Monte Carlo simulations of H_2 formation on grains of varying surface roughness

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- Mechanism for H_2 formation
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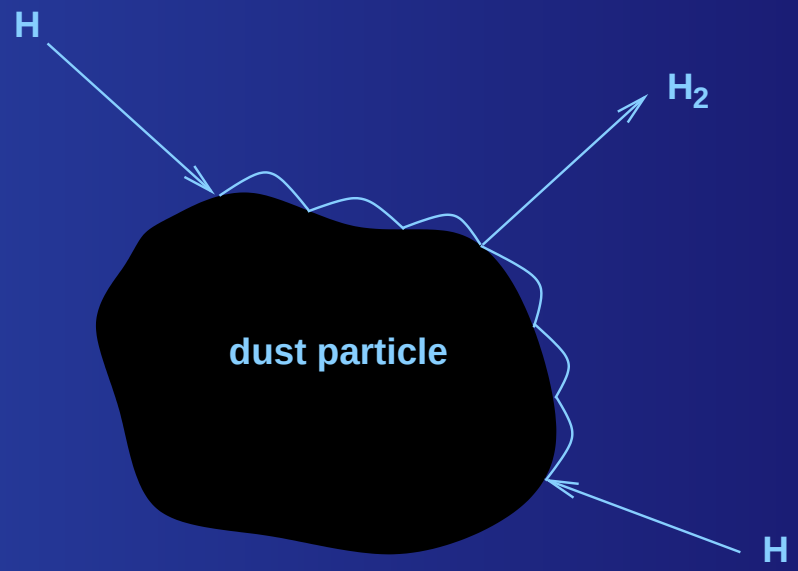
Molecular hydrogen formation

- Not possible in the gas phase
- Formed on interstellar grains
  - Two atoms land on dust particle
  - Move across the surface
  - Combine
  - H_2 evaporates



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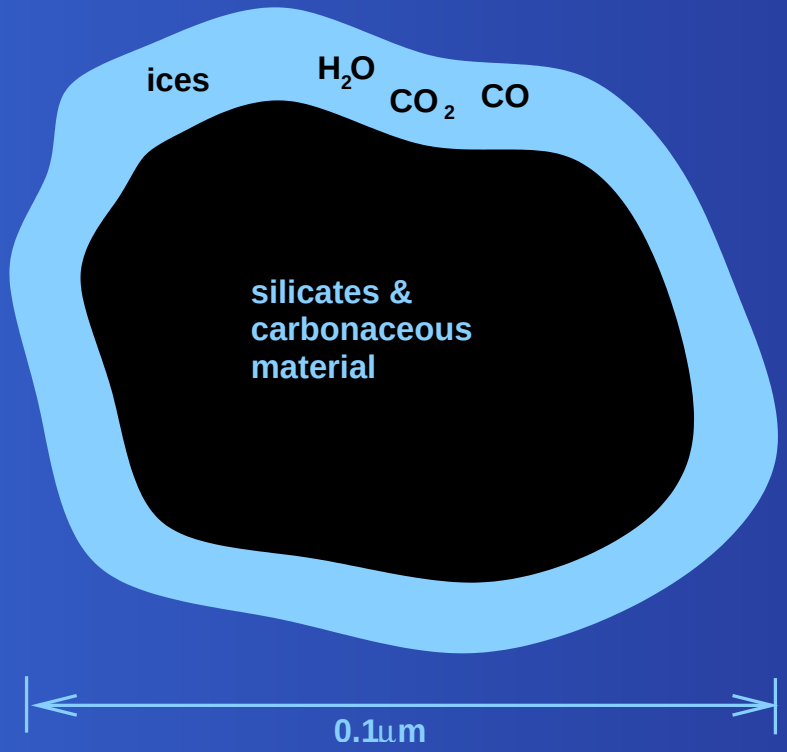
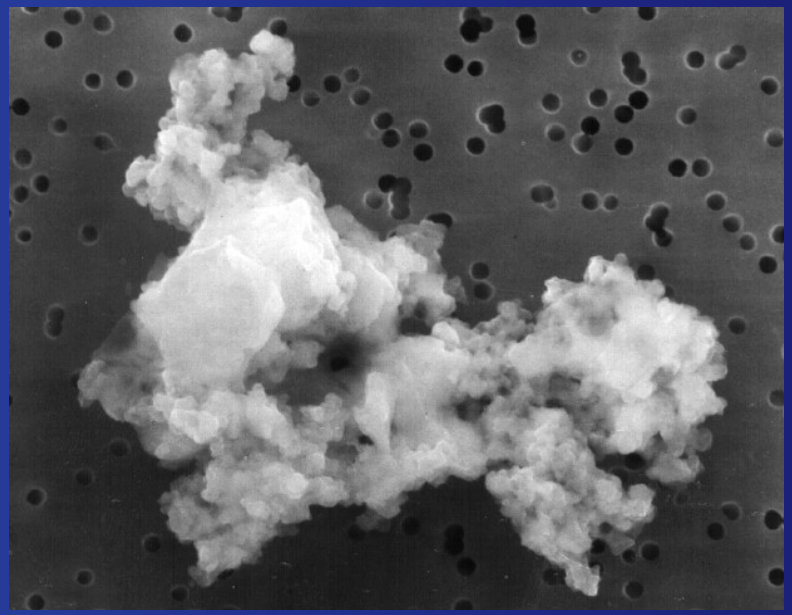
Interstellar grains

