Université de Rennes

UNIVERSITY OF GOTHENBURG

On the Impact of Atomic and Molecular Accretion on Cosmic Dust Growth

D. Bossion*, A. Sarangi, G. Nyman

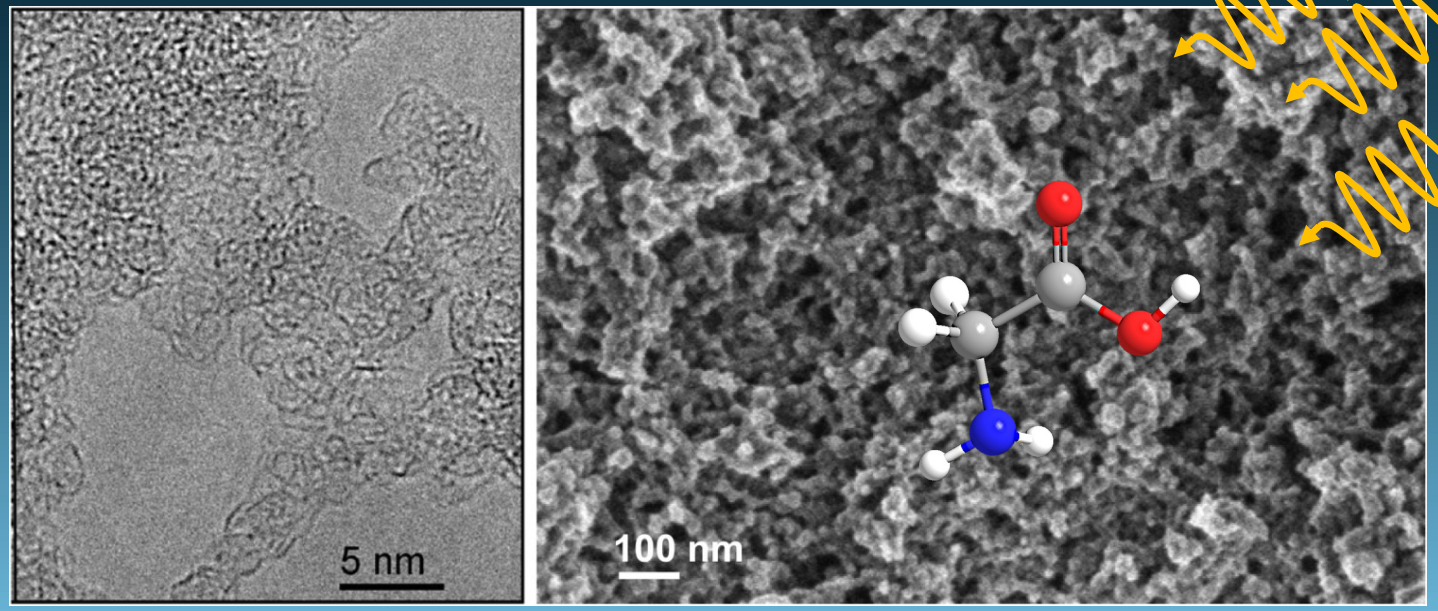
Département de Physique Moléculaire, Institut de Physique de Rennes, France

PCMI2024-Bordeaux, 28-31 October 2024

Cosmic Dust

❖ Ubiquitous in space (ISM, supernovae, near stars…), divides into 2 main types:

- O-rich star surrounding, C/O < 1 → Silicate dust (contains Si, Mg, Al, Fe, O, Ca… different seeds),
- C-rich star surrounding, C/O > 1 → Carbonaceous dust (amorphous carbon, graphite-like seeds).



Potapov & McCoustra, Intern. Rev. Phys. Chem., 40(2), pp. 299–364 (2021)

- ➢ Shields molecules from destructive radiations
- ➢ Provides a catalytic surface to form complex molecules (aminoacids, nucleobases…)
- ➢ Complexification of the chemistry in space → prebiotic molecules

Dust Formation

❖ Dust nucleation from gas phase in some environments:

- Winds of AGB stars, } T range 50 - 2500 K
- Ejecta of core-collapse SN. } Same dust & gas T

➢ No icy mantle

≠

❖ ISM conditions:

T range dust 3 - 300 K

T range gas 3 - 10 000+ K

➢ Some icy mantle

❖ Dust growth modeling (radius a): <u>accretion + desorption</u> of main colliders.

