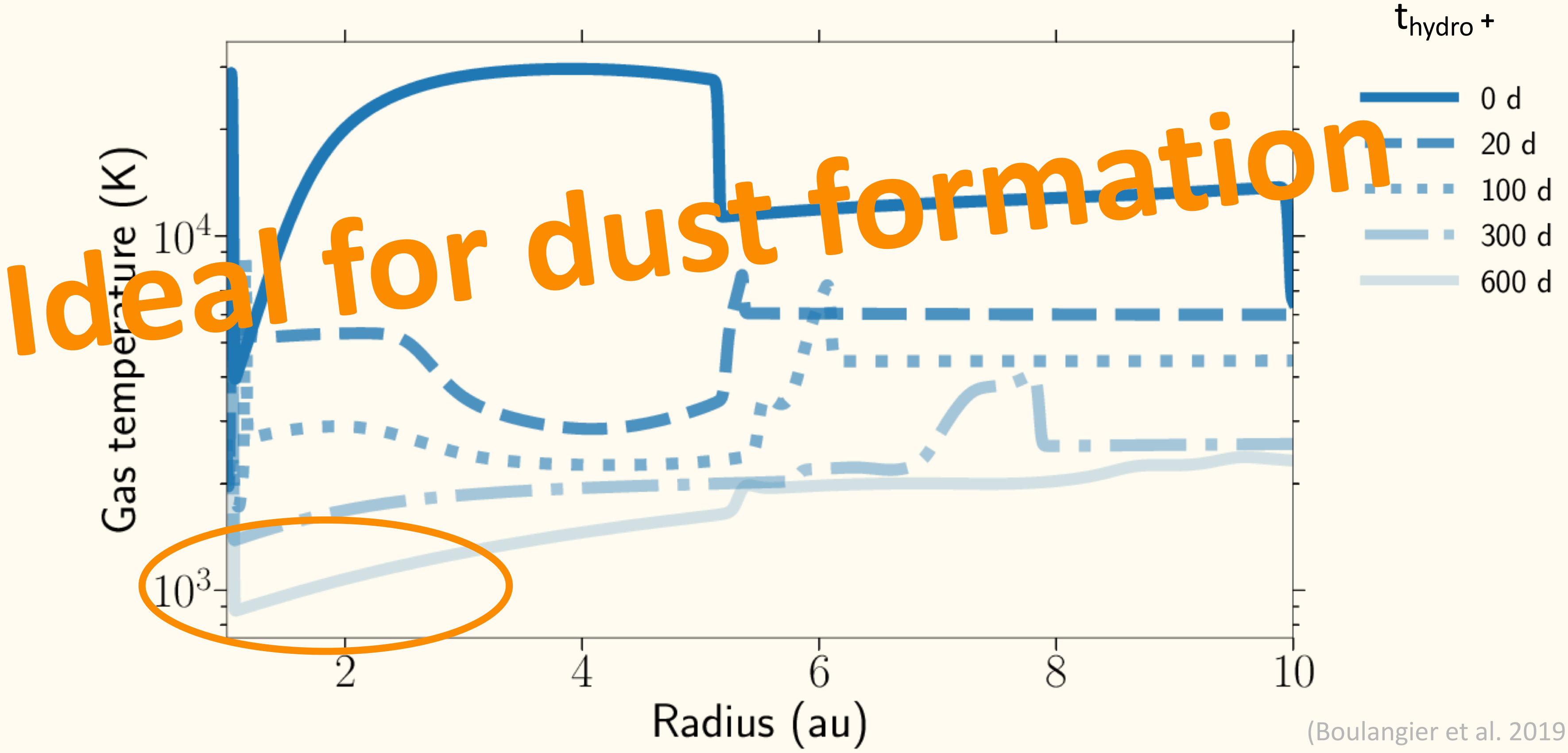
~1700 reactions
~160 species

→ **~250 reactions**
~70 species

Reduction algorithm