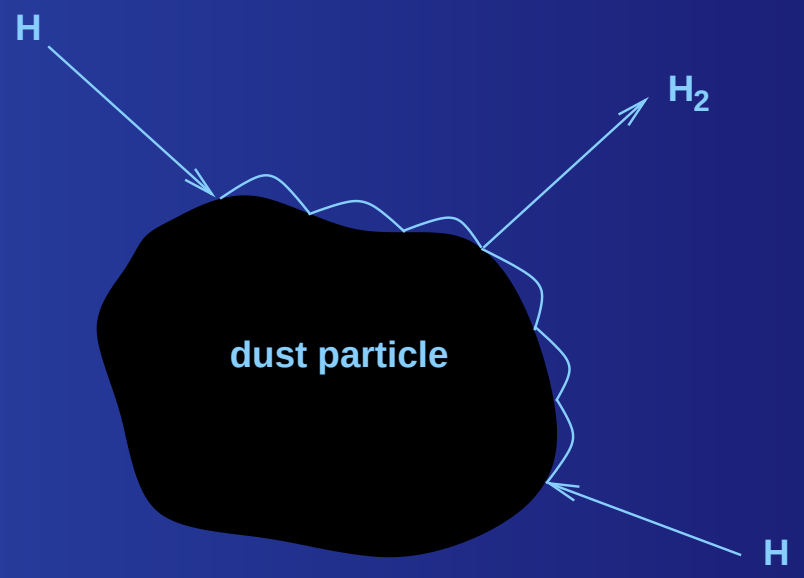




Interstellar dust particles are mostly amorphous.

H_2 formation on dust

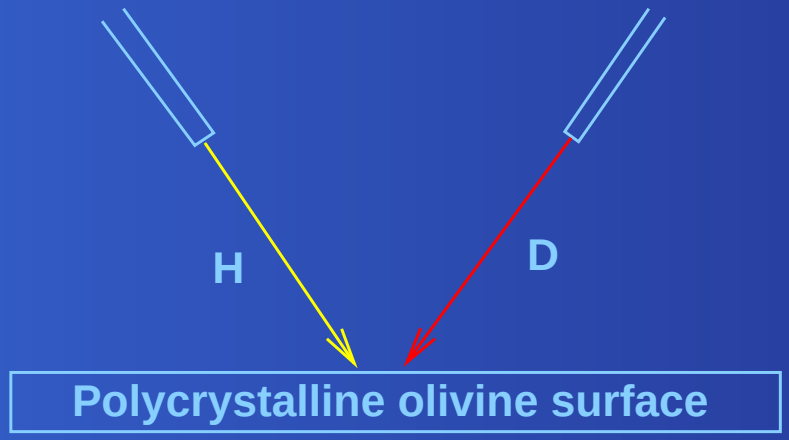
- temperature
- presence of ices
- material
- surface structure
  - evaporation barriers
  - hopping barriers