- Accretion rate of species i (density n_i, thermal velocity v_i^{th}):

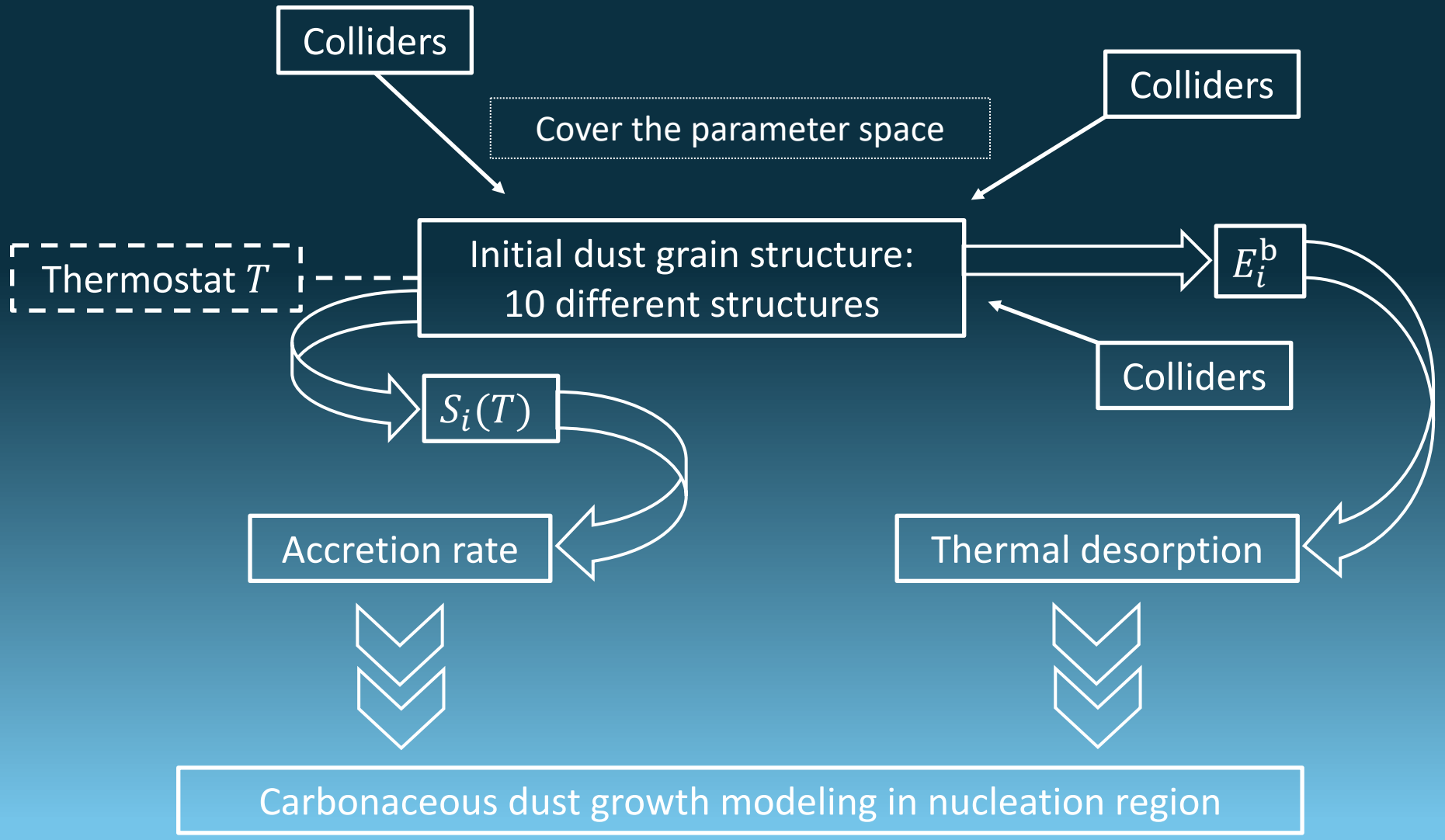
➢ $F_i(T) = \pi a^2 S_i(T) n_i v_i^{\mathrm{th}}(T)$ → $S_i(T)$ sticking coefficient (T- and i-dependent),

- Thermal desorption rate (Polanyi-Wigner formula, Λ_i surface atoms, ν_i escape frequency):

➢ $D_i(T) = \Lambda_i(a)\nu_i \exp -\frac{E_i^{\mathrm{b}}}{k_B T}$ → E_i^{b} binding energy (i-dependent).

