H_2 formation on stochastically heated grains

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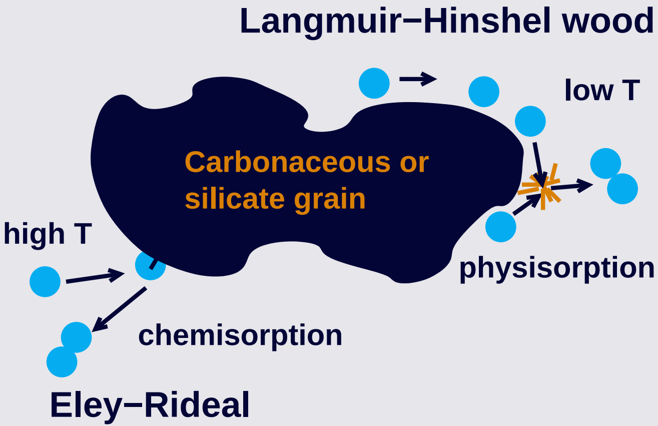
Problem of molecular hydrogen

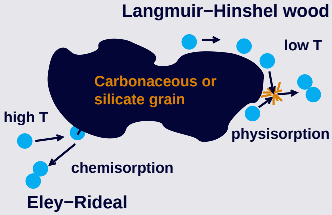
- H_2 is most abundant molecule in ISM
- H_2 is formed in diffuse clouds
- Gas phase reaction is not possible
- H_2 is formed by a surface reaction
- Rate constant α should be 2×10^{-17} cm^3 s^{-1} (Jura (1974))
    - Gas phase type reaction between grain and H atom

Molecular hydrogen formation

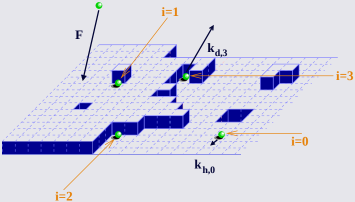


H_2 formation in diffuse clouds

- atomic H abundance (≈ 100 cm^{-3} $\approx 3 \times 10^6$ cm^{-2} s^{-1})
- gas temperature (60-100 K)
- grain temperature (≈ 20 K)
- energies of evaporation
- hopping barriers



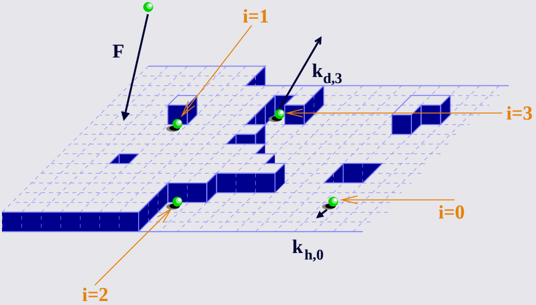
Monte Carlo simulations



$$R_{hop} = \nu \exp\left(-\frac{E_b(i)}{kT}\right)$$

$$R_{eva} = \nu \exp\left(-\frac{E_D(i)}{kT}\right)$$

- $+$ Surface structure can be included
- $+$ Individual atoms can be followed
- $+$ Laboratory and interstellar fluxes can be used
- $\pm$ All energy barriers have to be provided
- \- High demand of cpu
- \- No dynamical and structural information



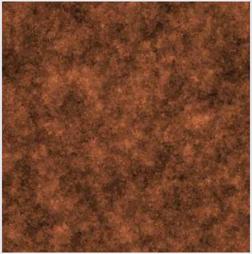
$$k_{hop} = \nu \exp\left(-\frac{E_h + iE_l}{kT}\right)$$

$$k_{des} = \nu \exp\left(-\frac{E_D + iE_l}{kT}\right)$$

Surfaces

flat

rough



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$$k_{des} = \nu \exp\left(-\frac{\mathbf{E_D} + i\mathbf{E_l}}{kT}\right)$$

Monte Carlo simulations

Sequence of processes is chosen using random numbers according to transition probabilities

Free parameters

- temperature
- flux
- surface
- energy barriers

Grain

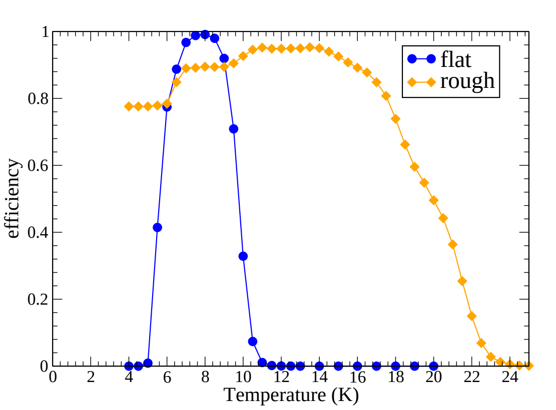
Hydrogen

Oxygen

Top view of the surface (50 $\times$ 50 sites)

