# Dust formation in AGB stars

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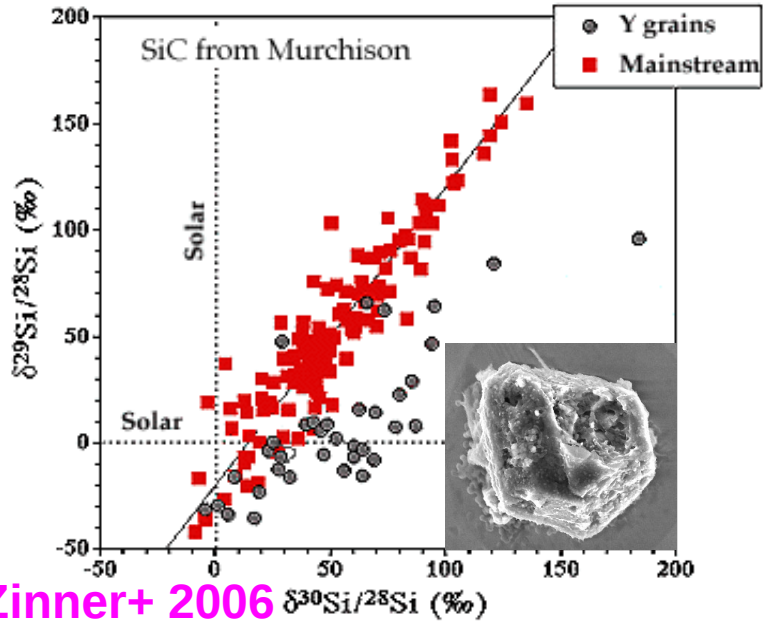
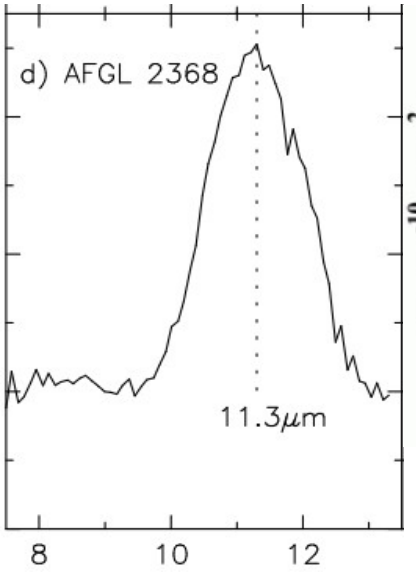
# Evidence for dust

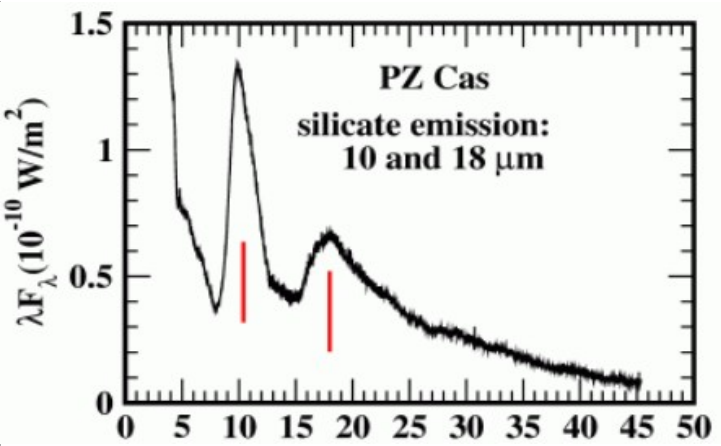
- In presolar meteoritic grains with particular isotopic signatures