This Study

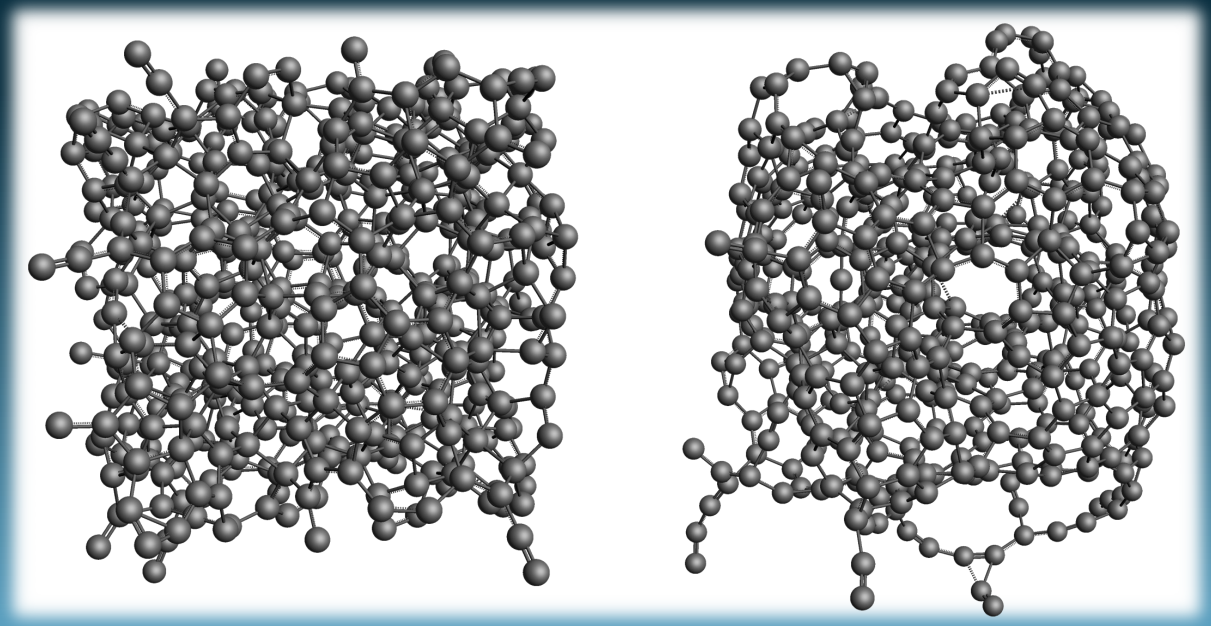
- Growth of pure amorphous carbon dust by sticking of common colliders H, H_2, C, O, CO.



Amorphous Carbon Structure

❖ 512 C-atom structures obtained by DFT coupled with ML → Deringer, V. L., et al., Chem. Mater., 30, 7438 (2018)

➢ 10 structures thermalized by reactive force-field (ReaxFF) with Nosé-Hoover chain (thermostat):



$T = 50$ K

$T = 2500$ K

Van Duin, A. C. T. et al., ReaxFF 2023.1, SCM 2023

➢ High 2500 K, structures resilient to T:

- Mainly 2D cyclic structures
- Some C-chains

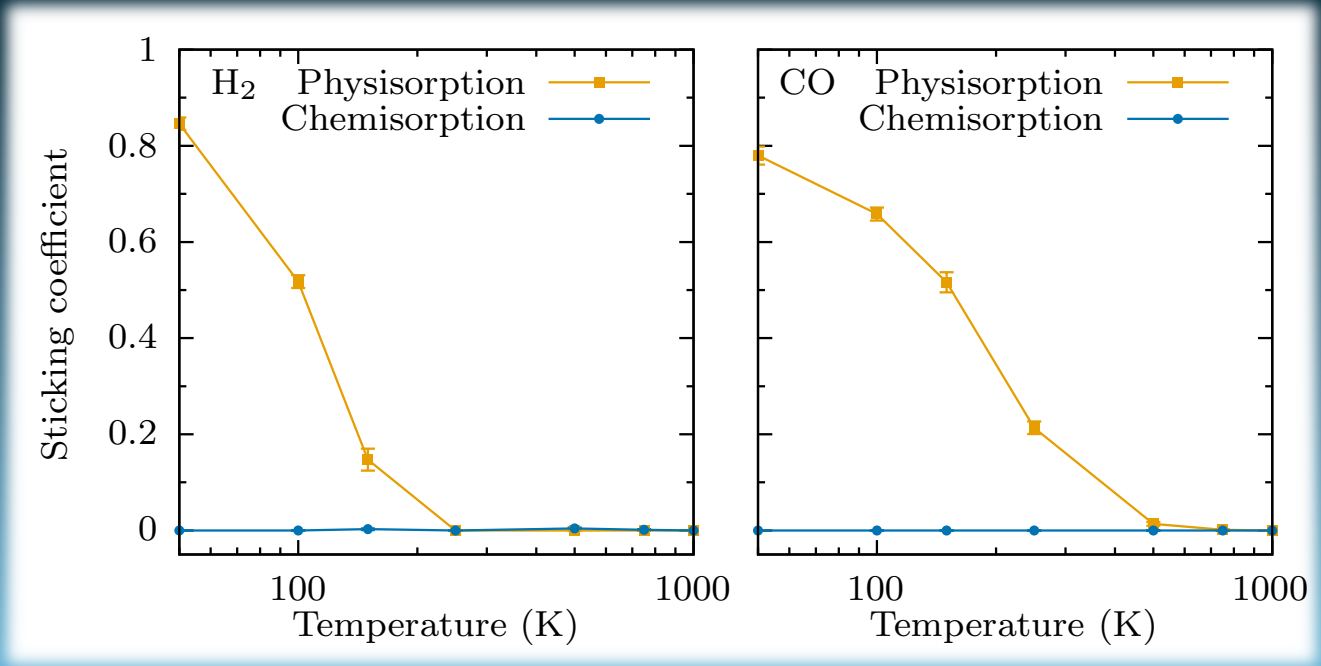
❖ Binding energy obtained from the force-field on amorphous carbon:

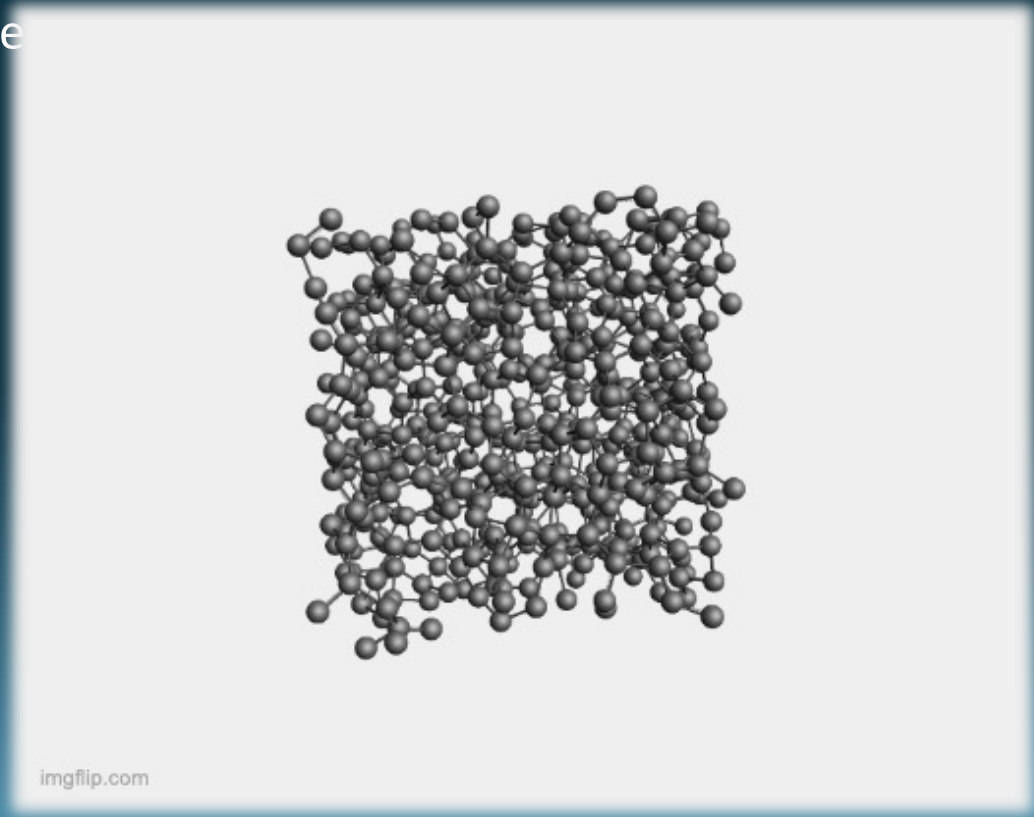
Species i	H	C	O
E_i^{b} (eV)	4.76 ± 0.12	7.55 ± 0.01	7.68 ± 0.21

Bossion, D. et al., A&A, *submitted*

Sticking Dynamics

- ReaxFF dynamics: 74 collisions/structure/species, 10 structure
- Main collisional partners: H, H_2, C, O, CO.
- Results: #chemisorbed, #physisorbed (growth from chemisorption).





