

# Dust formation around old stars and its feedback on the dust forming system

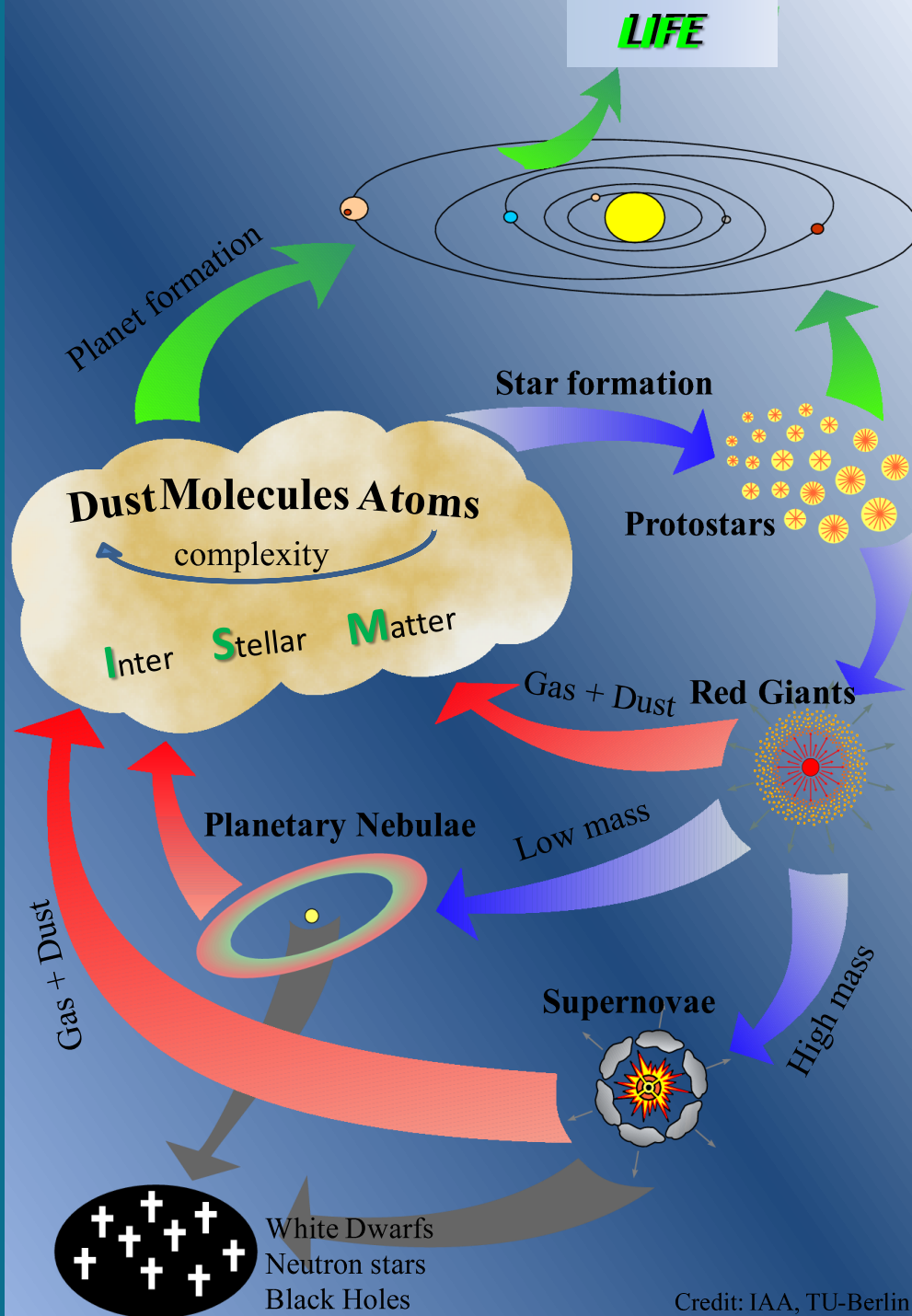


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# Necessary conditions for dust formation

- **suitable chemistry**  $\Rightarrow$  **condensing species (high-T condensate)**
- **„low“ temperature**  $\Rightarrow$  **stable clusters**
- **„high“ density**  $\Rightarrow$  **growth to macroscopic grains**

$\Rightarrow$  **Stellar sources of interstellar dust**

**Asymptotic Giant Branch stars**  
**Red Giant Branch stars, Red Supergiants**  
**ejecta of Supernovae and Novae**  
**Wolf-Rayet stars, RCrB stars**

**(also Brown Dwarfs, but the material is not injected to the ISM)**

# Two different approaches to describe dust formation

## nucleation theory

### Kinetic nucleation theory

Critical cluster

Moment equations

=>

**Possibility to construct self-consistent dust shell models**

Ex: Gail, Gauger, Patzer, Sedlmayr, Winters, Woitke

Dorfi, Feuchtinger, Höfner

## non-equilibrium chemistry

### Chemical pathway

Critical reaction

Rate network

=>

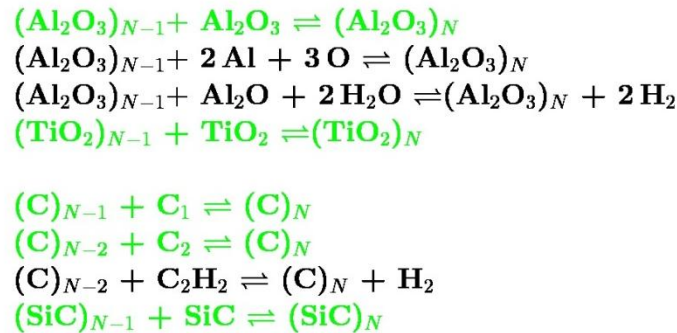
**Possibility to construct complex non-equilibrium chemical models under prescribed thermodynamical conditions**

Ex: Cherchneff, Gobrecht, Plane

# Dust formation

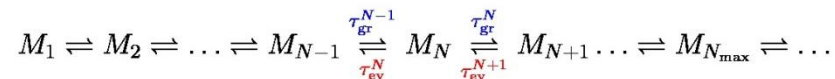
is a chemical process

E.g.:



...

Most simple case: **monomer addition**, linear chain,  $M_1$  is the monomer, e.g.,  $\text{Al}_2\text{O}_3$ ,  $\text{TiO}_2$ ,  $\text{C}_1$ ,  $\text{SiC}$ :  
 (heteromolecular processes: Gail & Sedlmayr 1988, A&A 206, 153,  
 chemical non-equilibrium: Patzer et al. 1998, A&A 337, 847)



Growth time scale:

$$\frac{1}{\tau_{\text{gr}}^{N-1}} = f_1 v_{N-1,1}^{\text{rel}}(T_g) A(N-1) \alpha(M_1, N-1, T_g, T_d(N-1))$$

Evaporation time scale:

$$\frac{1}{\tau_{\text{ev}}^N} = A(N) \beta(T_d(N))$$

# Stability

Thermodynamic equilibrium (phase equilibrium, thermal equilibrium ( $T_g = T_d$ ), chemical equilibrium, denoted by  $\circ$ ):

Detailed balance

$$\frac{1}{\tau_{ev}^{\circ N}} = \frac{1}{\tau_{gr}^{\circ N-1}}$$

$\Rightarrow$

$$\frac{1}{\tau_{ev}^{\circ N}} = f_1 v_{N-1,1}^{\circ \text{rel}}(T_d) A(N-1) \hat{\alpha}(T_d, T_d)$$