Zinner+ 2006




Speck+ 2006
SiC feacture

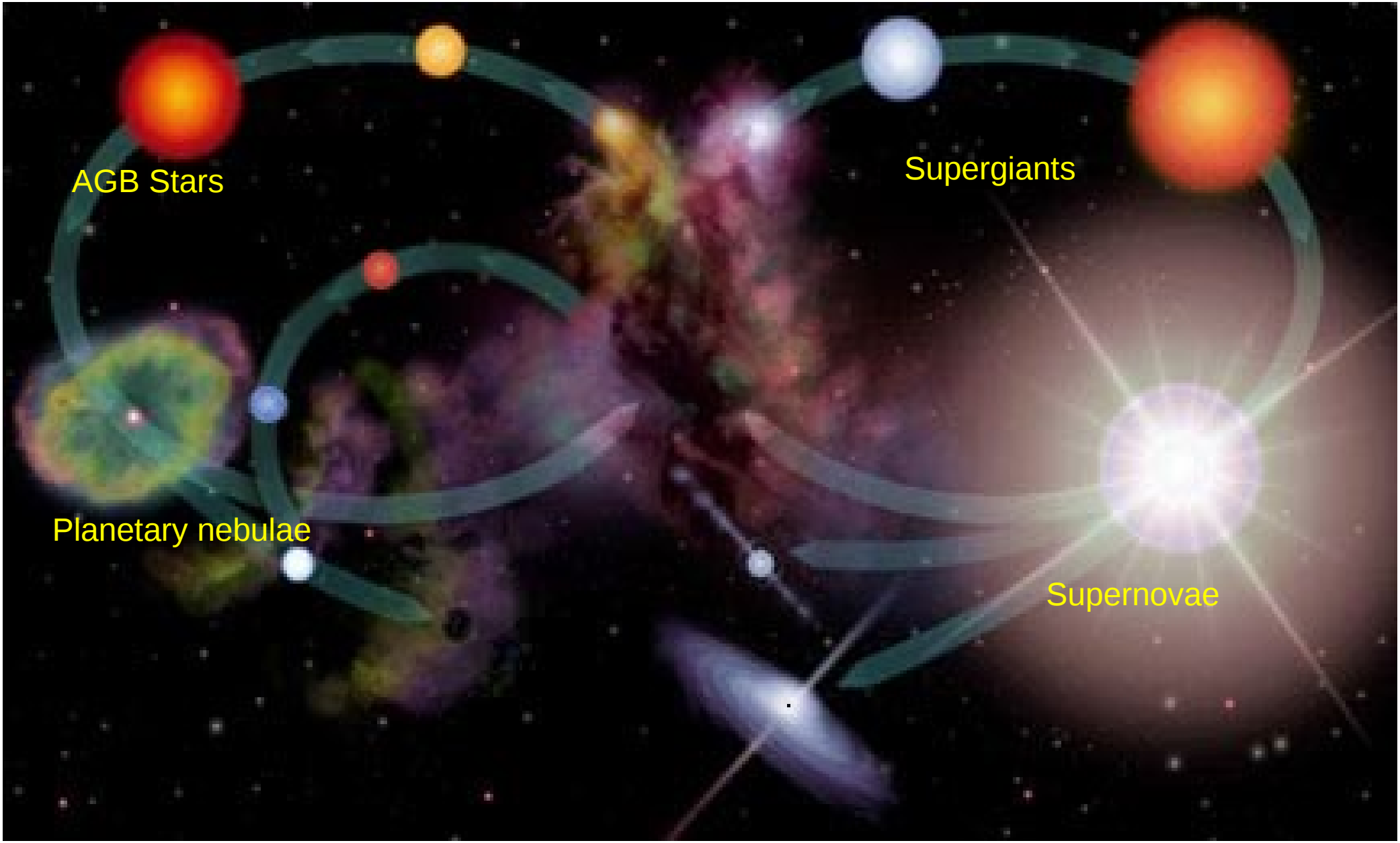



Volk+

Streching and bending modes of silicates

- Spectroscopic features
- Depletion of atoms and molecules (indirect)

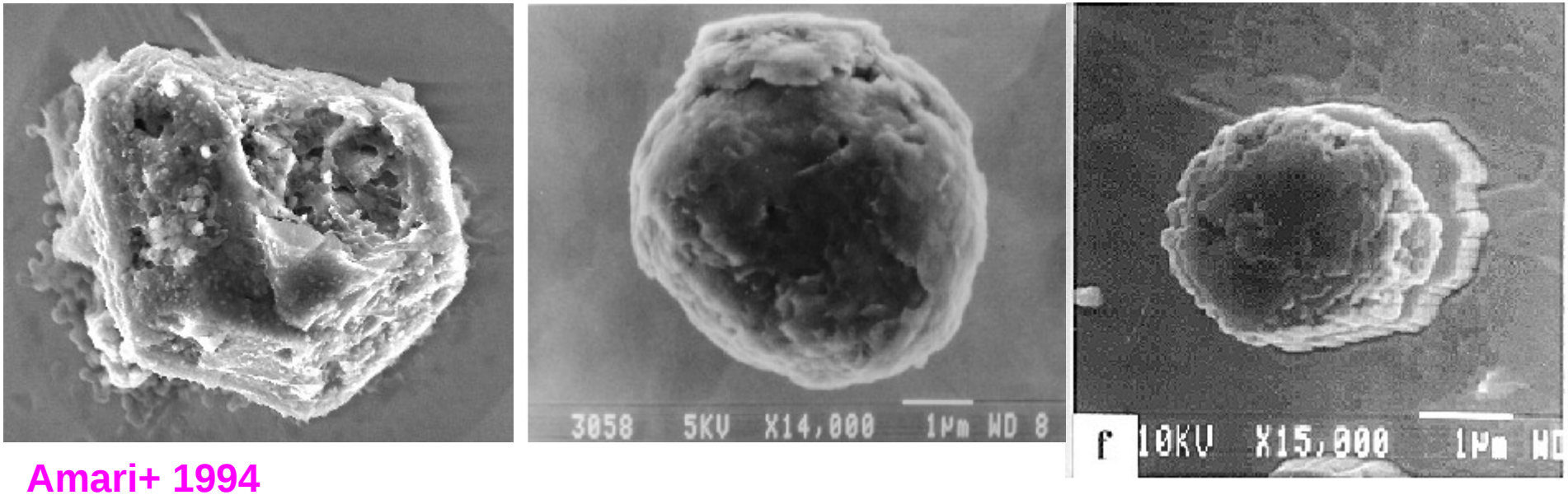
# Stellar sources of dust




wikipedia

# Types of dust

- C-rich dust: (hydrogenated) amorphous carbon, graphite, SiC
- O-rich dust: silicates (olivine, pyroxene) , metal oxides ($Al_2O_3$, $TiO_{(2)}$, $SiO_{(2)}$, FeO)
- Pure Metals: Fe, Mg, Al