$\sim$1 day

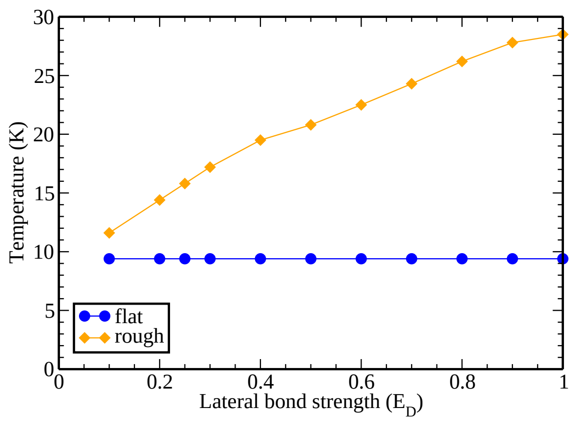
Results at constant temperature



- Efficient H_2 formation for rough surface

Cuppen & Herbst, MNRAS (2005), 361, 565-576

Influence of the lateral bond

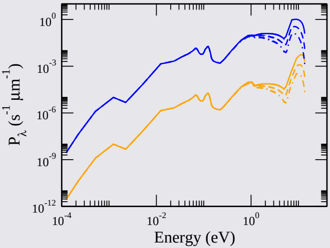


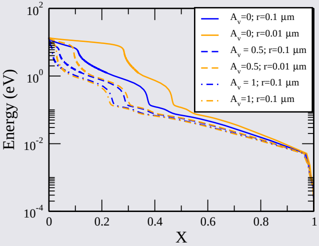
- Strong dependence of temperature range on lateral bond
- For small lateral bond still increase in temperature range

Cuppen & Herbst, MNRAS (2005), 361, 565-576

Stochastic heating in diffuse clouds

Interstellar grains are pulse heated by photons from stars in a stochastic manner

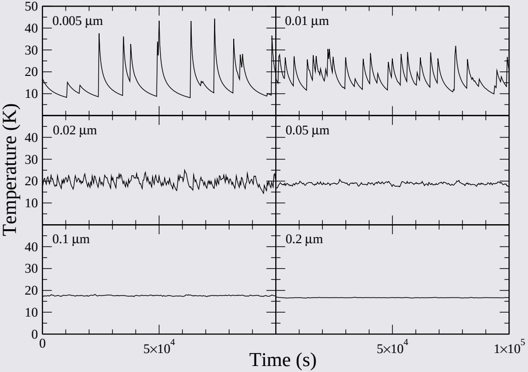




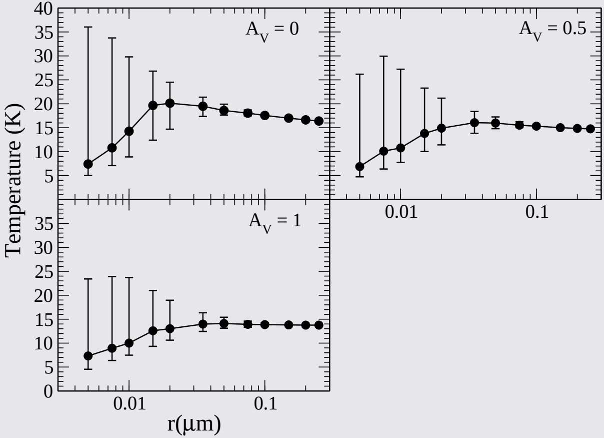
$$P_\lambda = \pi r^2 I_\lambda Q_{abs}(\lambda) D_\lambda$$

Stochastic heating in diffuse clouds

Interstellar grains are pulse heated by photons from stars (Draine, ARAA, 41 (2003) 241)

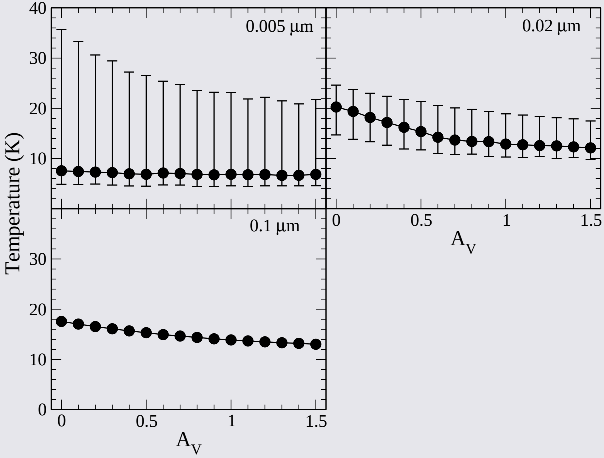


Grain temperature



- Small grains have a lower temperature most of the time.
- Small grains have a stronger temperature fluctuations.