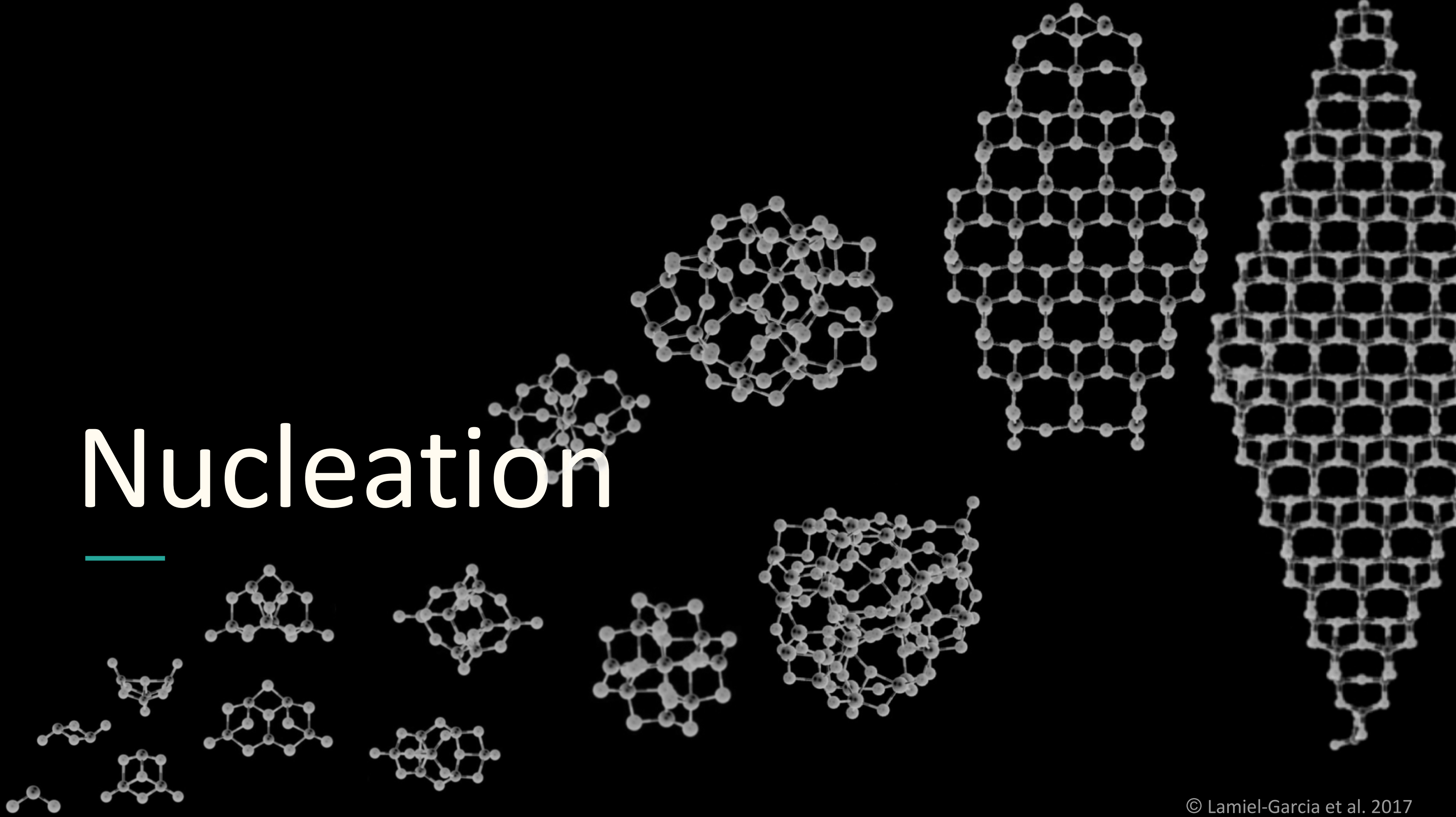
Speed-up factor ~20

Cooling is super efficient



(Boulangier et al. 2019)