Laboratory experiments

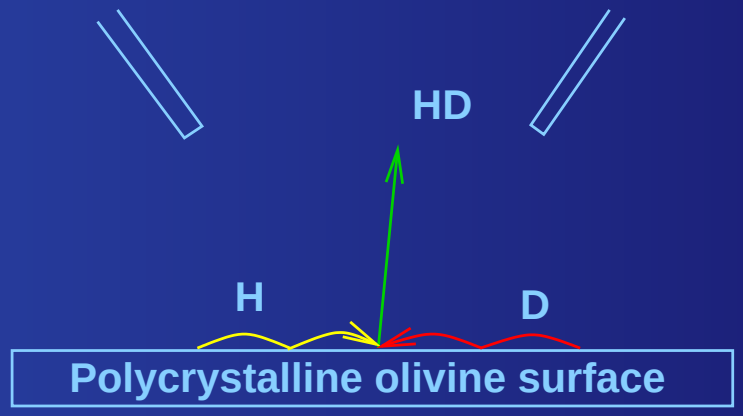
Temperature Programmed Desorption

Phase 1



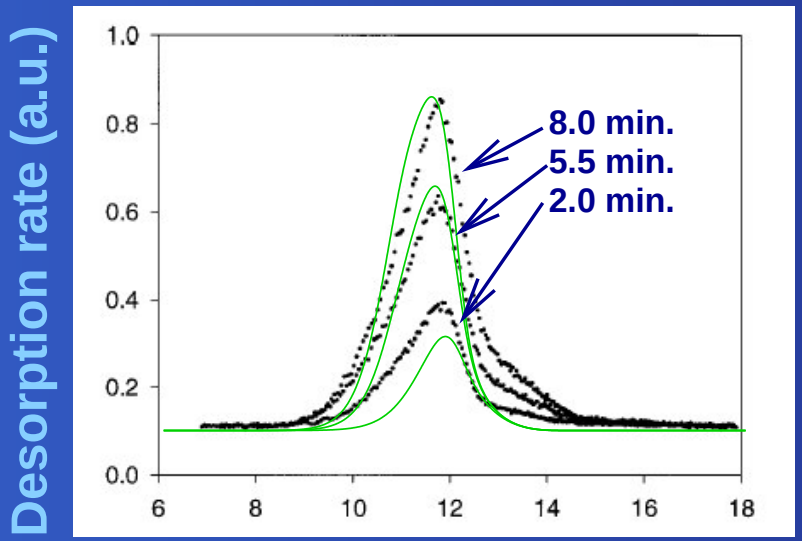
Constant low temperature of 6 K

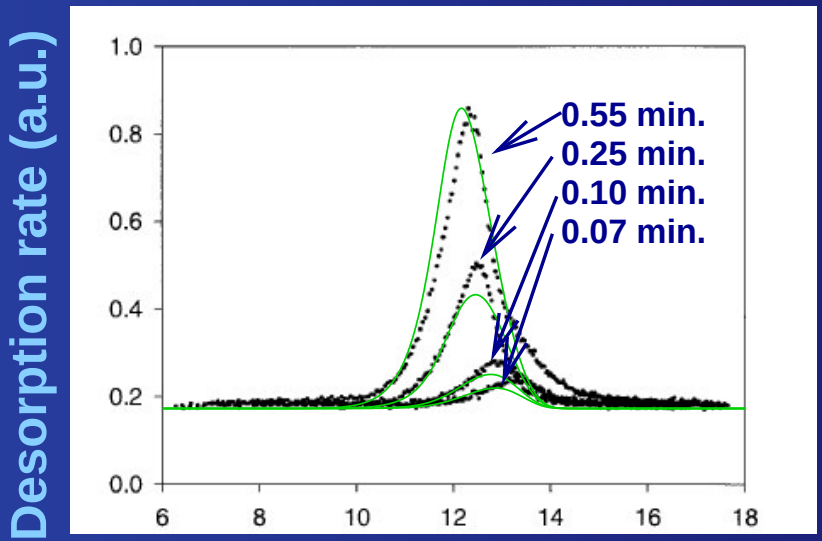
Phase 2



Temperature is raised with 0.6 Ks^{-1}

TPD experiments





Graphs taken from Pirronello et al., Astrophys. J. 483 (1997) L131

Fits by Katz et al., Astrophys.J. 522 (1999) 305

Problem: with the barriers found only molecular hydrogen production possible between 6-10 K.