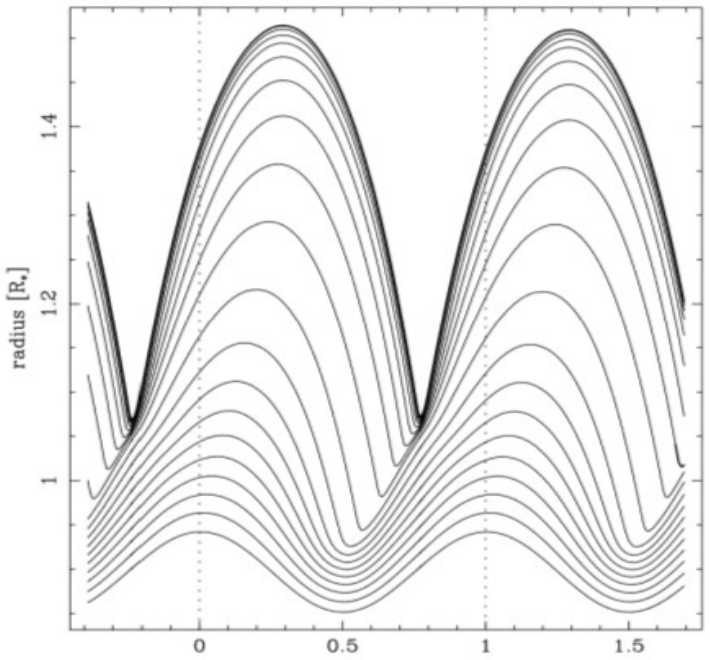

Amari+ 1994

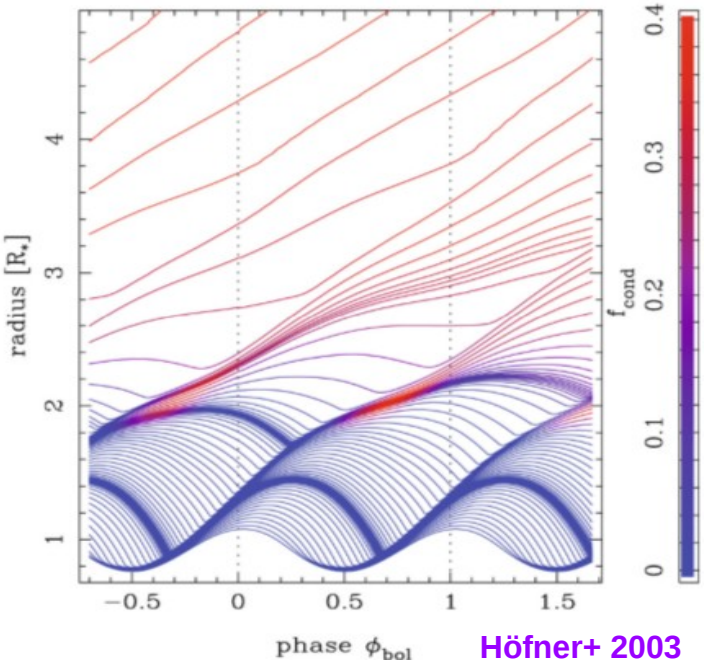
# Conditions for dust formation

- Low temperatures (< 2000 K) to afford condensation
- Sufficient high densities (~$10^{10}$ – $10^{16}$ $cm^{-3}$)to allow for coalescence
- Availability of atoms, molecules & clusters for the specific condensate
- Sufficient time for dust clusters and grains to grow (time scales)

→ such conditions prevail in the inner envelopes of AGB stars

# Pulsational shocks



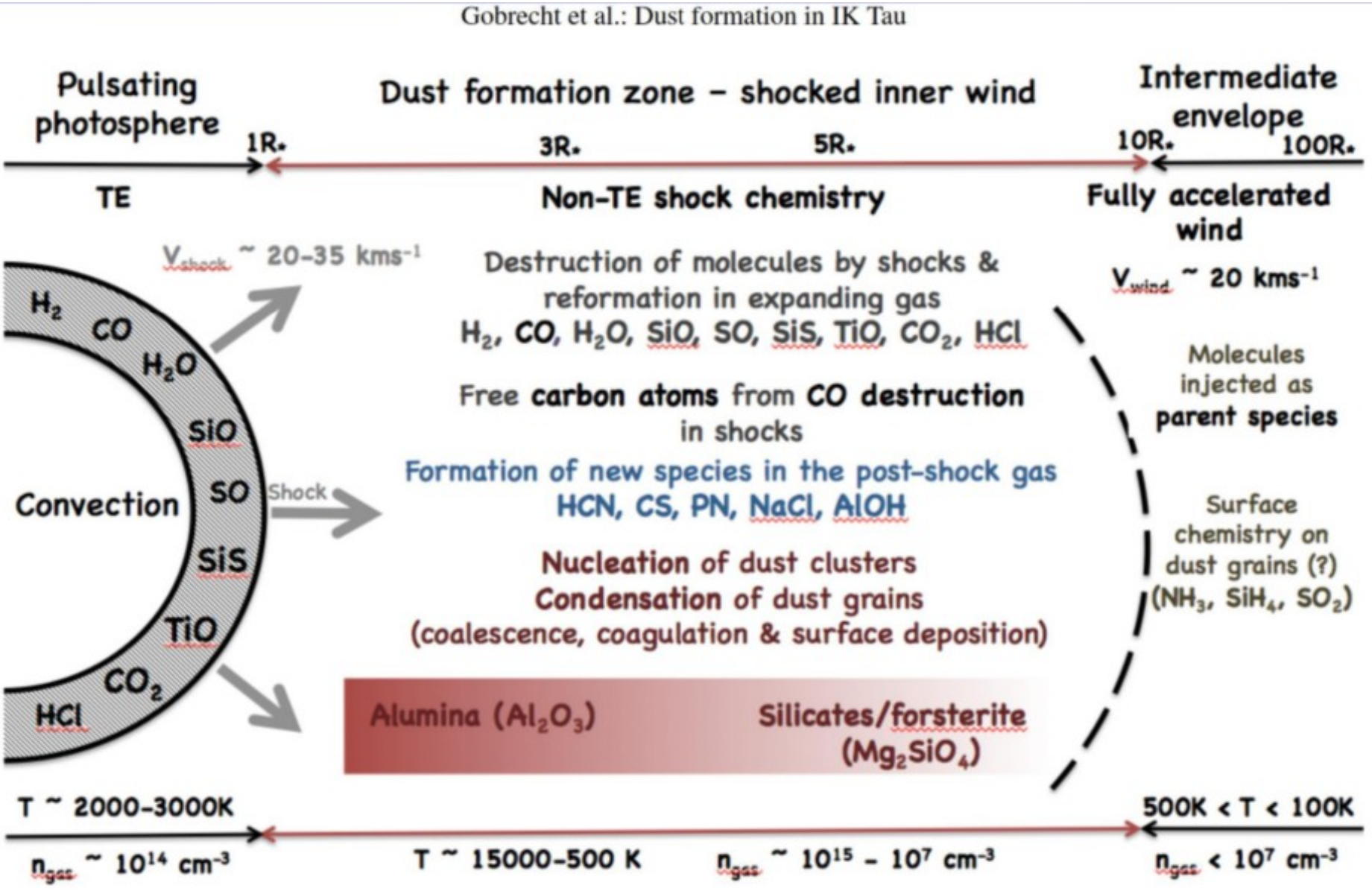

Höfner+ 2003
Nowotny+ 2010

Periodic pulsations compress, heat and accelerate the ambient medium

→ dense molecular layers form in the cooling post-shock gas

→ favourable conditions for dust formation

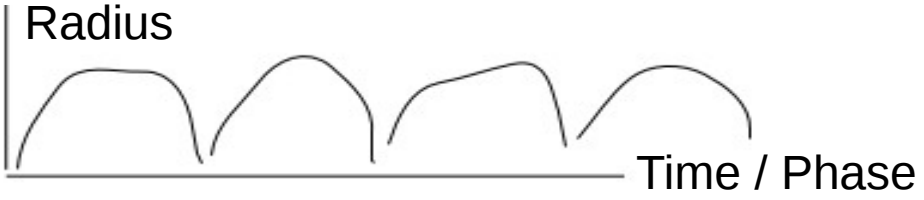
# Circumstellar envelope



# IK Tau: circumstellar model

- Periodic pulsation model of the extended atmosphere of an O-rich AGB + chemical-kinetic network with 100 species and 440 processes including dust cluster formation