$\Rightarrow$

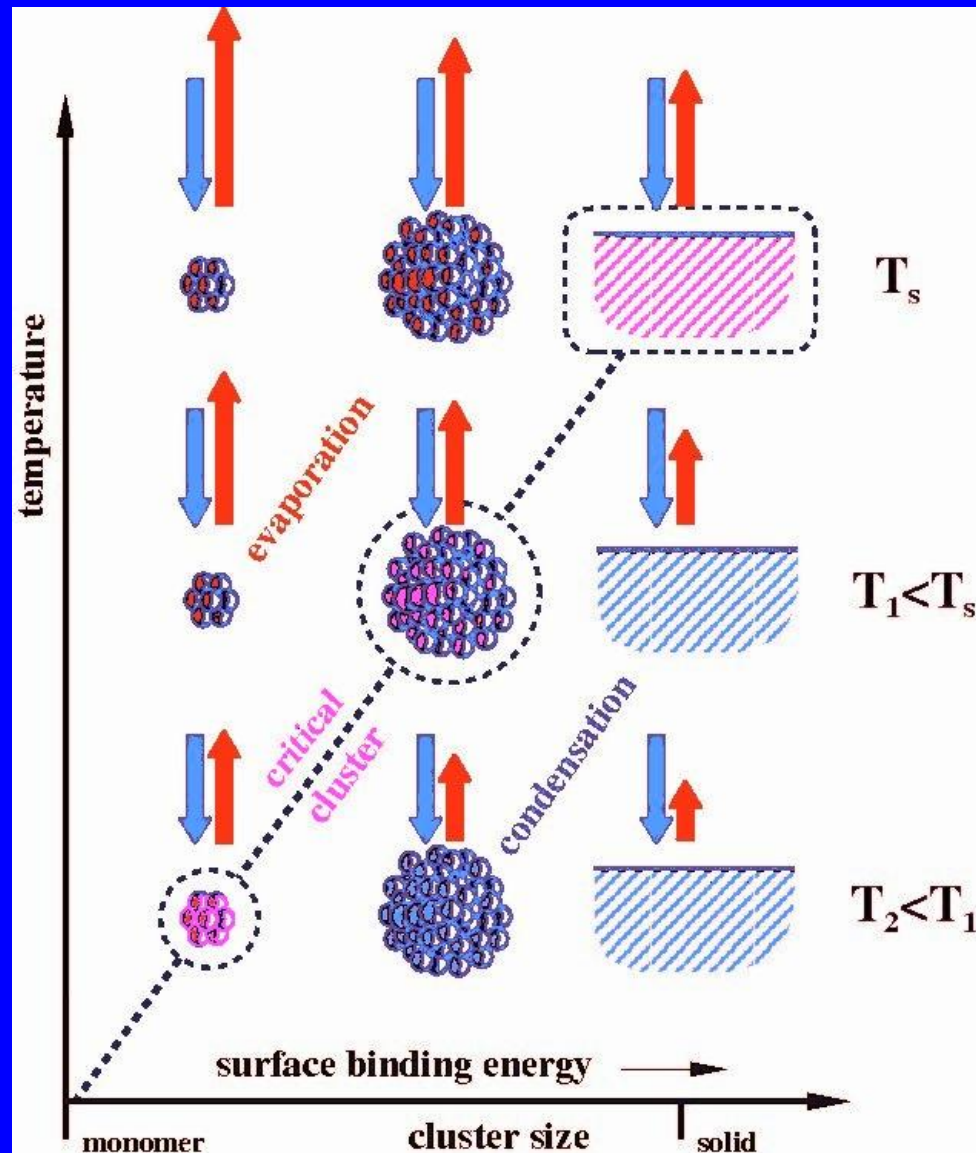
Net growth rate:

$$\begin{aligned} \frac{1}{\tau} &= \frac{1}{\tau_{gr}^{\circ N-1}} - \frac{1}{\tau_{ev}^{\circ N}} = \frac{1}{\tau_{gr}^{\circ N-1}} \left[ 1 - \frac{p_{\text{vap}}(T_d) v_{N-1,1}^{\circ \text{rel}}(T_d) \hat{\alpha}(T_d, T_d)}{f_1 k T_d v_{N-1,1}^{\text{rel}}(T_g) \alpha(T_g, T_d)} \right] \\ &= \frac{1}{\tau_{gr}^{\circ N-1}} \left[ 1 - \frac{1}{S} \frac{1}{b_{\text{therm}}} \frac{1}{b_{\text{chem}}} \right] \end{aligned}$$

$$S = \frac{f_1^{\text{CE}} k T_g}{p_{\text{vap}}(T_g)}, \quad b_{\text{therm}} = \frac{p_{\text{vap}}(T_g) T_g v_{N-1,1}^{\circ \text{rel}}(T_d) \hat{\alpha}(T_d, T_d)}{p_{\text{vap}}(T_d) T_d v_{N-1,1}^{\text{rel}}(T_g) \alpha(T_g, T_d)}, \quad b_{\text{chem}} = \frac{f_1}{f_1^{\text{CE}}}$$

$$S b_{\text{therm}} b_{\text{chem}} \begin{cases} > 1 : \text{net growth} \\ = 1 : \text{stable} \\ < 1 : \text{net evaporation} \end{cases}$$

# Critical cluster



Credit: A. Goeres

# Two-step process

Nucleation barrier at the *critical cluster* of size  $N_*(T)$  ( $O(10)$ )  
separating the *nucleation regime* from the *growth regime*

high supersaturation ratios are required

⇒ Dust formation can be conceived as a two-step process:

1. **Formation of the critical cluster (“nucleation”)**

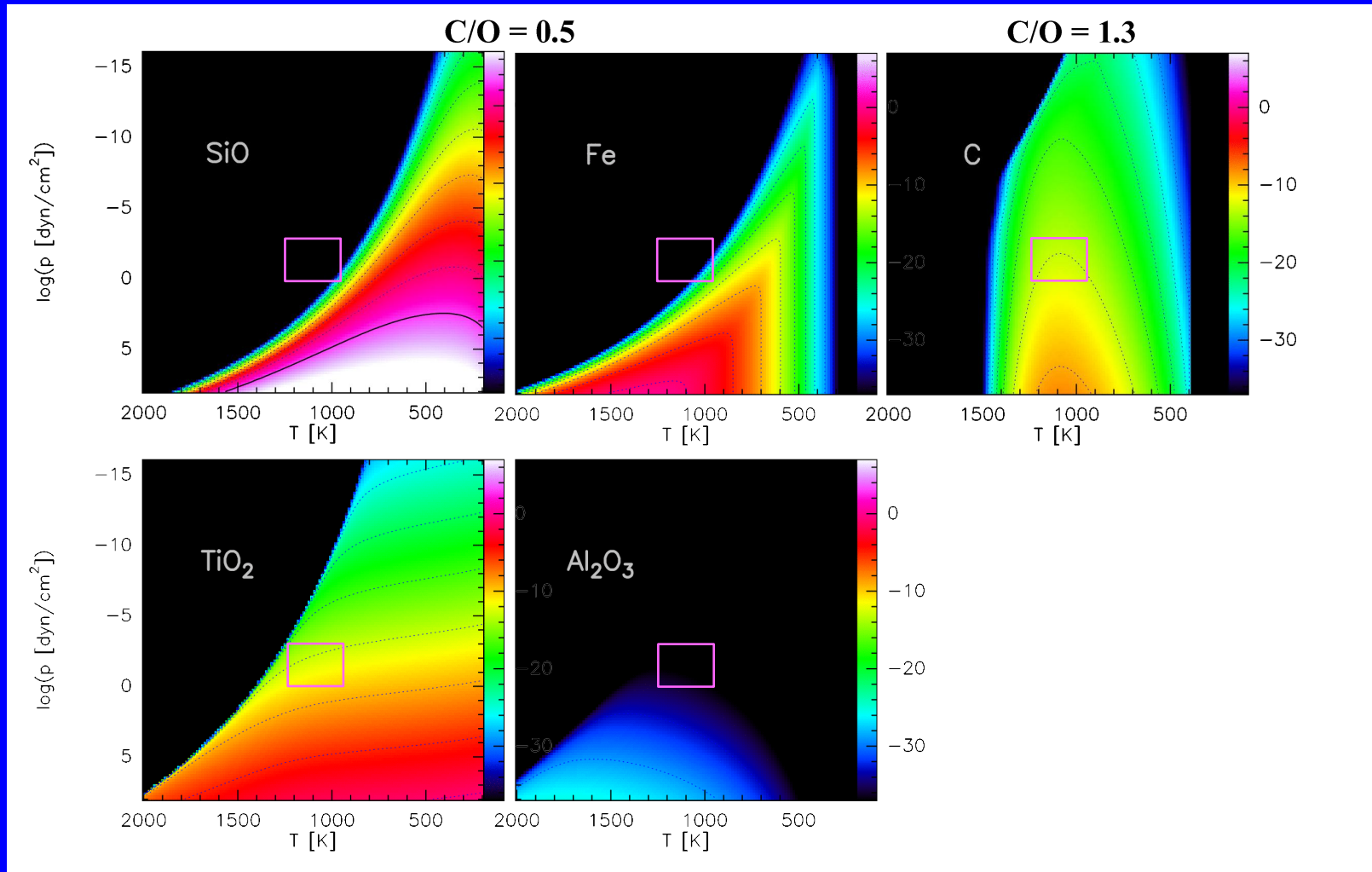
- Stationary process in circumstellar dust shells
- Properties of the clusters have to be known