Possible explanation for discrepancy

Due to model:

- Only one barrier is used for hopping and evaporation
- Spatial distribution of H atoms is not taken into account

Lab setup cannot be translated to interstellar case

- Large surfaces vs. small particles
- Polished vs. “fluffy”
- Polycrystalline vs. amorphous

Monte Carlo simulations

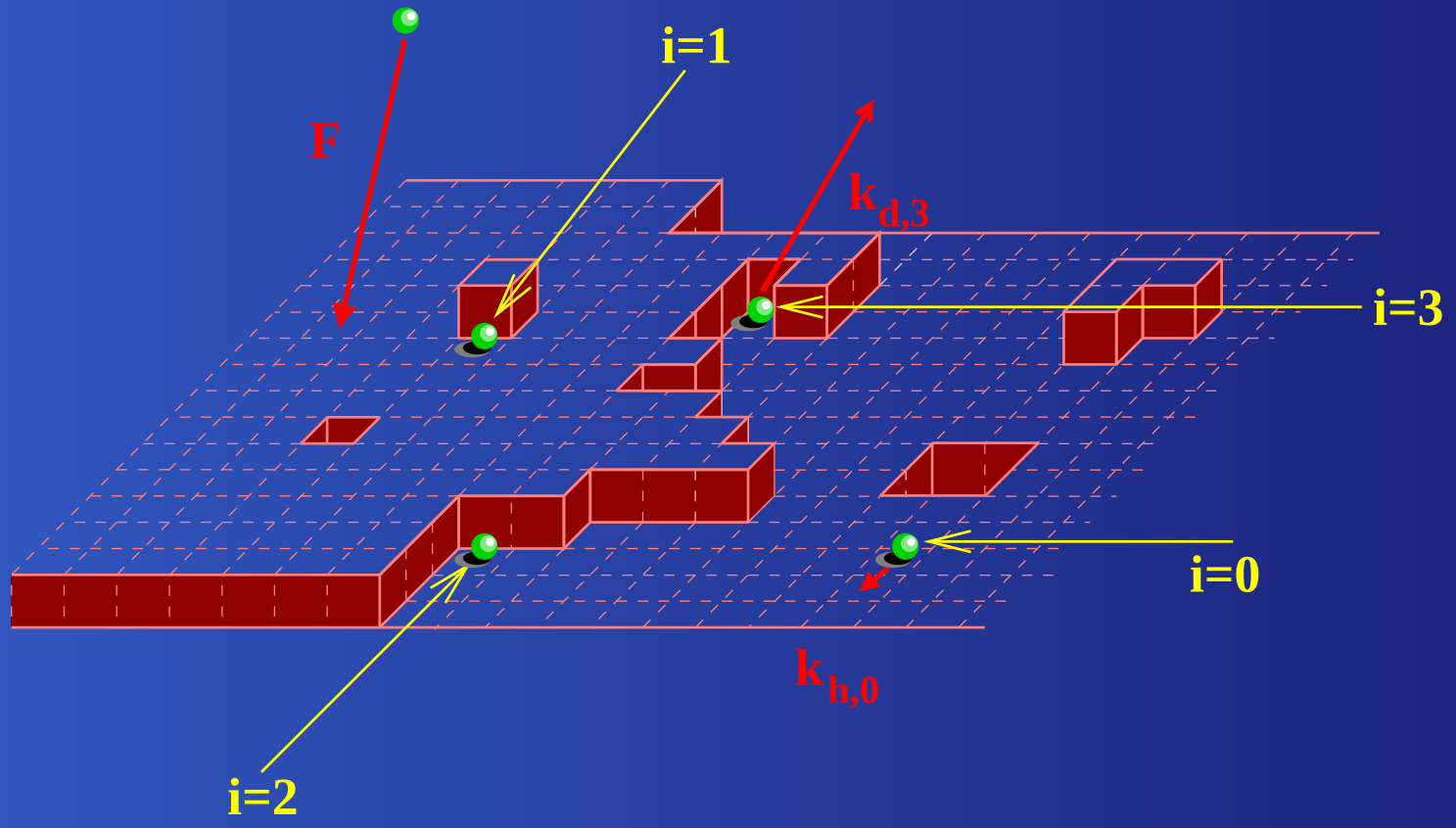
Advantages

- Surface structure can be included
- Individual atoms can be followed