Dynamics of O colliding at 250 K

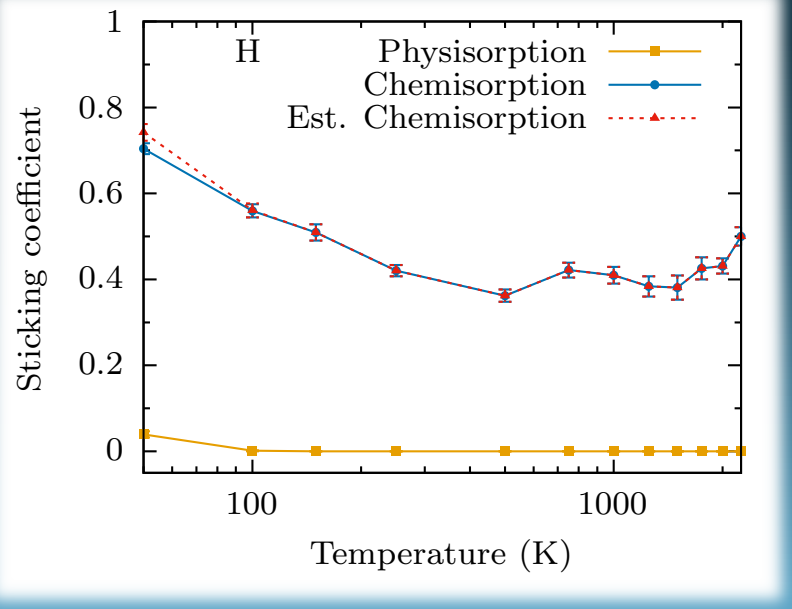
Bossion, D. et al., A&A, *submitted*

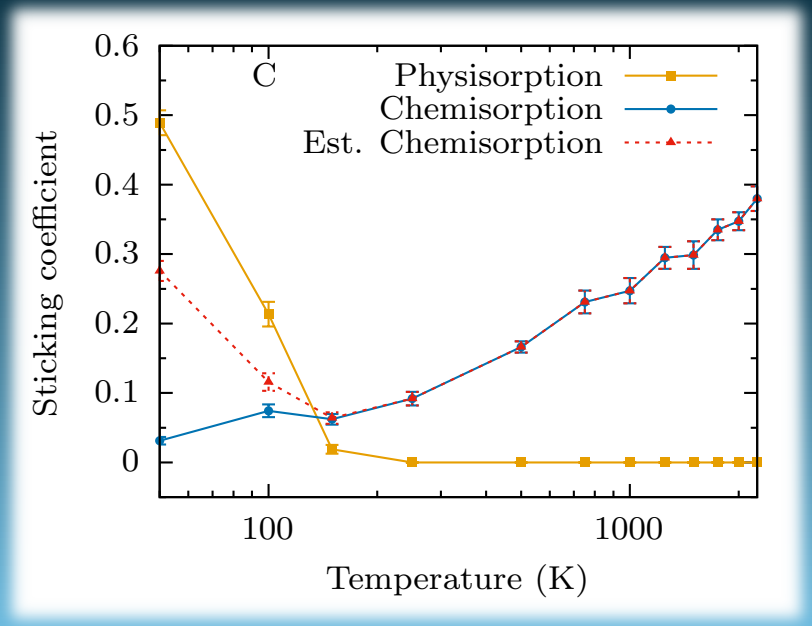
➢ No growth from H_2, CO (saturated valence, strong bond).