Nucleation



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

Current nucleation

Steady-state

Bulk/Modified bulk/ Quantum mechanical properties

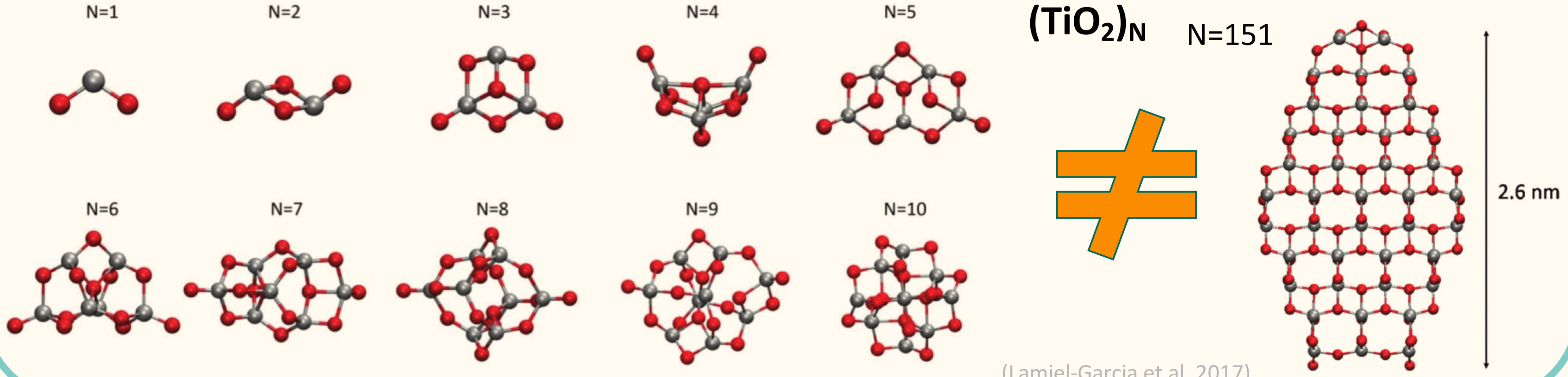
Monomer interactions

3 step improvement

Time-dependent

Quantum mechanical properties

Polymer interactions



(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

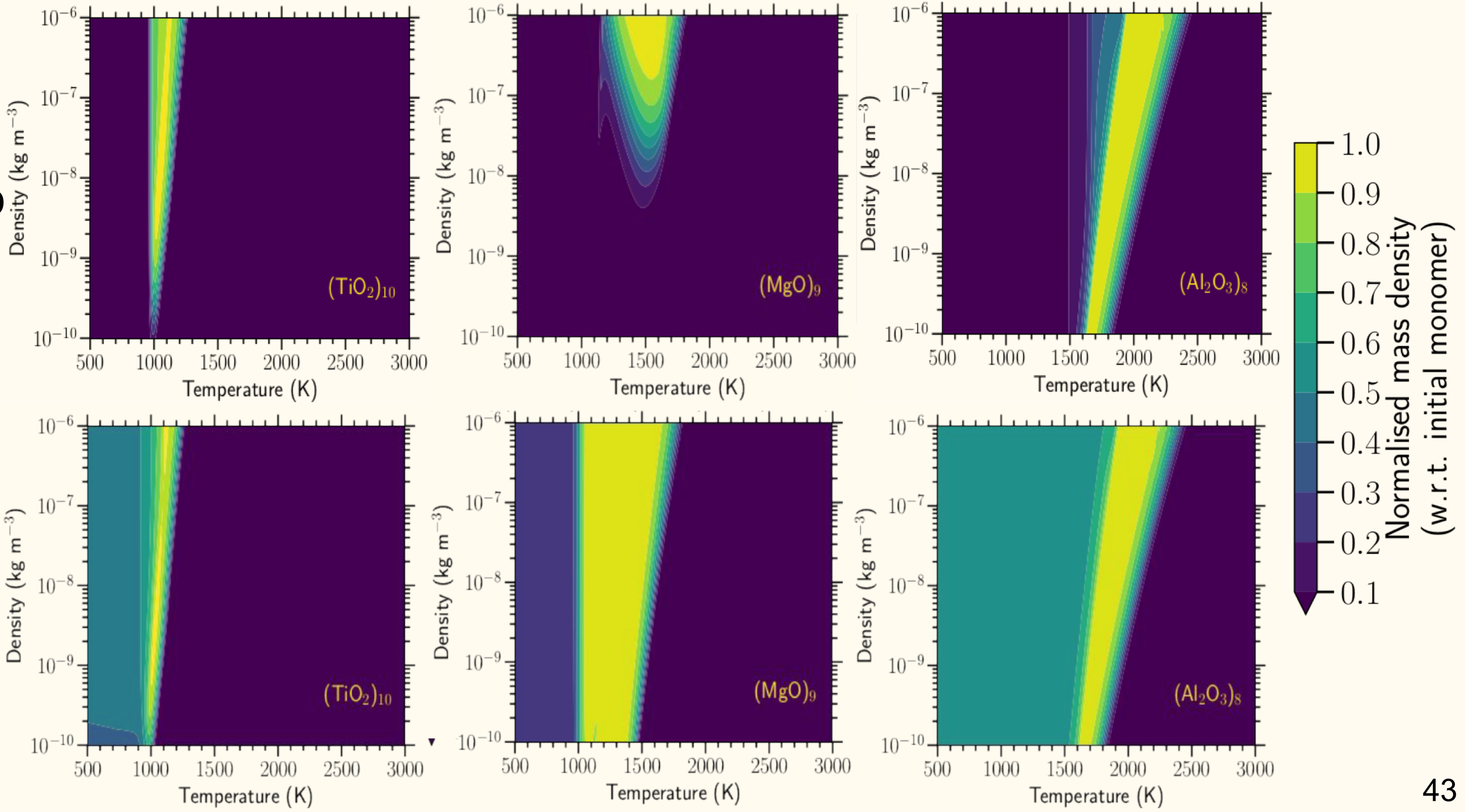
Presolar grains + High bond energies + Atomic abundances