Disadvantage

- High demand of cpu

Monte Carlo simulations



Hopping and evaporation is dependent on number of neighbors on the surface

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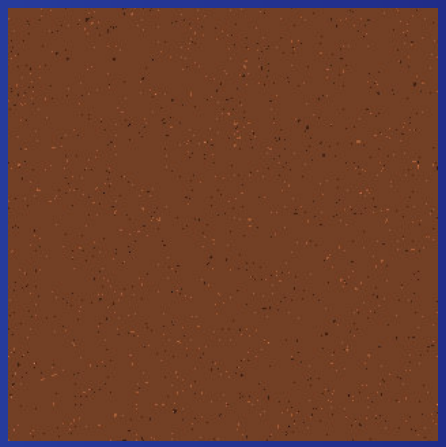
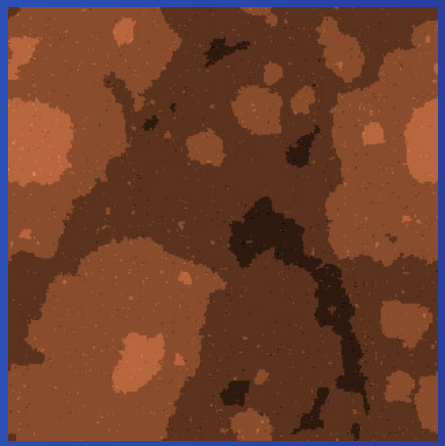
Surfaces

(a)

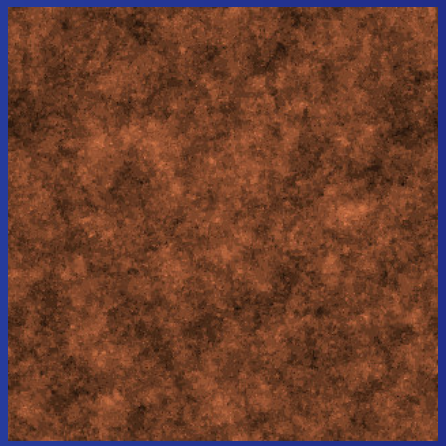
(b)



(c)

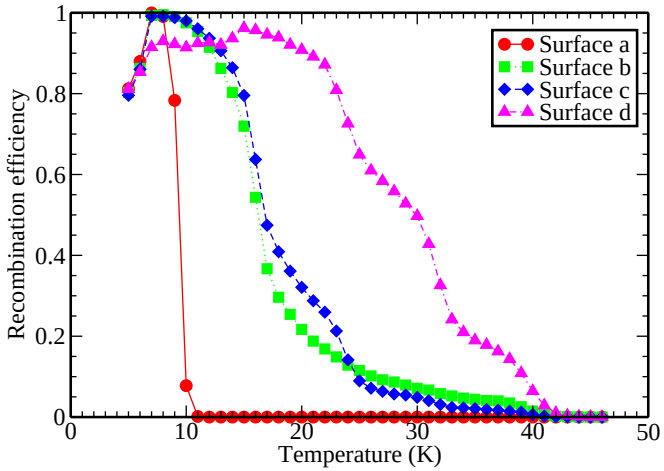


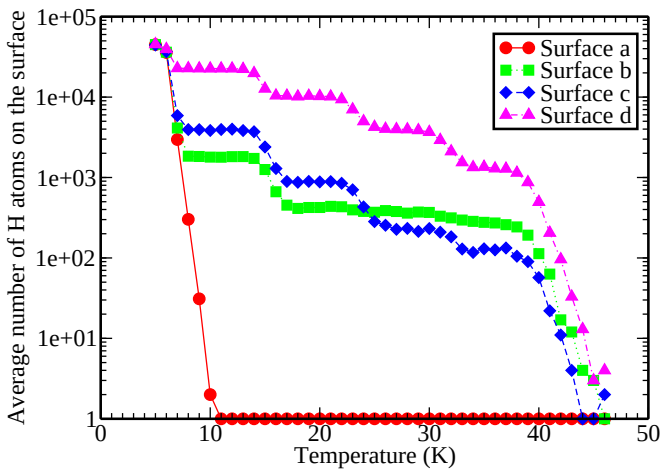
(d)