| | | |
|---|---|---|
| **Star** | | |
| $M_{\star\,ZAMS}$ | 1.5 $M_\odot$ | 1 |
| $R_\star$ | $2.5 \times 10^{13}$ cm | 2 |
| C/O | 0.75 | 3 |
| P | 470 days | 4 |
| $T_{eff}$ | 2200 K | 2 |
| **Wind** | | |
| $r_s$ | 1 $R_\star$ | 3 |
| $V_s$ | 32 km s$^{-1}$ | 3 |
| $\dot{M}$ | $8 \times 10^{-6}$ $M_\odot$ yr$^{-1}$ | 2 |
| $v_{esc}$ | 17.7 km s$^{-1}$ | 2 |
| $\gamma$ | 0.98 | |
| $\alpha$ | –0.6 | 3 |
| $n_{gas}(r_s)$ | $3.62 \times 10^{14}$ cm$^{-3}$ | 3 |
| $T_{gas}(r_s)$ | 2200 K | – |

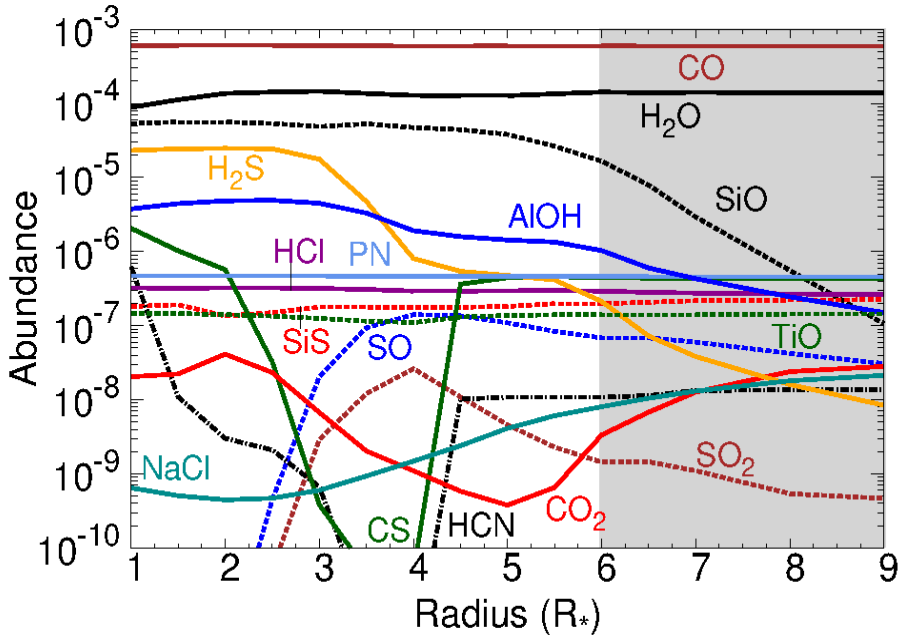


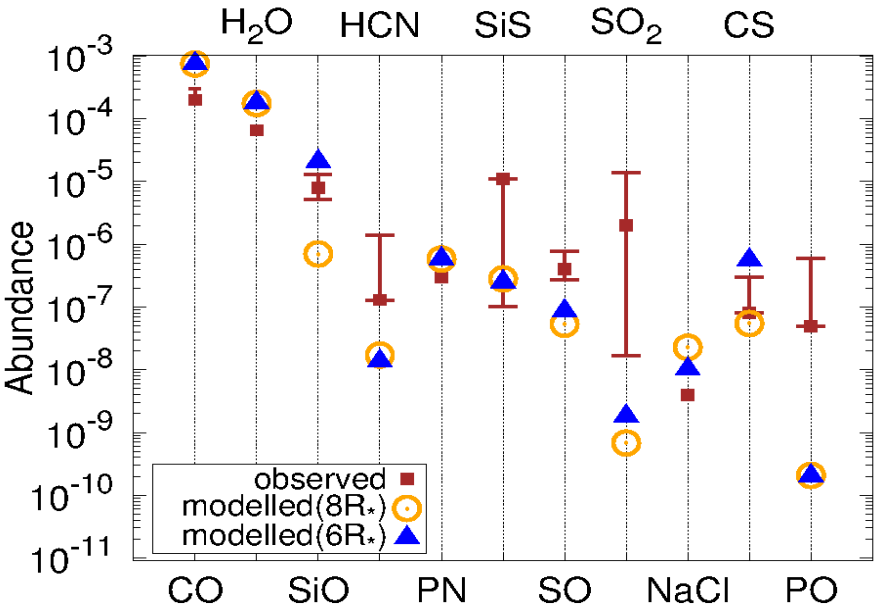

| Reaction type | Reaction | formulation | Gas conditions |
|---|---|---|---|
| *Unimolecular* | | | |
| Thermal decomposition | AB | → A + B | High T |
| *Bimolecular* | | | |
| Neutral-exchange | AB + C | → A + CB | T dependent |
| Collisional dissociation | AB + M | → A + B + M | High T |
| Radiative association | A + B | → AB + $\gamma$ | T independent |
| *Termolecular* | | | |
| Termolecular formation | A + B + M | → AB + M | (Very) high n |

Bertschinger&Chevalier 1985
Cherchneff 1992,2006,2012
Duari 1999, Gobrecht 2016

# IK Tau: results on molecules

- Non-equilibrium: Carbon-bearing species like HCN, CS or $CO_2$ form in the inner envelope
- Modelled abundances at 6-8 $R_*$ agree well with observations