	$(TiO_2)_N$	$(SiO)_N$	$(MgO)_N$	$(Al_2O_3)_N$
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**

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

Mono

Poly



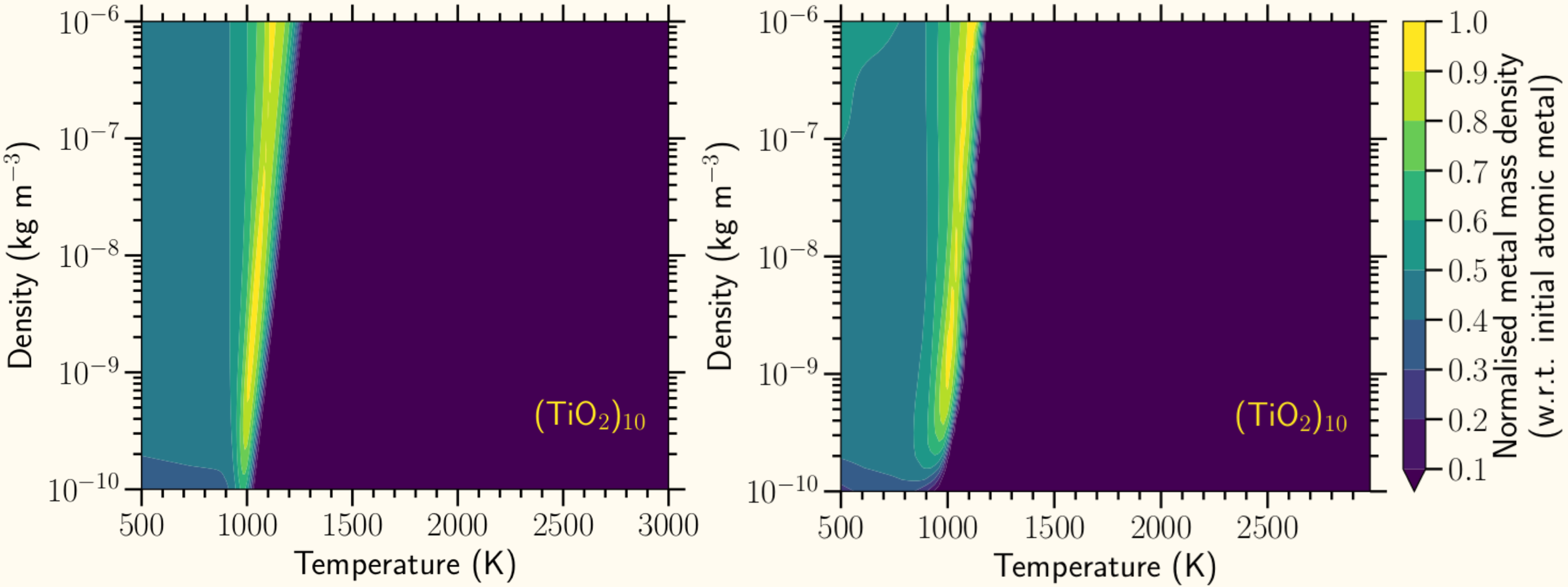
What if combined with network?