2. **Growth of these clusters to macroscopic grains**

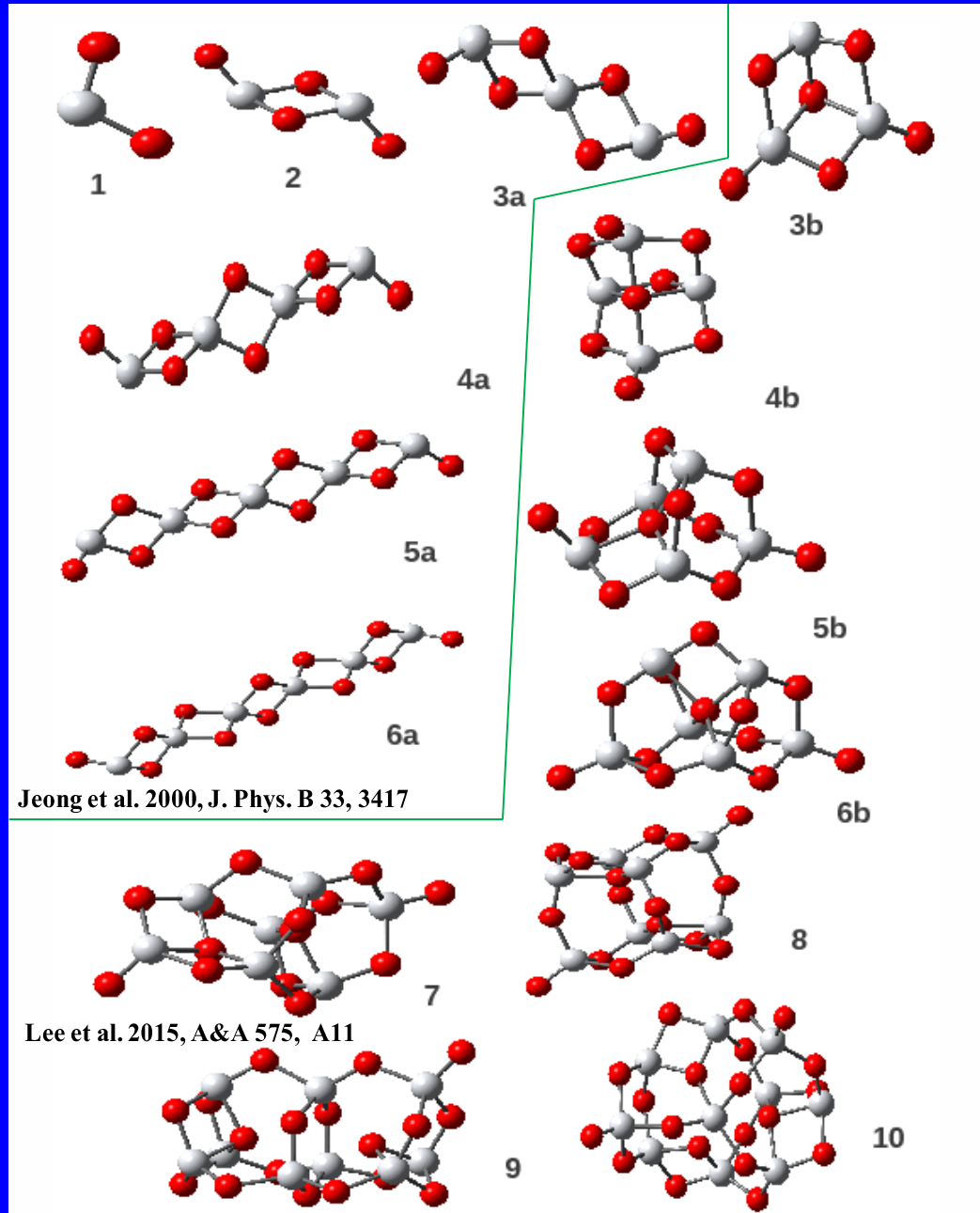
- Time dependent treatment necessary
- Thermodynamic description appropriate



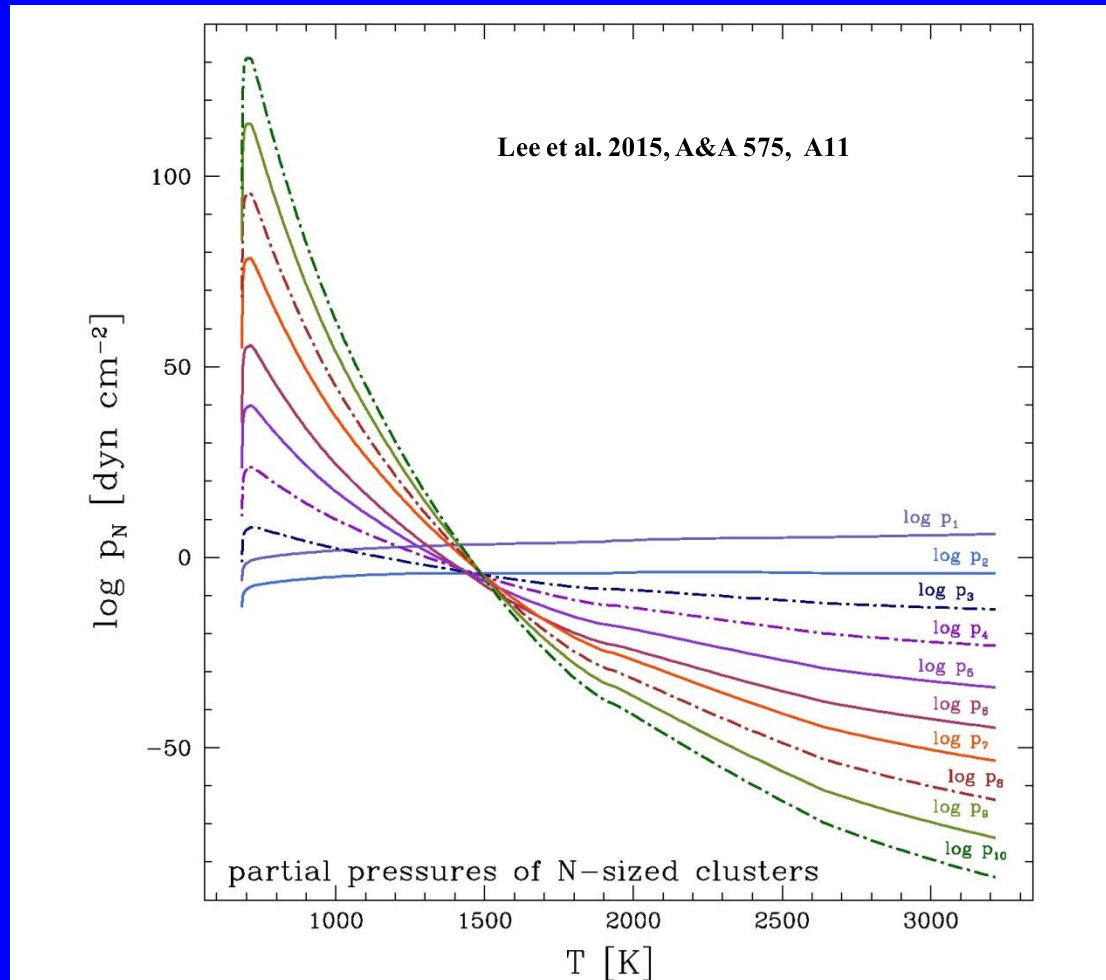
# Nucleation rates in the p-T plane (=> chemical equilibrium)