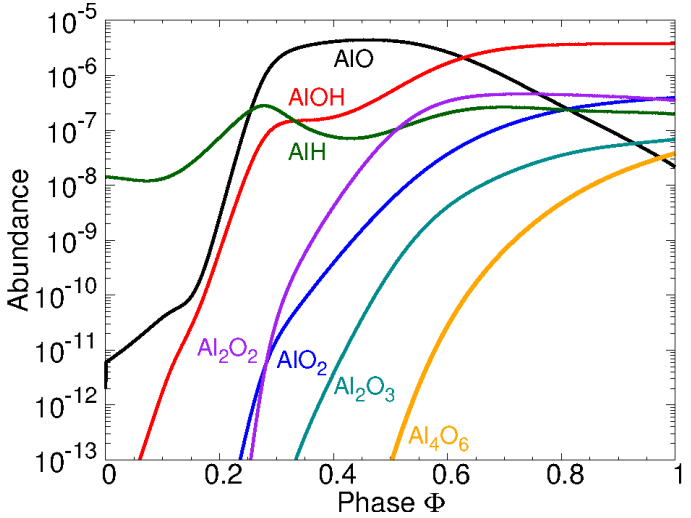




Decin+ 2010A, 2010B De Beck+ 2013 Milam+ 2007
Schoeier+ 2007, 2013

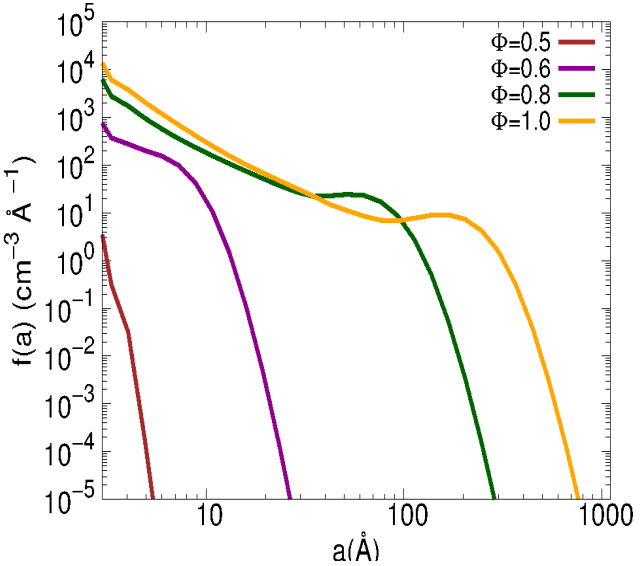
# IK Tau: results on clusters and dust

- Clusters of alumina ($Al_2O_3$) form and condense close to the star in the cooling post-shock gas
- Forsterite grains ($Mg_2SiO_4$) form at larger radii ($4R_*$) in greater amounts, but lower size

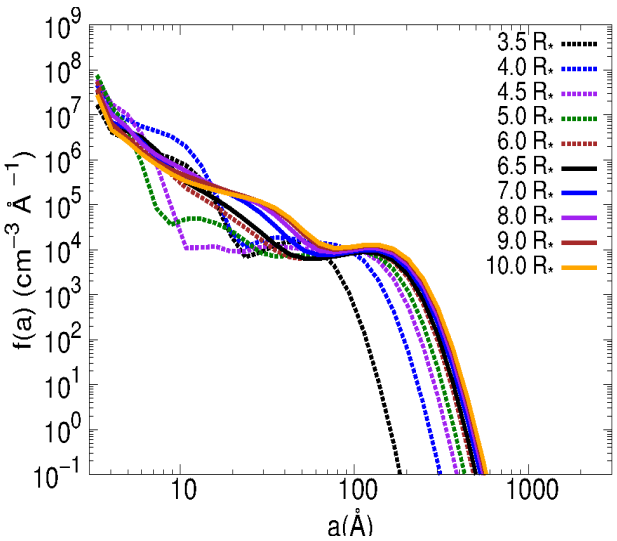
1 R*




ψ = 2.7e-5




ψ = 2.2e-3




Gobrecht+ 2016

# Conclusions (part I)

- Molecular abundances including non-equilibrium species HCN, CS and $CO_2$ well reproduced, expect $NH_3$, PO and ($SO_2$)
- Large grains of alumina dust form close to the star that is too low to exclusively explain the observed mass loss rate / dust-to-gas ratio
- Forsterite grains form around 4 $R_*$ in amounts comparable to observations, although their mean size rather low

# Dust Clusters

- Link between molecules and dust grains:

  e.g. $Al_4O_6$, $Mg_4Si_2O_8$, $Si_{16}C_{16}$
- Many body-problem: $H\psi(r) = E\psi(r)$

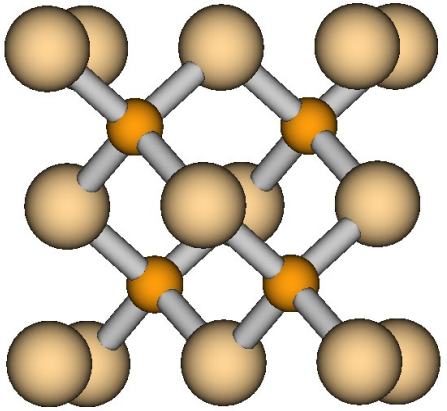
  → no exact solution

  → parallelized supercomputers required to perform full quantum calculations

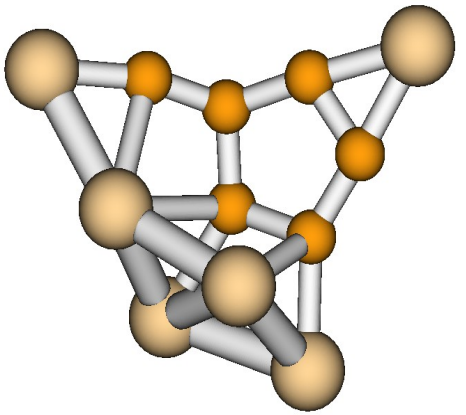
  → structures, energetics, reactivity are not well characterized

# Silicon carbide (SiC) clusters

Crystalline bulk versus clusters



4.4 Å



Clusters: Quantum effects, surface-to-volume ratio, unsaturated bonds

Candidate structure search by Molecular dynamic & Monte-Carlo simulations

→ subsequent refinement on the quantum DFT level of theory

# SiC: Molecular dynamics

- Tersoff potential:

Tersoff 1989

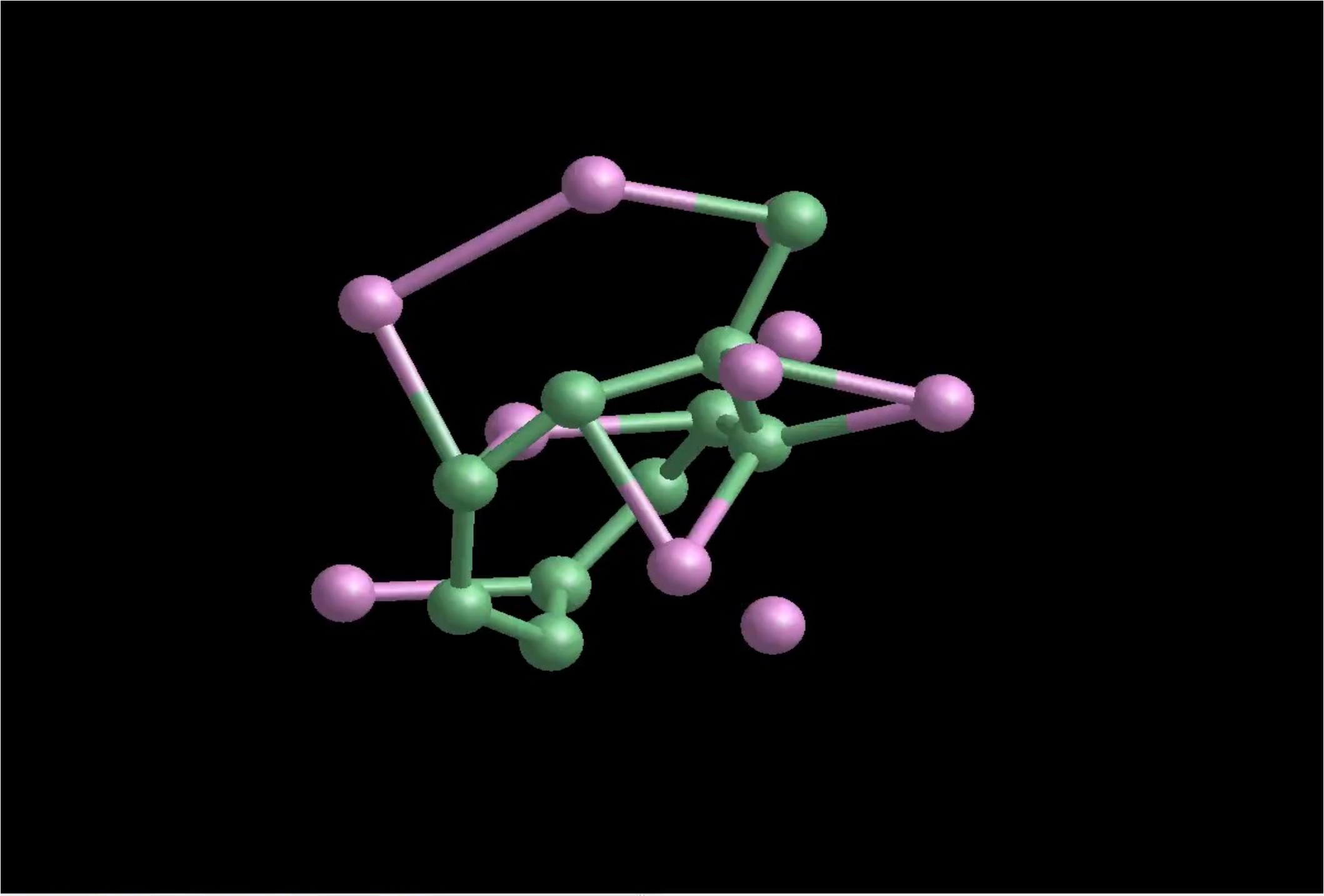
$$V_{ij} = f_C(r_{ij})\left[V_{rep}(r_{ij}) + b_{ij}(\theta_{ijk})V_{att}(r_{ij})\right]$$

→ accounts for covalent character of clusters

→ segregation of Si and C atoms, $C_5$ and $C_6$ ring formation

- Simulated annealing: High-temperature (2000-3000 K) molecular dynamics and subsequent decrease of temperature with the program GULP (General Utility Lattice Program)

Gale+ 1997



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# Monte-Carlo candidate structures

- Buckingham pair potential:

$$\Phi_{12}(r) = A\exp(-Br) - \frac{C}{r^6} + \frac{q_1 q_2}{4\pi\varepsilon_0 r}$$

