Monte Carlo simulation to investigate the formation of various deuterated species on interstellar dusts

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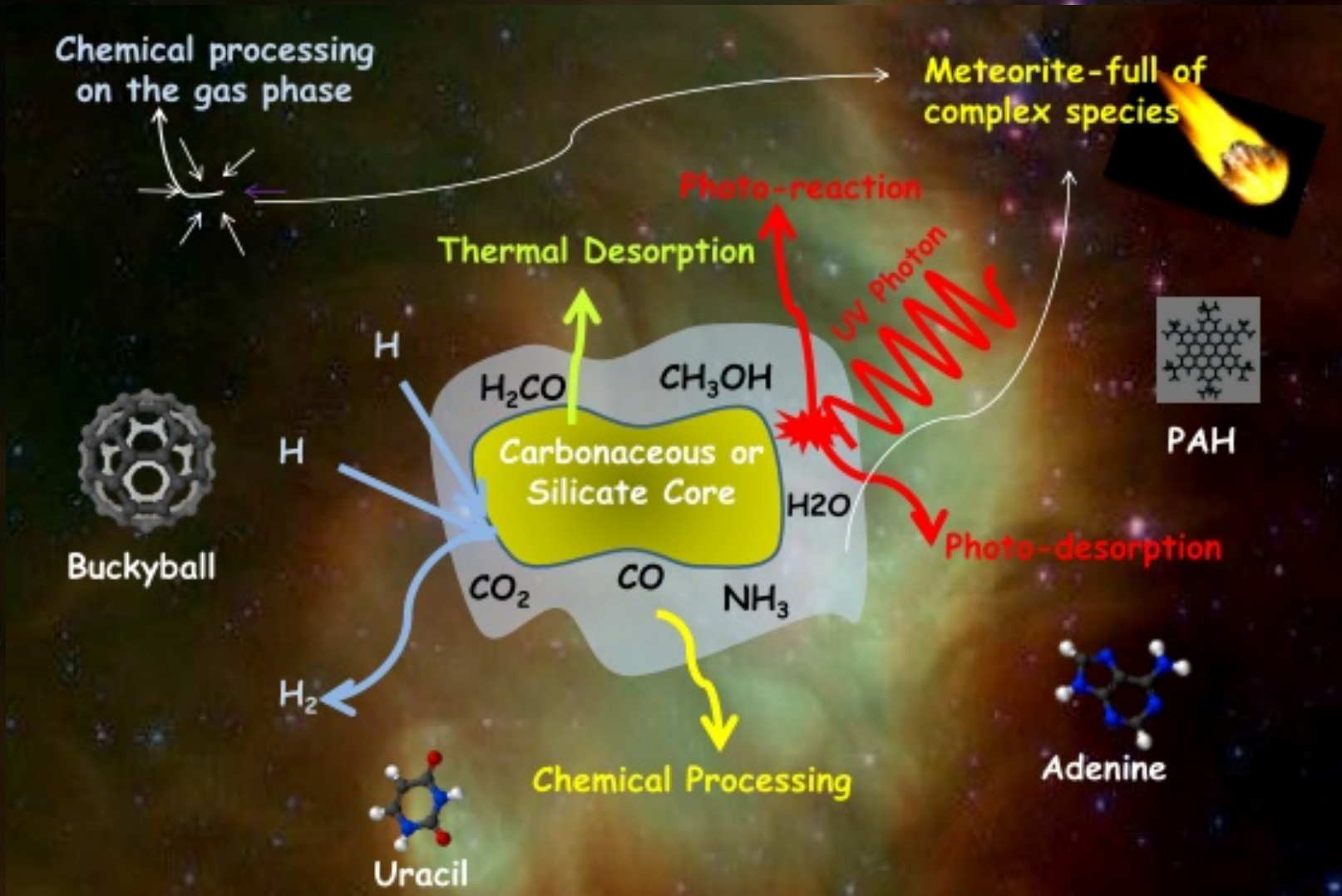
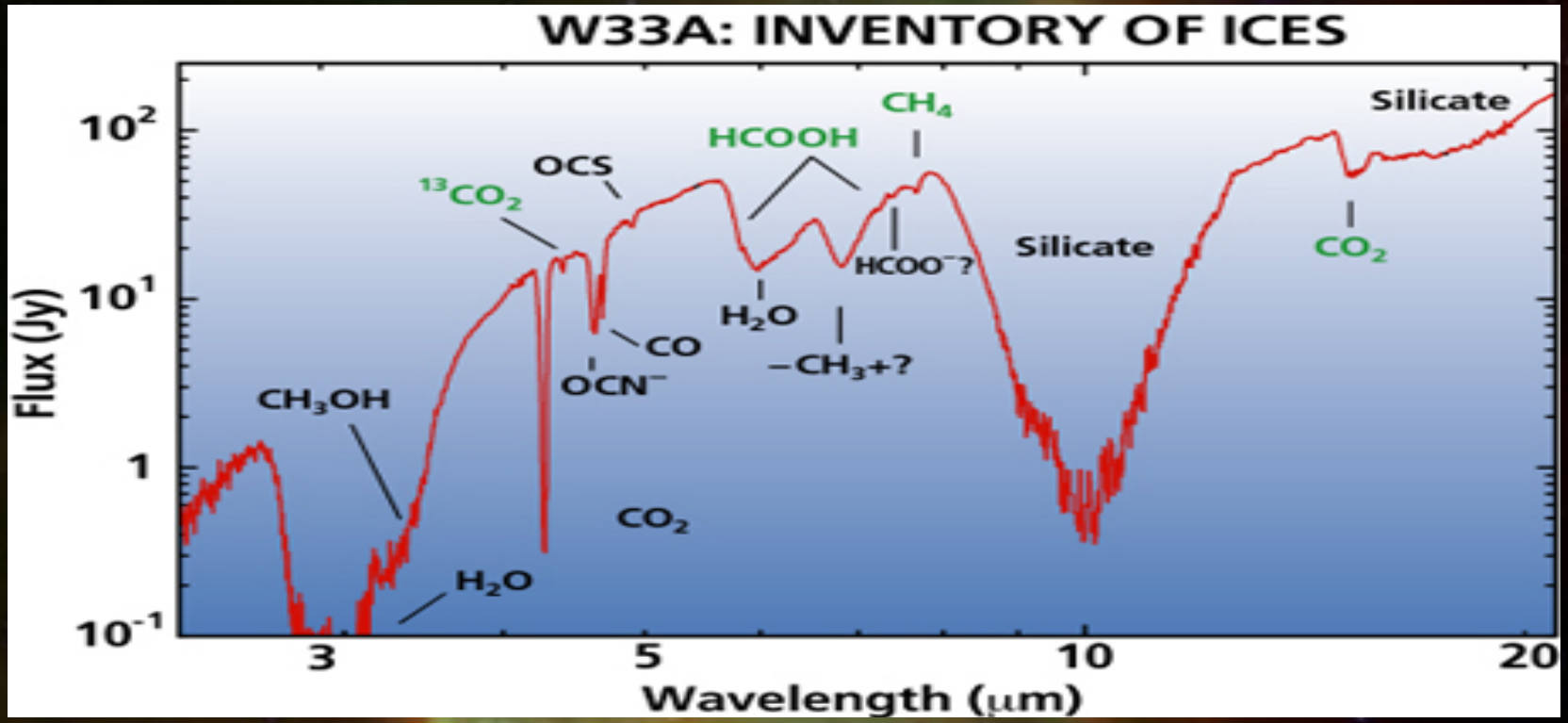
Plan of this presentation