# Equilibrium geometries of $(\text{TiO}_2)_N$ compounds



# $(\text{TiO}_2)_N$ cluster distribution

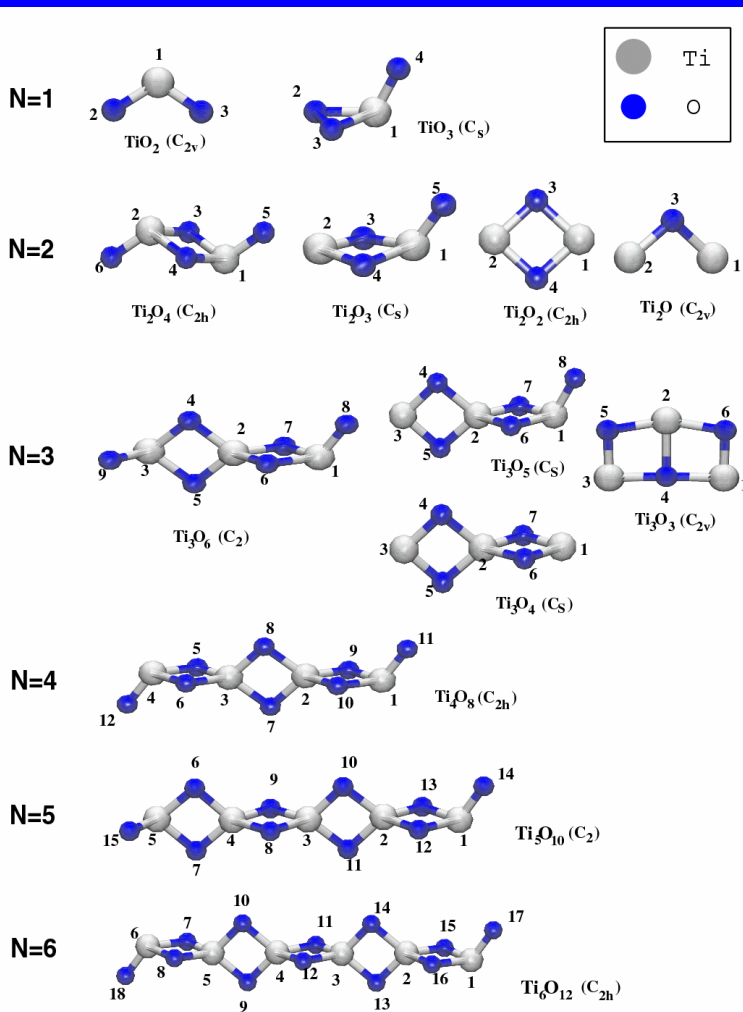


# TiO<sub>2</sub> in VY CMa

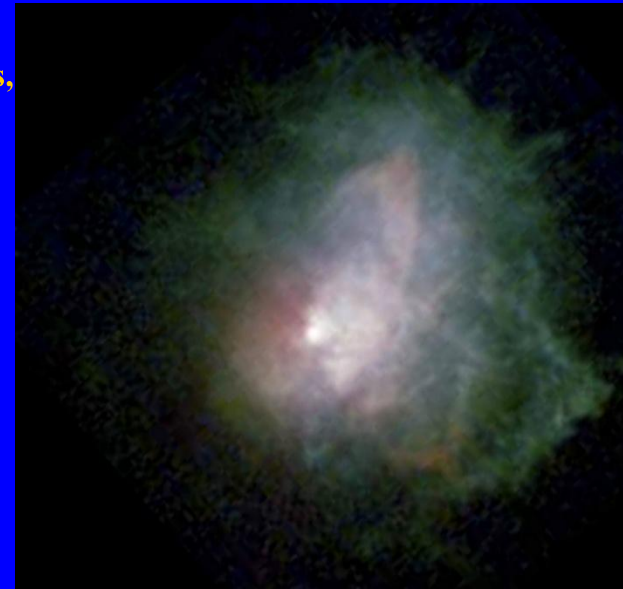
Mass-losing red supergiant VY CMa

## Equilibrium structures of Ti<sub>x</sub>O<sub>y</sub> systems

(Jeong et al. 2000, J.Phys.B 33, 3417)

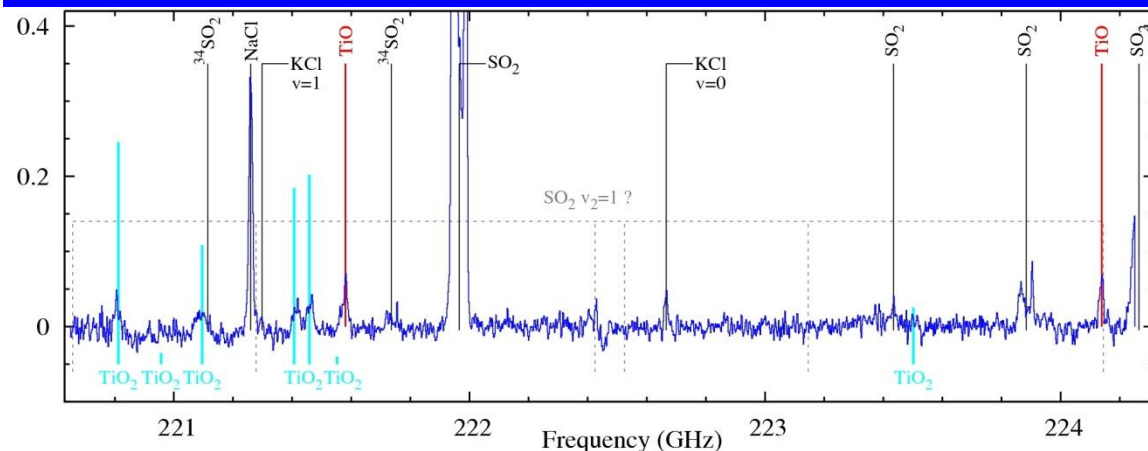


“...it is shown that titanium oxides, especially TiO<sub>2</sub> molecules, are the most probable candidates to form the primary condensates in circumstellar shells of M stars”  
 (Gail & Sedlmayr 1998, Faraday discussions 109, 303)

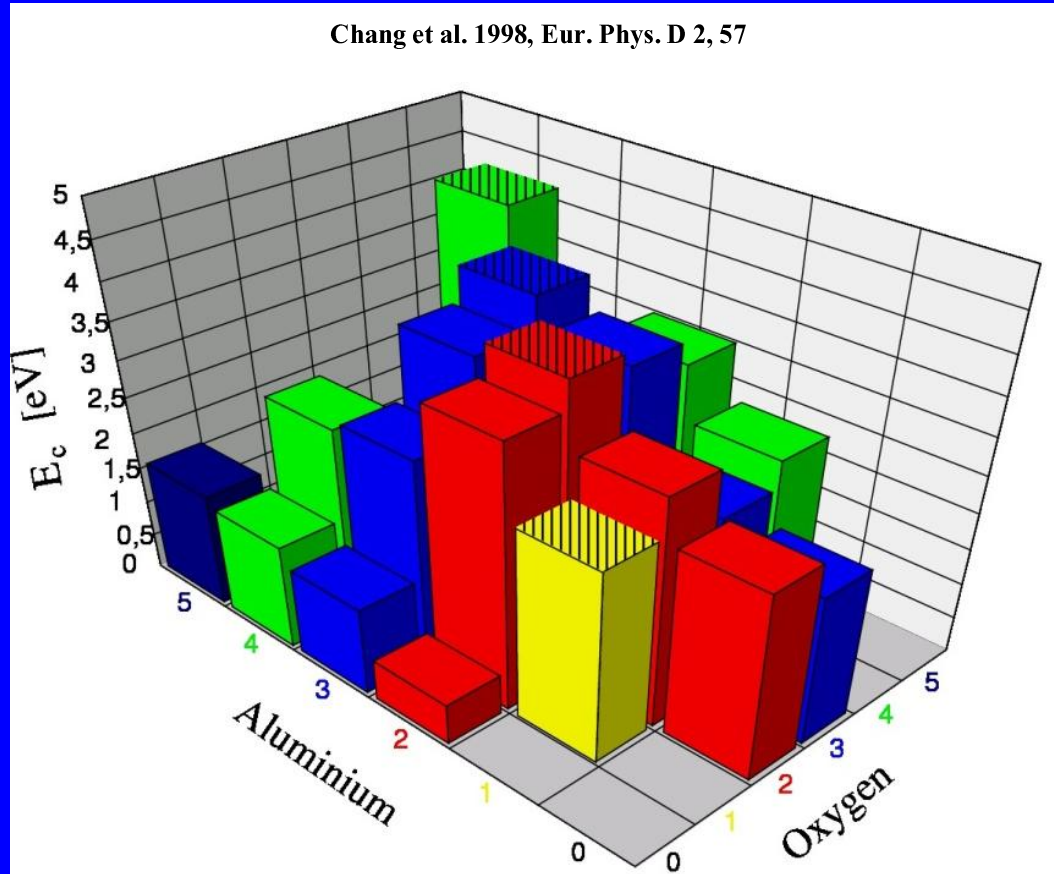


## First detection of TiO<sub>2</sub> in space (NOEMA/SMA)

(Kaminski et al. 2013, A&A 551, A113)