Buckingham 1938

→ account for ionic character of clusters

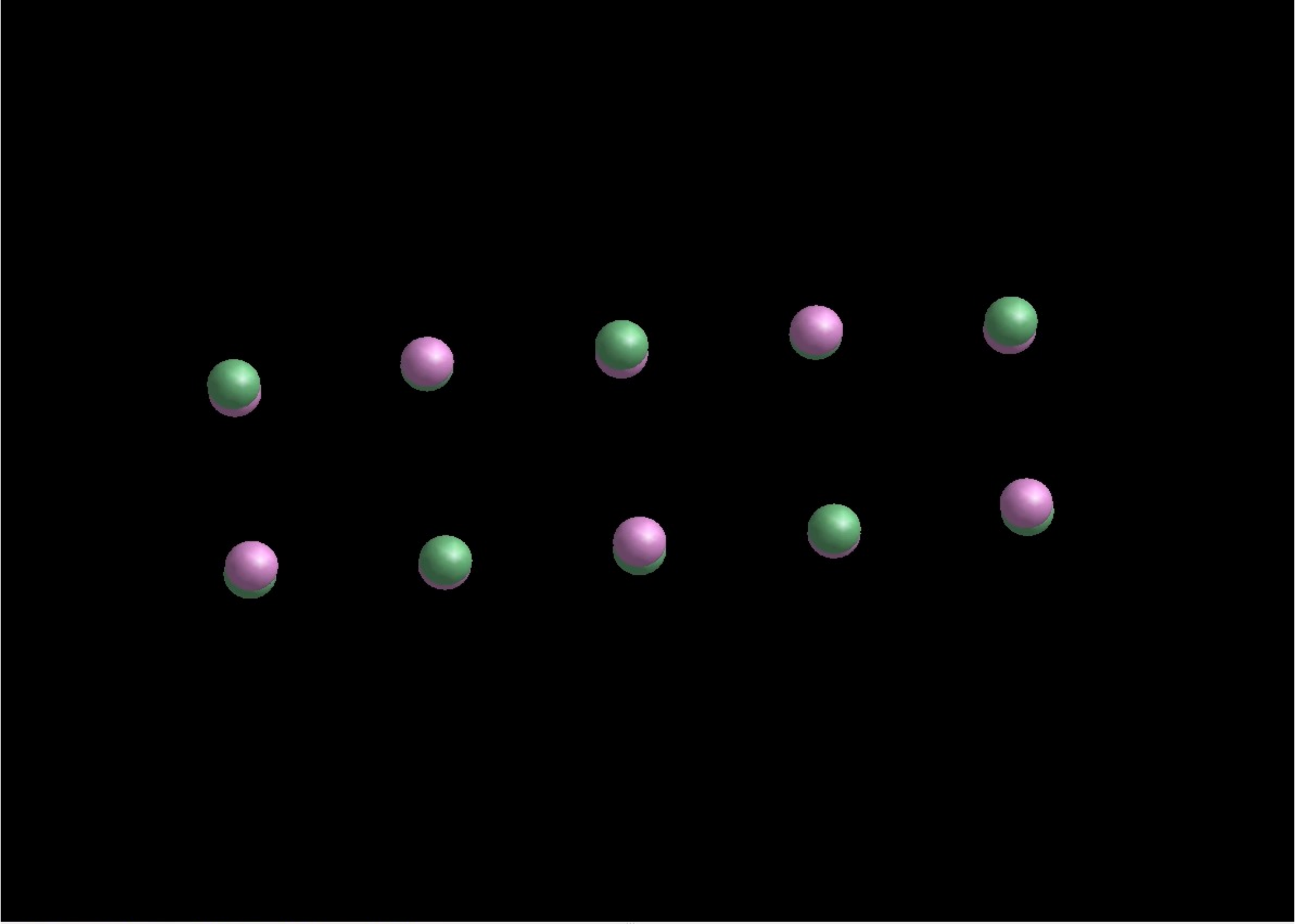
→ alternating Si-C bondings

- ZnS (zinkblende) analogy, charge transfers between C and Si ions as large as 2.5 e

Watkins 2009

- Monte-Carlo exploration of the potential landscape with the Basin-Hopping algoritm

Wales 1997
Bromley 2005



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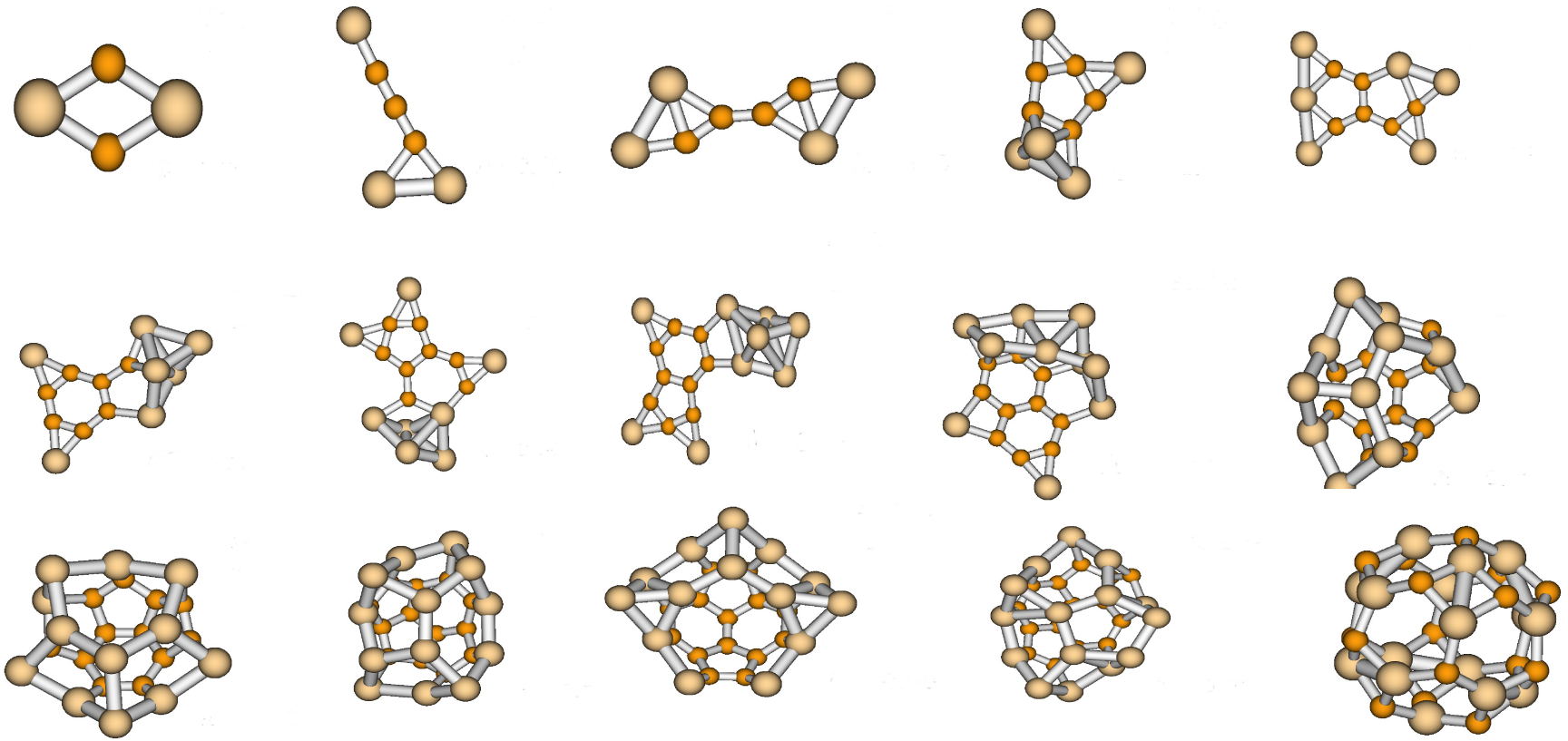
# SiC clusters: preliminary results