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

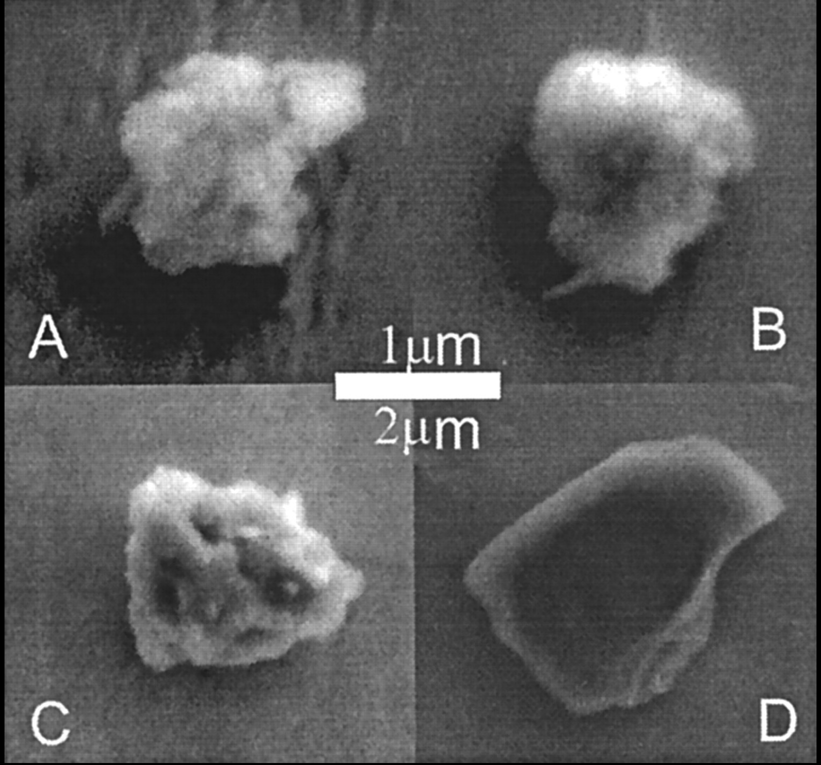
TiO_2-clusters are the best candidate

A priori TiO_2 existence

Combined in large network



Planet Earth – Meteorites



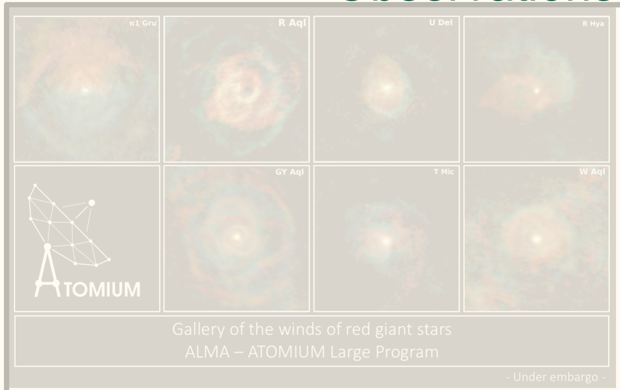
Al_2O_3-clusters are best candidate

- 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 circumvent $(Al_2O_3)_{n=1}$