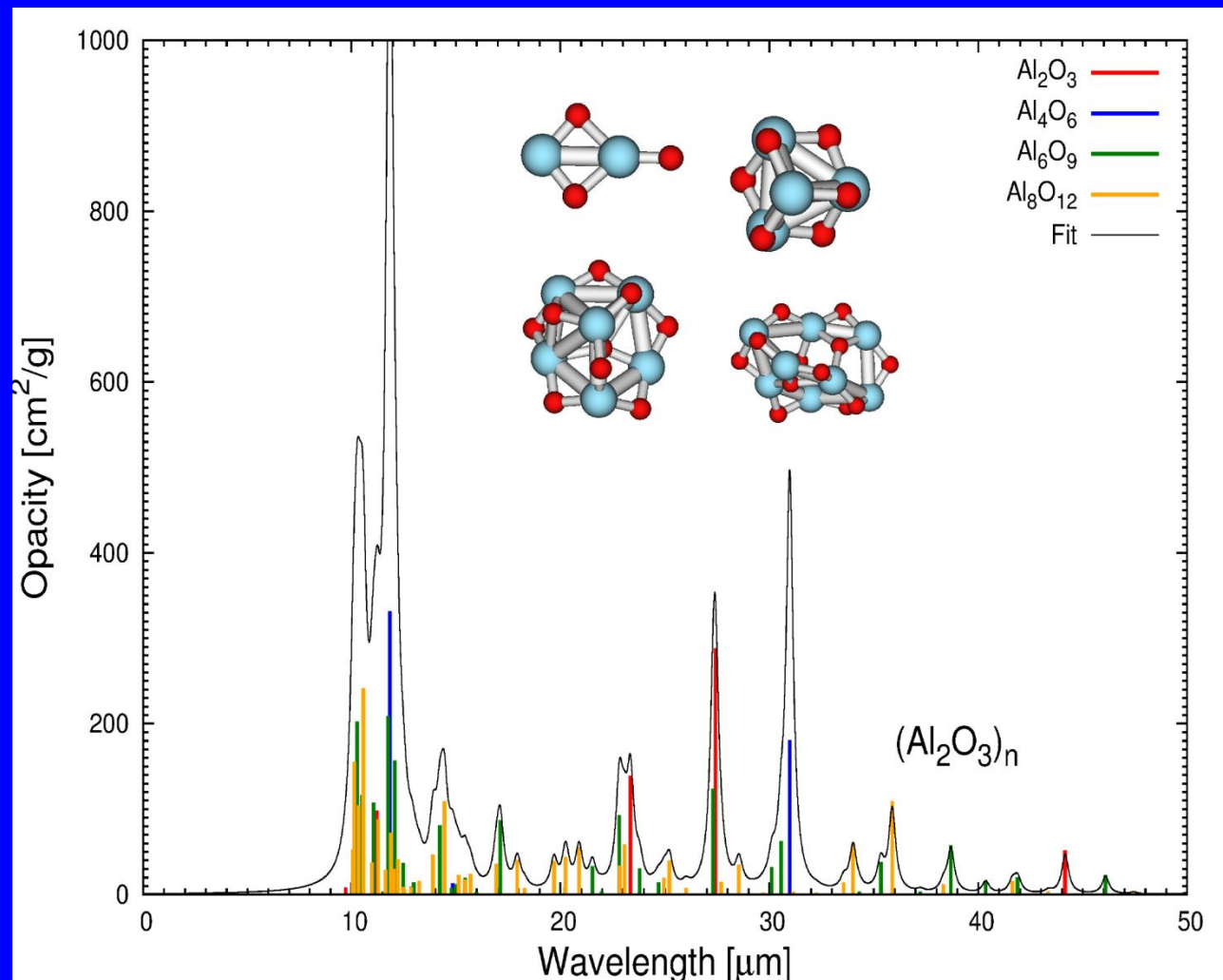


# Binding energies of $\text{Al}_x\text{O}_y$ compounds



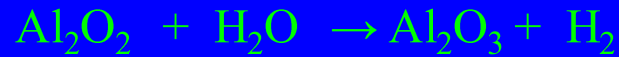
# Equilibrium geometries of $(\text{Al}_2\text{O}_3)_n$ clusters and vibrational transitions

(Decin et al. 2017, A&A 608, A55)

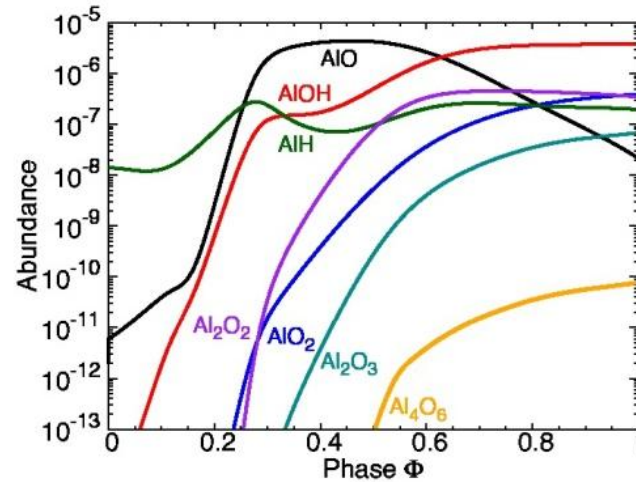
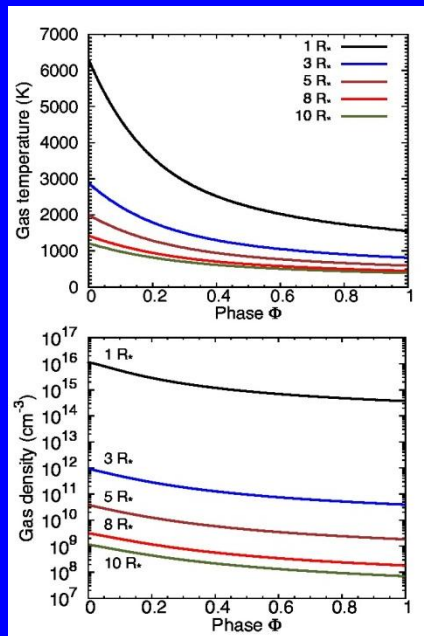