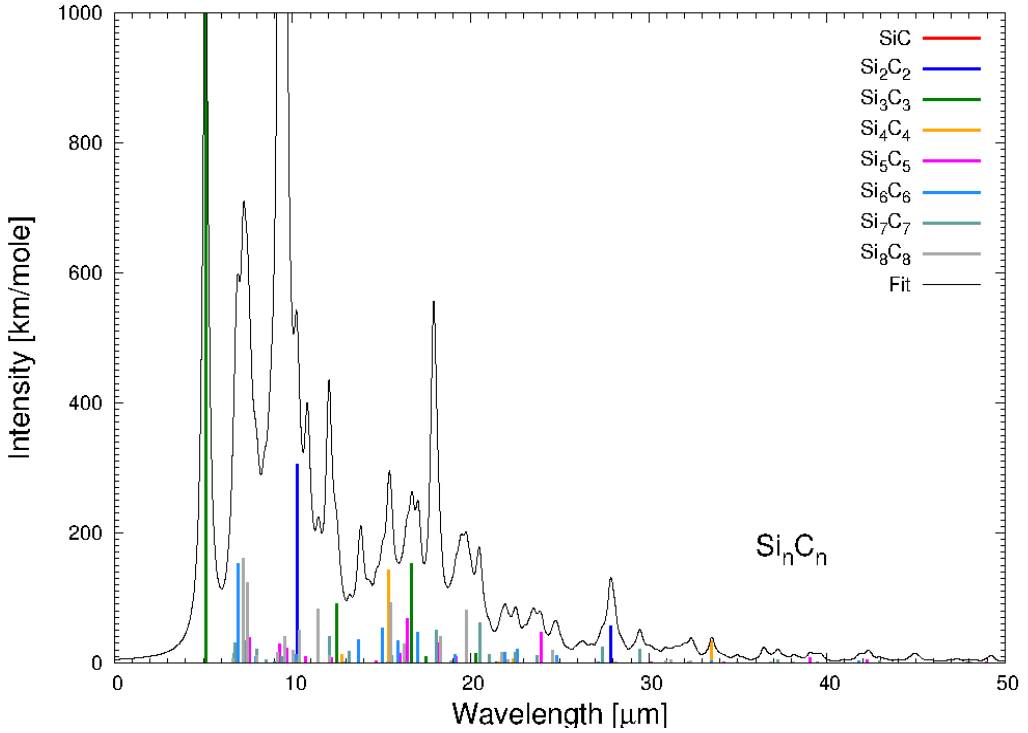
- Most stable $Si_nC_n$ structures exhibit segregation of C atoms forming chains, $C_5$ and $C_6$ rings and cage-like configurations with increasing size

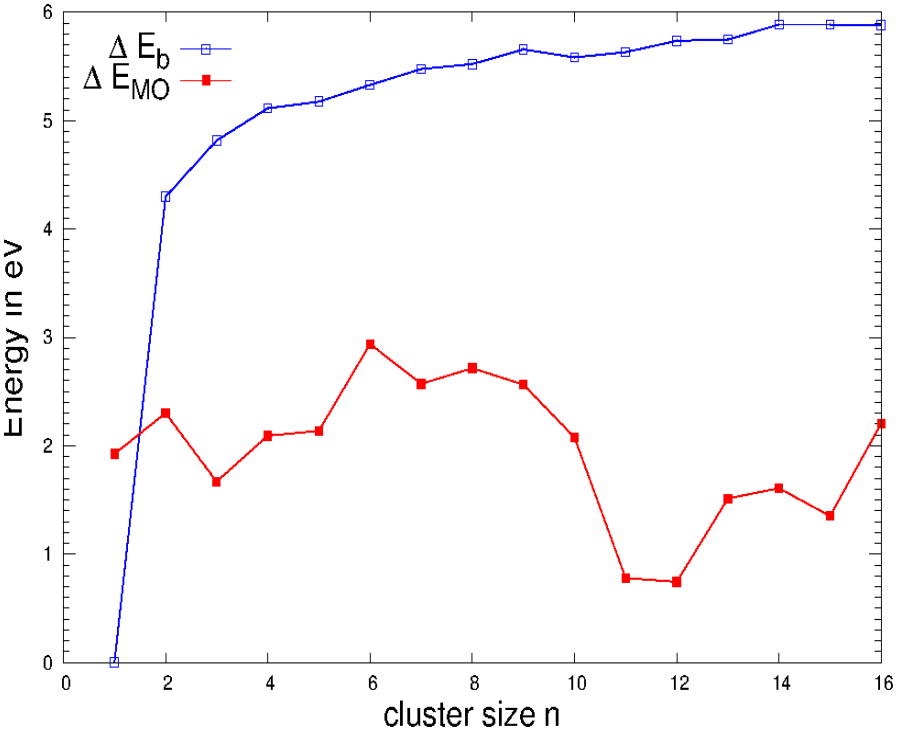
Gobrecht in preparation



# SiC clusters: preliminary results II

- DFT calculations → Potential energy, HOMO-LUMO gap, Vibrational IR spectra, theoretical reaction rate determination



# Conclusions (part II)

- We found new, stable $(SiC)_n$ with $n \leq 16$ clusters with the lowest potential energies
- Segregated clusters with $C_5$ /$C_6$ rings dominate the SiC cluster chemistry for $n \leq 16$
- However, for n=12 and n=16 very stable clusters with alternating Si-C bonds and bulk-like properties are found
- These clusters indicate the sizes / length scales, where the transition of quantum-effect dominated clusters and bulk-SiC (found in meteoritic inclusions) may occur

# Still to be finalized ...

- Comparison with observations (e.g. 11.3 μm feature)
- Theoretical rate (temperature & density dependent)
- Formation routes via $Si_nC_m$, $m \neq n$ ($SiC_2$ and $Si_2C$ observed)

THANK YOU FOR YOUR ATTENTION!