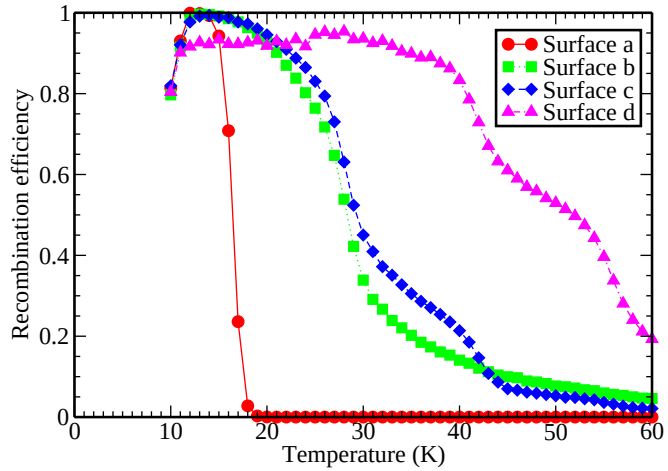
Results

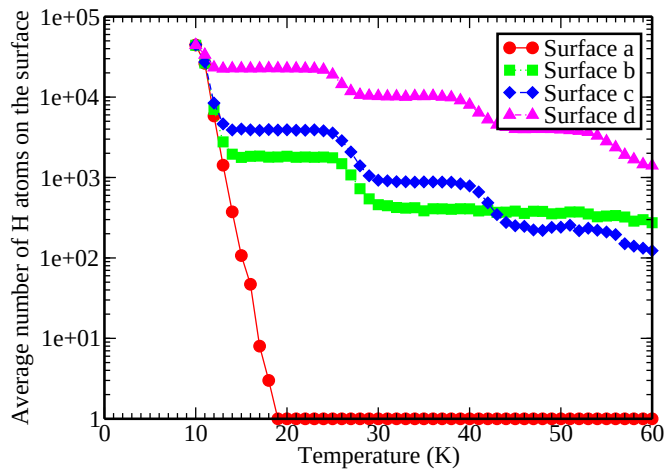
Olivine



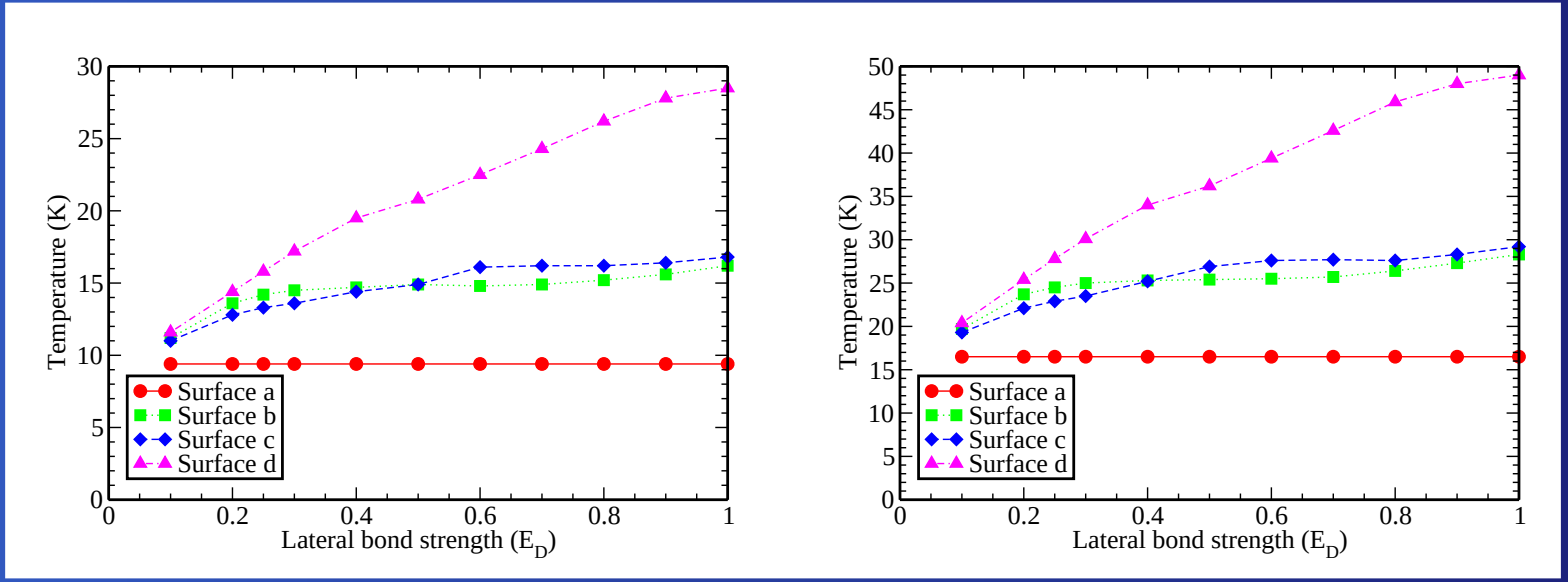


Amorphous carbon



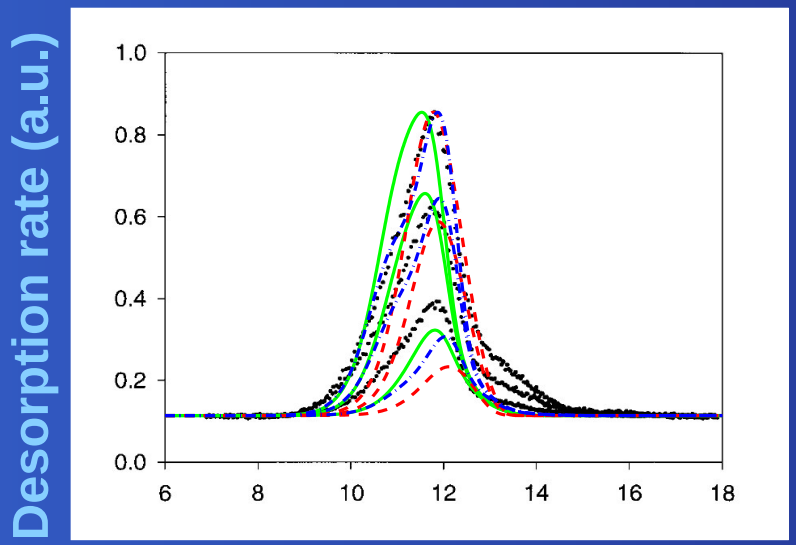


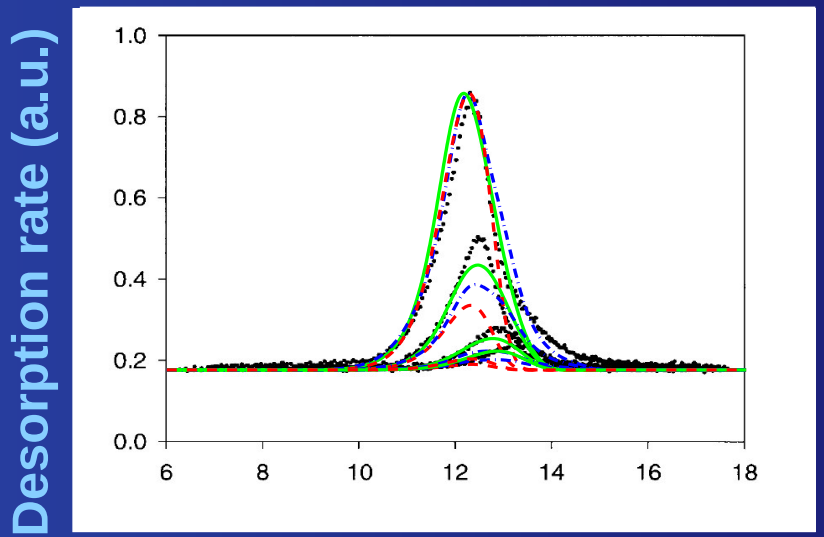
Influence of the lateral bond



- For low lateral bond still increase in temperature range
- For surface d stronger dependence than b and c

Model compared with TPD data





orginal fit by Katz et al.

new model with $E_I = E_D$

new model with $E_I = 0.09\ E_D$

Summary and Future plans

- Using the model with only one barrier, it is not possible to reproduce hydrogen formation in a large temperature range.
- If surface roughness is included using Monte Carlo simulations, this range is much larger depending on the lateral bond strength.

Future plans

- Other species
- Influences of ice mantle
- Comparison with new TPD measurements