# Non-equilibrium chemistry of AlO bearing species

at  $r = 1R_*$

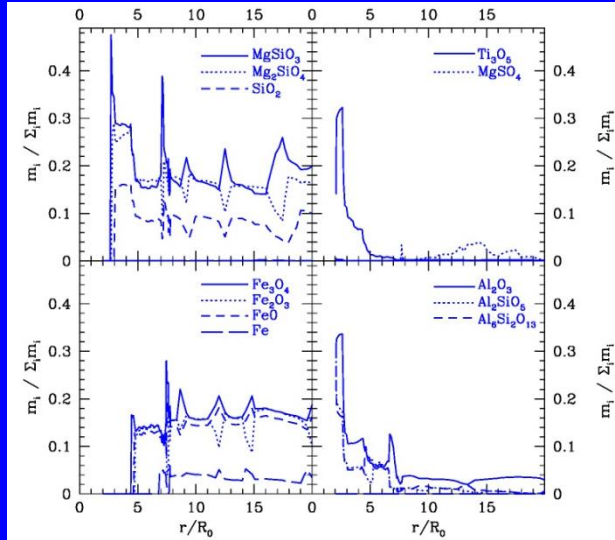


critical reaction



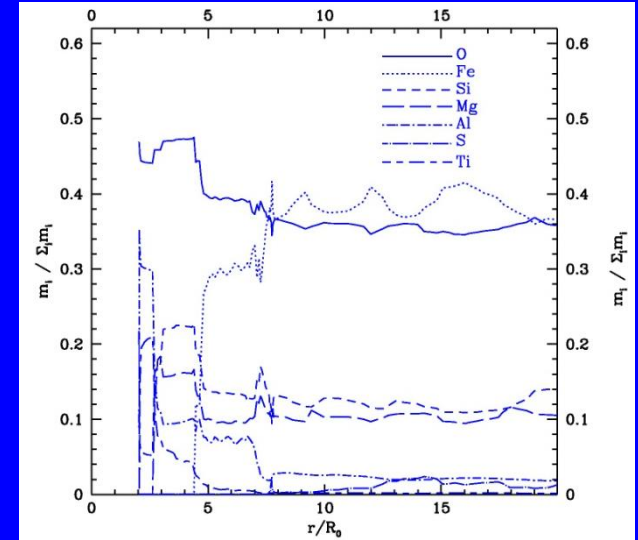
Gobrecht et al. 2016, A&A 585, A6

# Condensates in an oxygen-rich model calculation



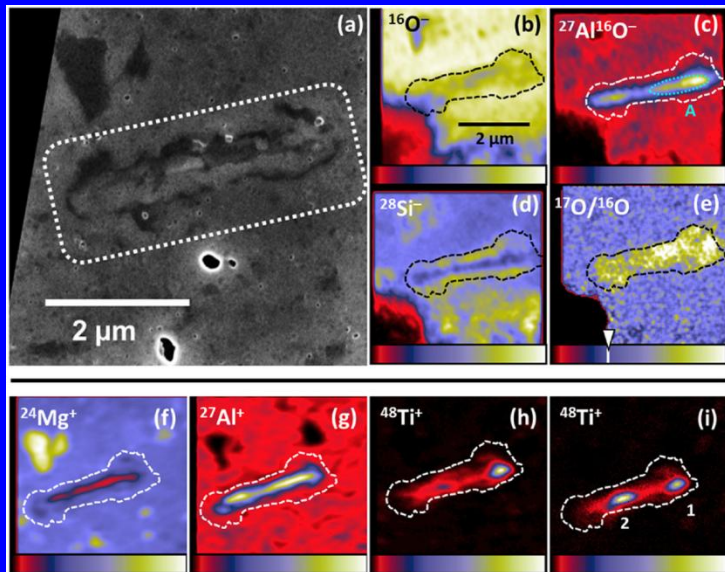
(Jeong et al. 2003, A&A 407, 191)

TiO<sub>2</sub> seeds,  
Mantle growth by  
Ti<sub>x</sub>O<sub>y</sub>, Al<sub>x</sub>O<sub>y</sub>,  
MgSiO<sub>3</sub>, Mg<sub>2</sub>SiO<sub>4</sub>,  
SiO<sub>2</sub>, Fe<sub>x</sub>O<sub>y</sub>...



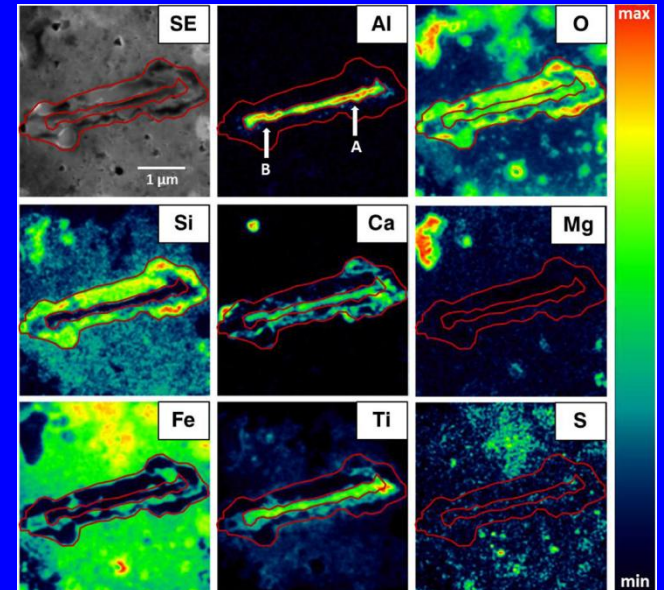
## Presolar O-rich grain from Krymka LL3.2 chondrite

(Leitner et al. 2018, Geochim. Cosmochim. Acta 221, 255)



Core: O, Al, Ti,  
Mantle: O, Si, Fe

Core:  
44% Al<sub>2</sub>O<sub>3</sub>, 44% TiO<sub>2</sub>  
In mantle only: Si, Fe

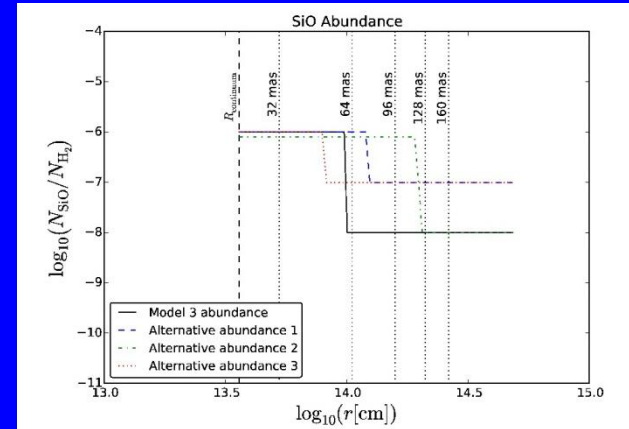
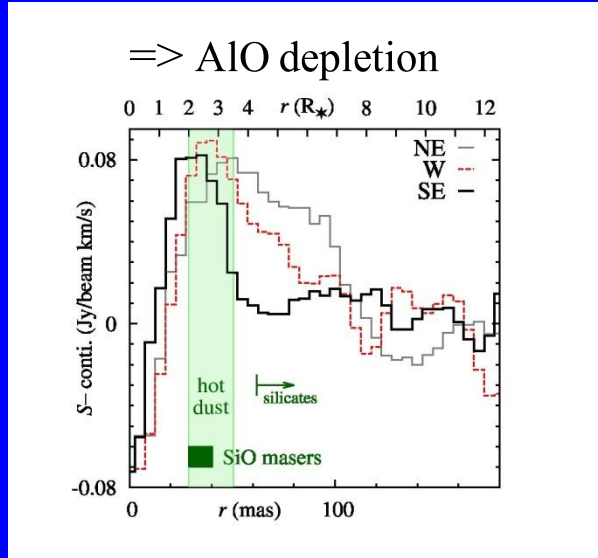




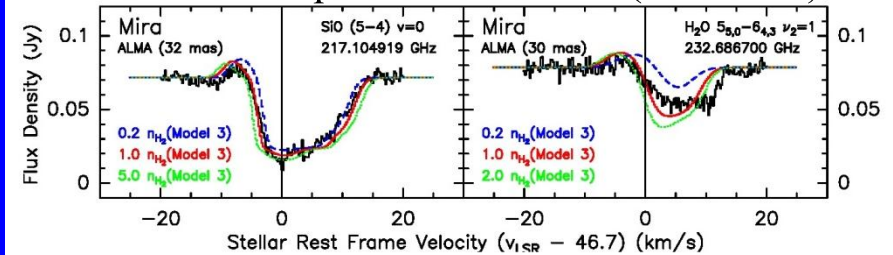
# Observational study of dust formation in $\circ$ Ceti

Wong et al. 2016, A&A 590, A127

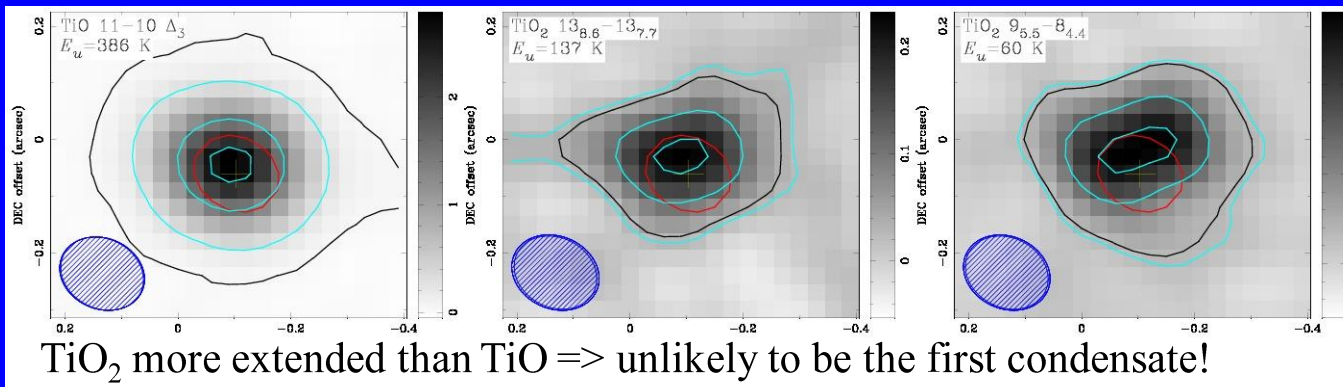
AlO(6-5): Kaminski et al. 2016, A&A 592, A42