Corundum = Conundrum

Future

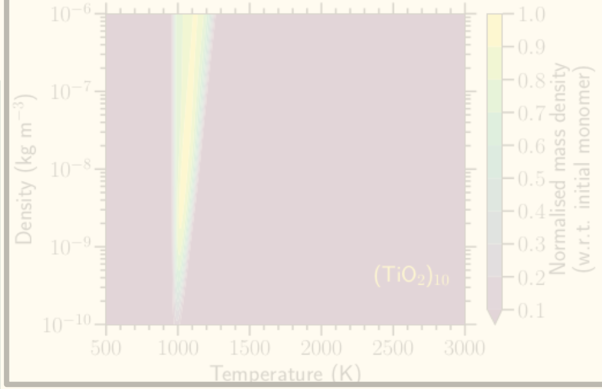
Observations

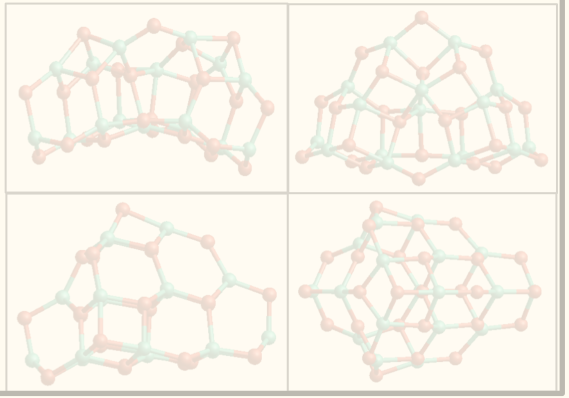


Laboratory

parsec

nanometer

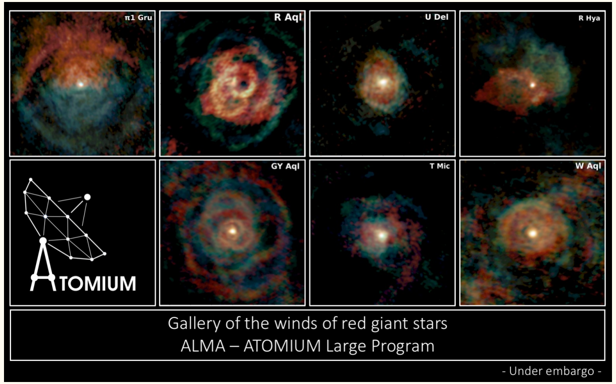




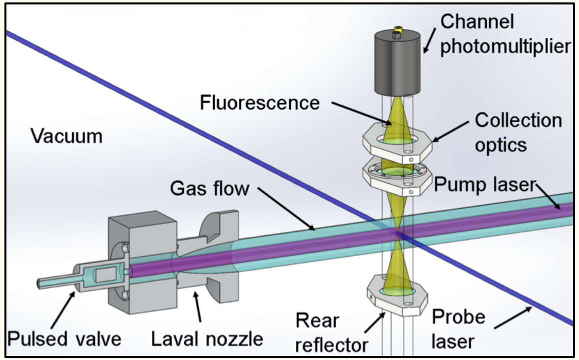
Simulations

Theory

Observations



Laboratory

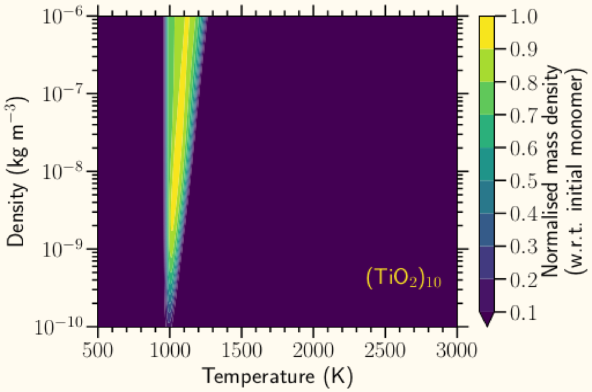


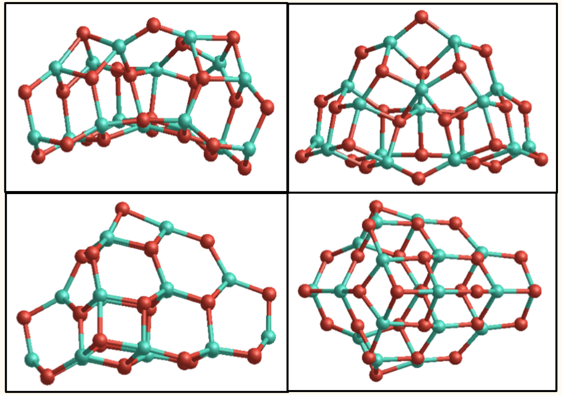
THANKS!

parsec

team

nanometer





Simulations

Theory