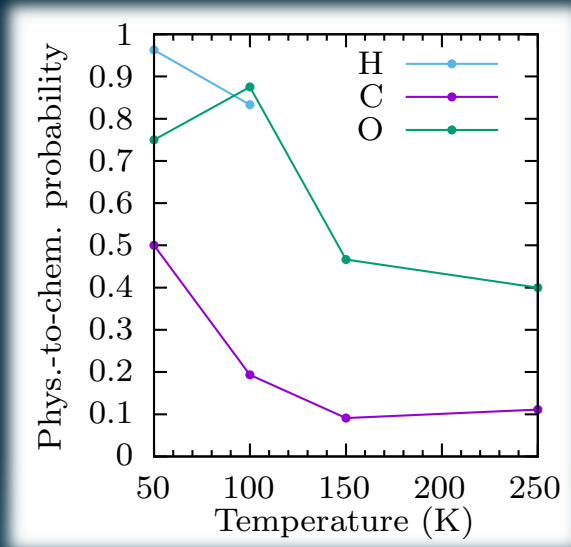
Sticking Coefficients

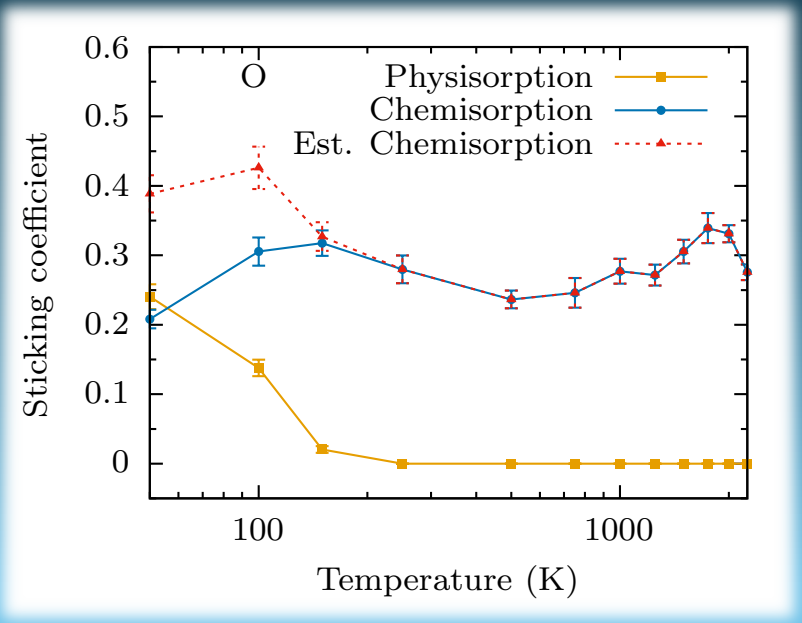
- When chemis. and phys. → phys. species can chemisorb or desorb.
- $\bar{\tau}_{\mathrm{coll}} \gg \bar{\tau}_{\mathrm{phys}\rightarrow\mathrm{chem/des}}$ → asymptotic sticking coeff. when #phys.$= 0$
- ➢ Estimated chem. from prob. $P_{\mathrm{phys}\rightarrow\mathrm{chem}}$