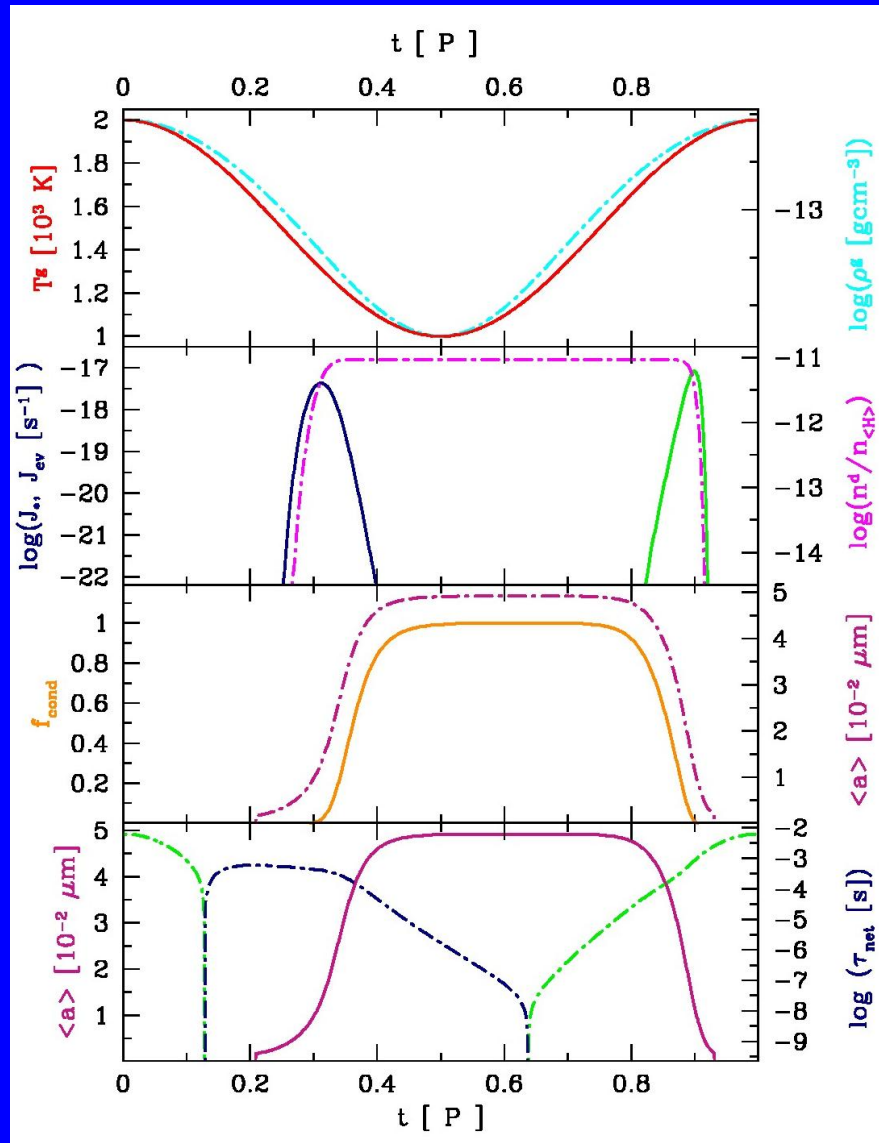
=> SiO depletion at  $r > 4 R_*$  ( $T \leq 600\text{K}$ )