Grain temperature



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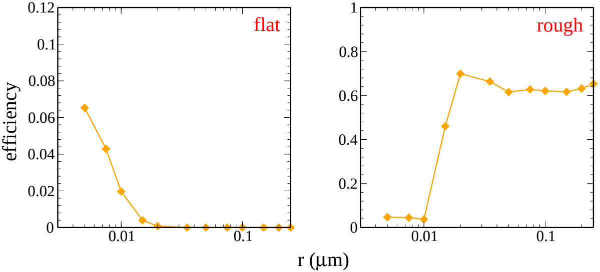
Results for stochastic heating



Efficiency is highly grain size dependent

Cuppen, Morata and Herbst, MNRAS (2006), 367, 1757

Results for α

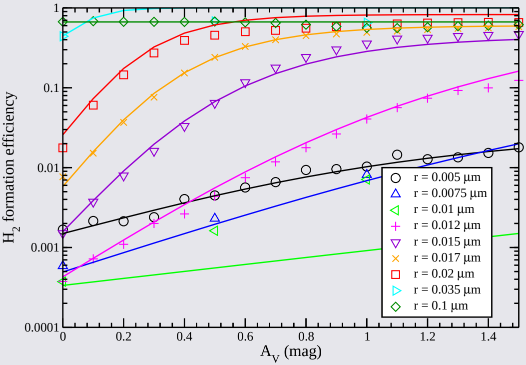
	$A_V = 0.5$	$A_V = 0.5$	$A_V = 0.5$
flat	6.50×10^{-19}	1.99×10^{-18}	2.91×10^{-18}
rough	3.12×10^{-17}	4.75×10^{-17}	5.62×10^{-17}

α should be 2×10^{-17} cm^3 s^{-1}

Rate is high enough for the rough surface to explain observations

Results for stochastic heating

- Introduction
- Monte Carlo simulations
- Results
- Stochastic heating
- Extra



$$\eta = a_0 \exp\left(a_1 \tanh(a_2 A_\mathrm{V})\right)$$

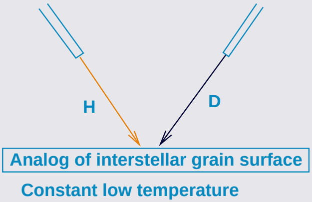
$$a_0 = \exp\left(\min(2.13 \arctan(281(r - 0.02)) - 3.656, 62000(r - 0.01) - 8)\right)$$

$$a_1 = \min(24.2 \exp(-97.18 r), 1423 r - 4.11)$$

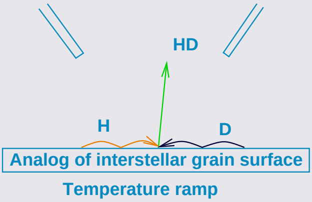
$$a_2 = \max(-134 r + 1.43, 299 r - 2.88)$$

Temperature Programmed Desorption

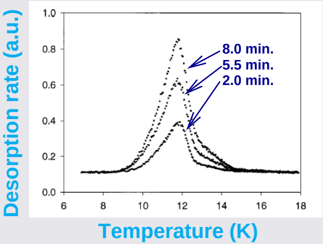
Phase 1

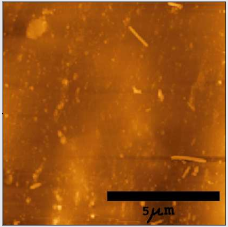


Phase 2



$$H + D \rightarrow HD$$





Pirronello et al., ApJ. 483 (1997) L131

Desorption under laboratory conditions

Analysis of TPD experiments

- Fitted with simple rate equations
- Translated to interstellar conditions (very low fluxes)

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$\longrightarrow$ Only efficient for 6-10 K

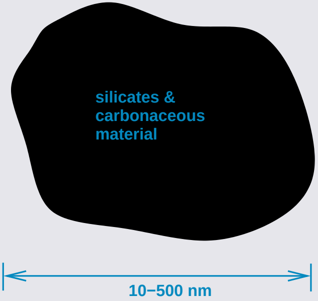
Analysis of TPD experiments

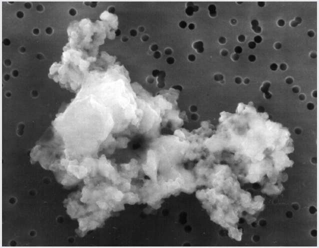
- Fitted with simple rate equations
- Translated to interstellar conditions (very low fluxes)

$\longrightarrow$ Only efficient for 6-10 K
$\longrightarrow$ Not a possible formation route

Interstellar grains

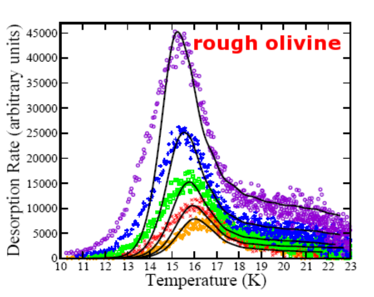
- have a "fluffy" shape
- are bare in these conditions



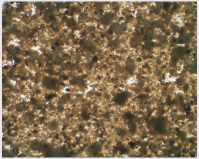


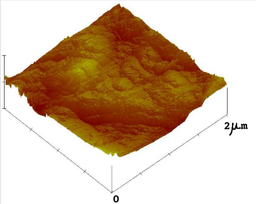
TPD experiments

H + D → HD



Vidali et al. J. Phys. Chem. A (2007) 111, 12611





Experimental confirmation of simulation results at higher temperatures