Results for H, C, O with $T = 50 - 2250$ K









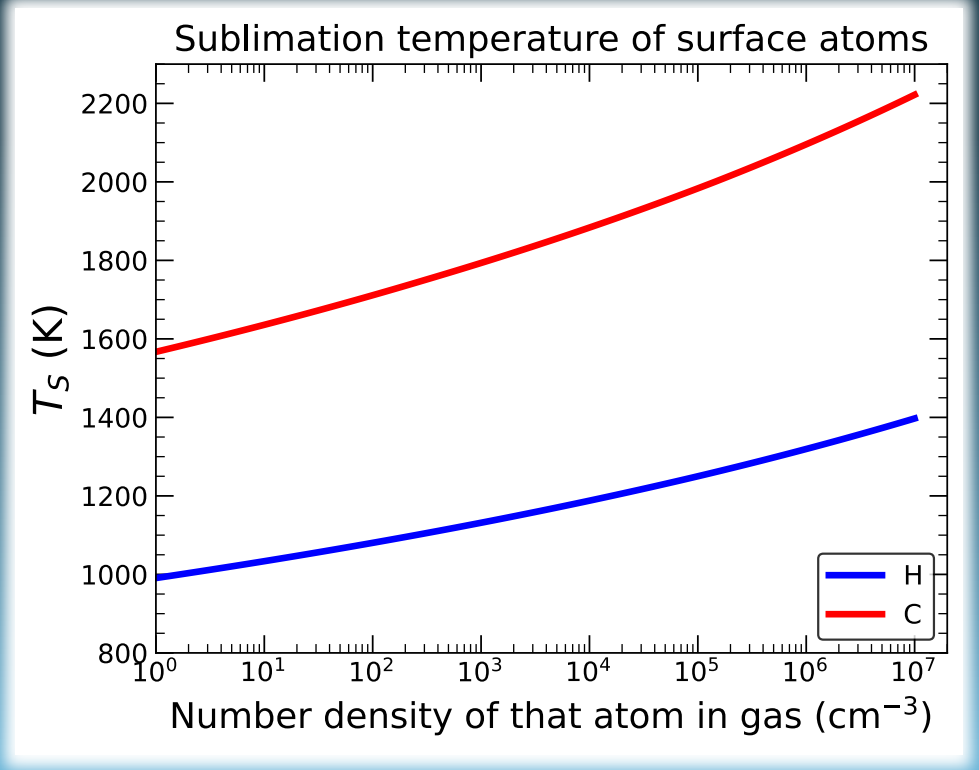
Bossion, D. et al., A&A, *submitted*

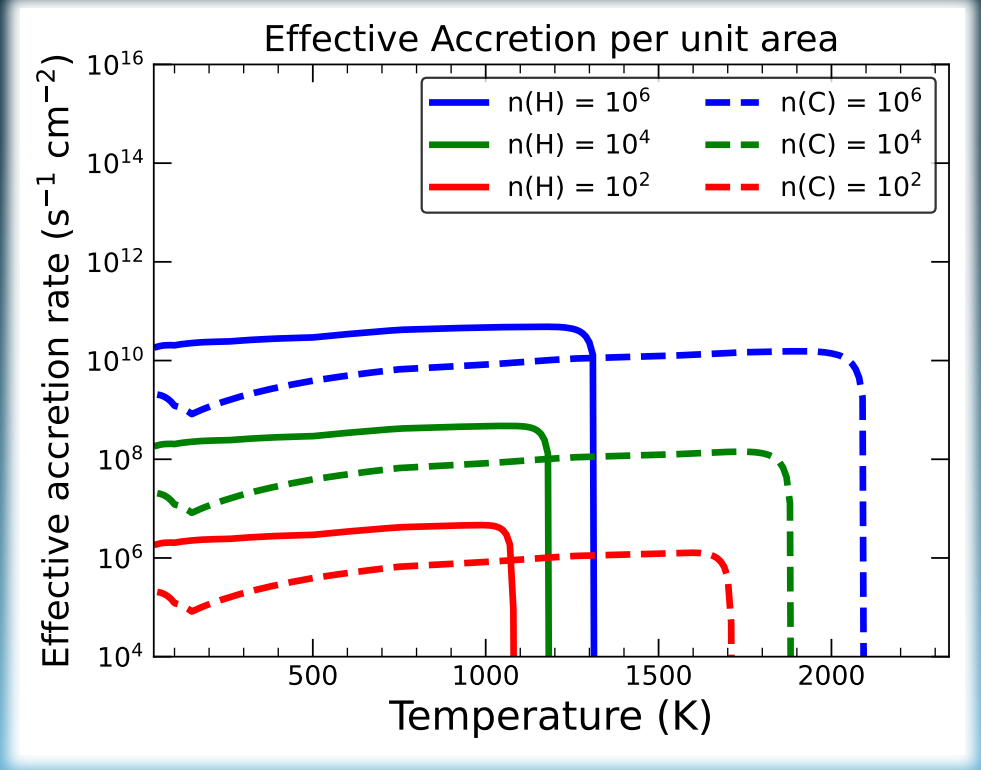
Dust Growth Through Accretion and Desorption

- Sublimation T when accretion & desorption rate of a species equalize:

$$F_i(T_{\rm subl}) = D_i(T_{\rm subl}).$$

- Effective accretion rate including accretion & desorption:
  - Dust composition, dust size at any T.