Kaminski et al. 2017, A&A 599, A59

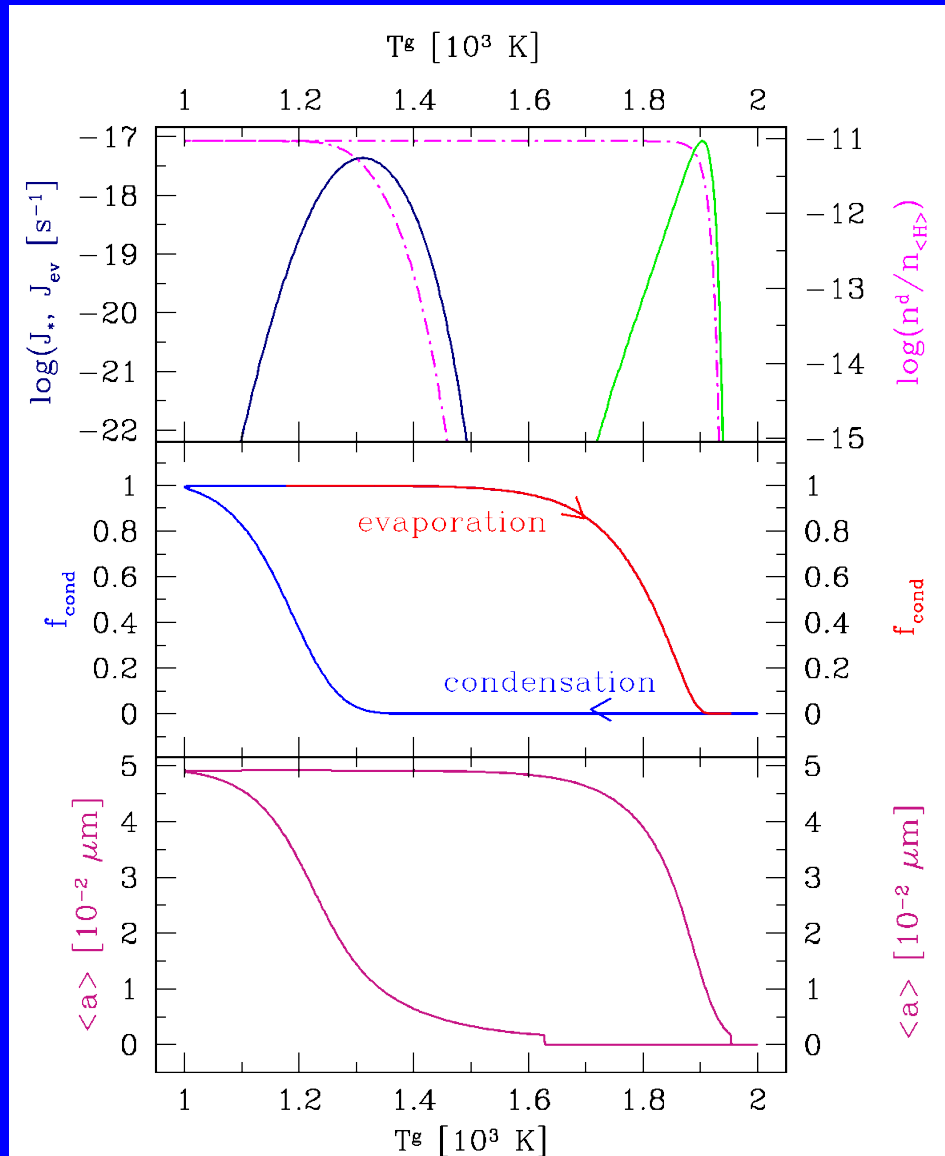


# Carbon dust formation in a gas box with oscillating thermodynamic conditions

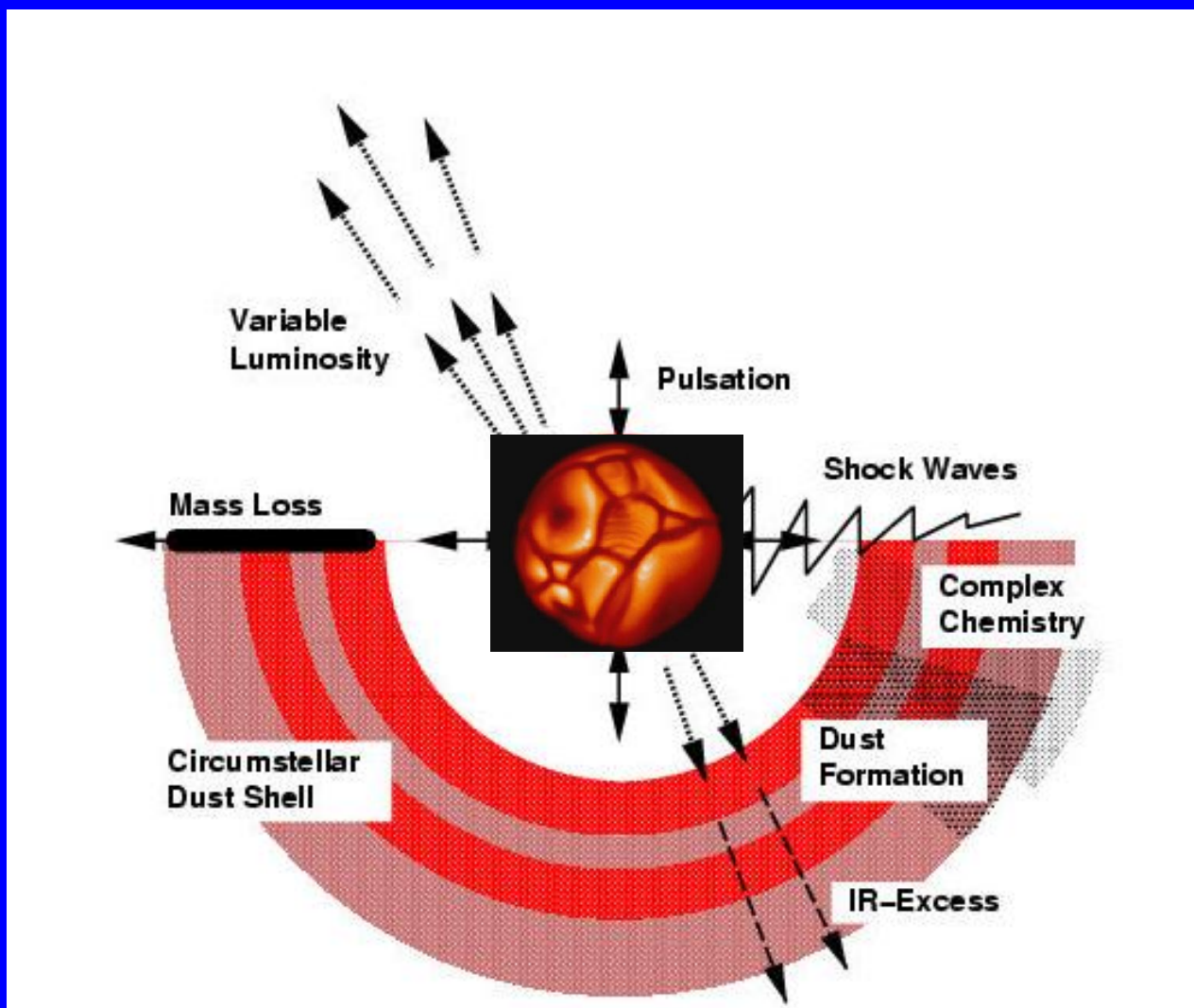


# Carbon dust formation in a gas box

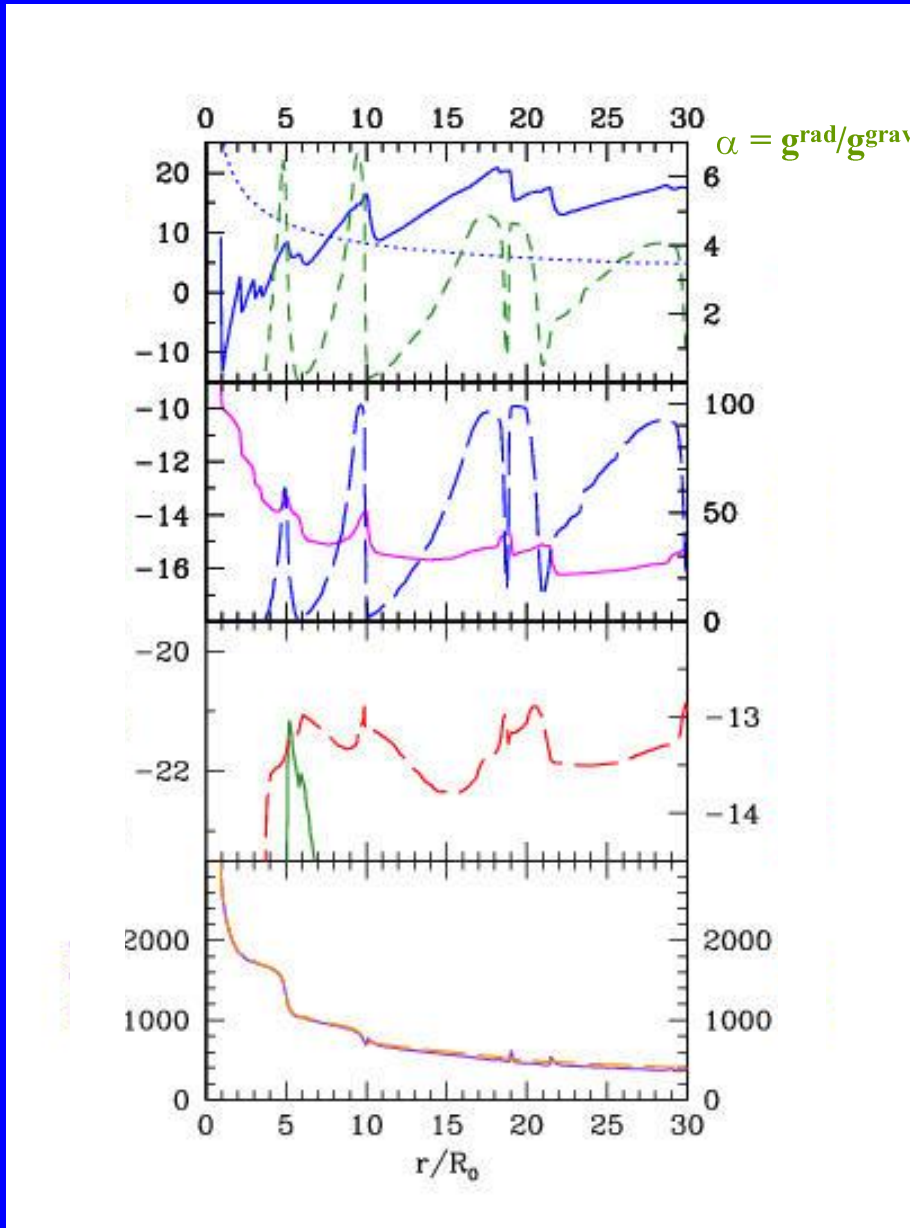
## Supercooling => hysteresis



# Scenario of a dust forming circumstellar shell



# Radial structure of a high mass-loss rate model



$$M_* = 0.8 M_\odot$$

$$L_* = 1.5 \cdot 10^4 L_\odot$$

$$T_* = 3000 \text{ K}$$

$$\epsilon_C/\epsilon_O = 1.30$$

$$P = 650 \text{ d}$$

$$\Delta v_p = 8 \text{ km/s}$$

$$\dot{M} = 4.5 \cdot 10^{-5} M_\odot/\text{yr}$$

$$v_{\text{exp}} = 17.3 \text{ km/s}$$

$$\rho^d/\rho^g = 1.1 \cdot 10^{-3}$$

2D carbon-rich models:  
Woitke 2006, *A&A* 452, 537

# Summary and conclusions

**Two different physical descriptions of the astrophysical dust formation problem are at hand**

**The required input data start to become available**

**Dust formation has to be treated in a consistent way, i.e. taking into account the coupling of the dust component to its surroundings**

**Time-dependent hydrodynamic models of pulsating, dust forming circumstellar shells reveal nonlinear phenomena induced by the self-regulating dust formation process:**

**spatial structuring of the dust shell**

**dust induced shocks**

**back-warming**

**temporal structuring of the shell, eigen-timescale**

**Chemical non-equilibrium calculations start to reproduce observed molecular abundances**

**Both approaches seem ready to be combined!**