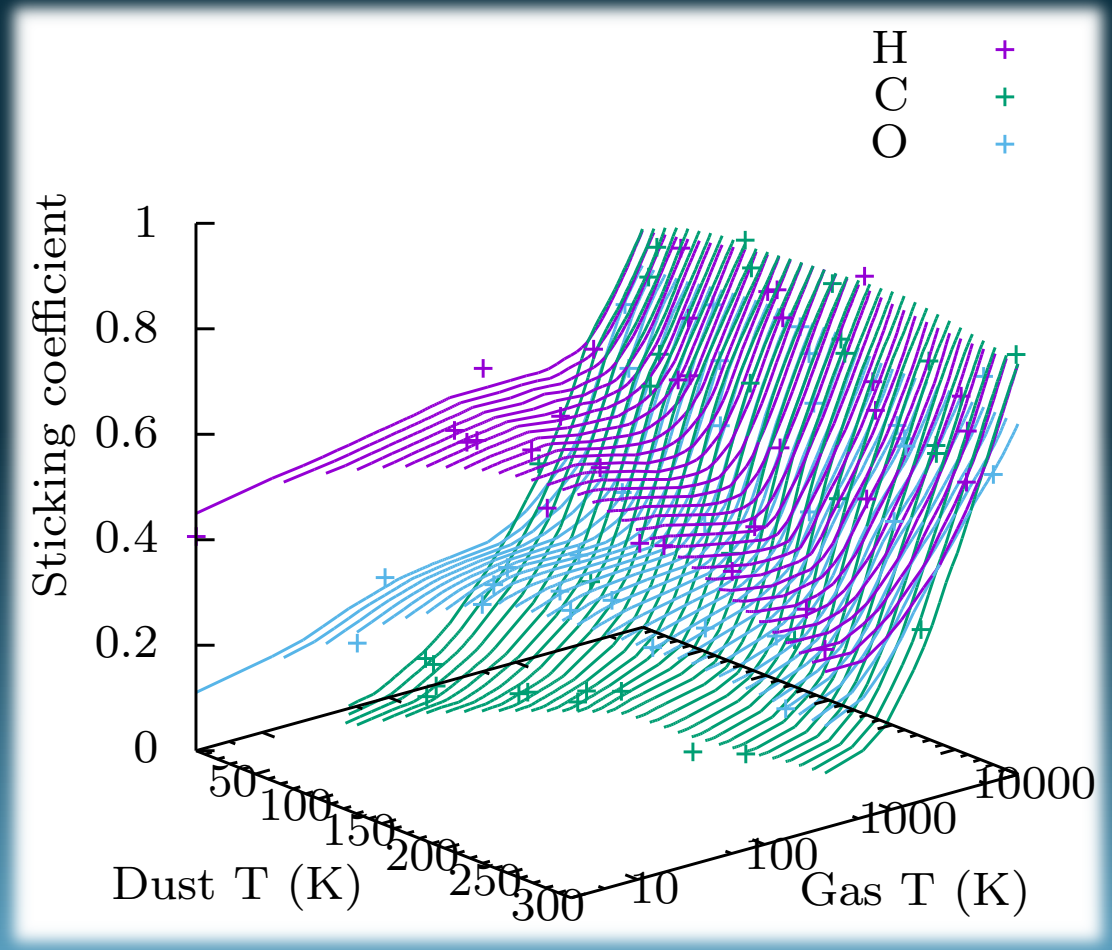




Bossion, D. et al., A&A, *submitted*

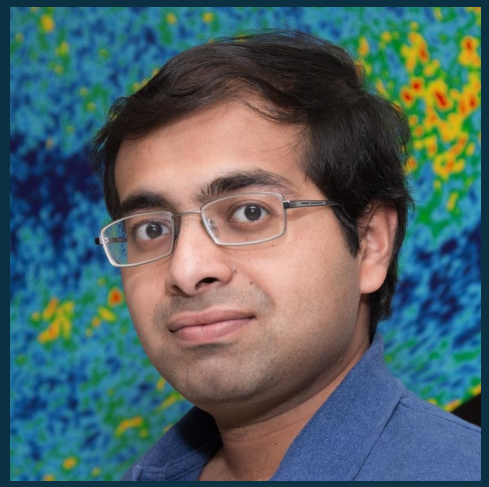
Future Directions

- ❖ Sticking coefficient for other colliding partners (like Fe, Mg…)
- ❖ Extend conditions to ISM: $T_{\mathrm{dust}}(3-300\ \mathrm{K}) \neq T_{\mathrm{gas}}(3-10\ 000\ \mathrm{K})$
- ➢ Ongoing, use of ML (Multi-layer Perceptron) to predict sticking coefficients for many (T_{dust}, T_{gas}) and species (N-D interpolation).
- ❖ Extend the study to silicate type dust (ongoing, more structures).



Collaborators

Gunnar Nyman
Molecular physics,
University of Gothenburg, Sweden



Arka Sarangi
Dust modeling,
Niels Bohr Institute, Denmark,
Indian Institute of Astrophysics, India

and

The Origin and Fate of Dust in Our Universe Collaboration

Funded by

Knut and Alice Wallenberg Foundation

Thank you for your attention!