- Introduction and basic process on interstellar dust
- Formation of most simplest molecule, H_2
- Formation of complex molecules on interstellar dust
- Deuterium enrichment of grain mantle
- Conclude

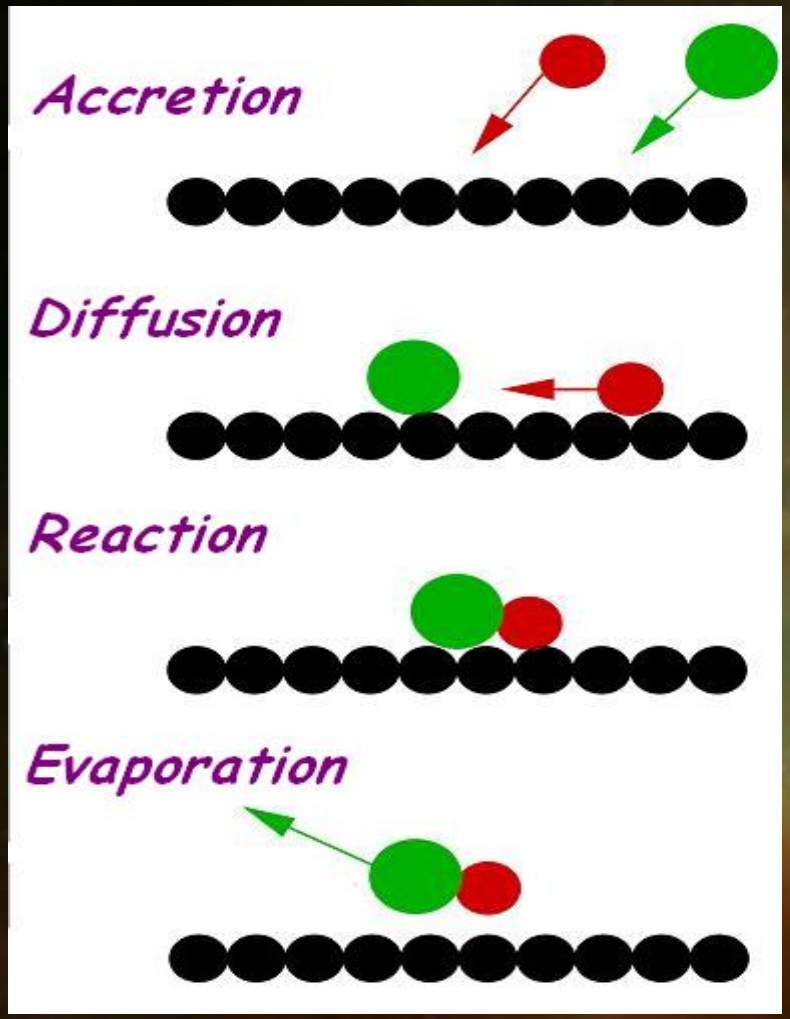
Cartoon diagram of the interstellar process





Gibb et al. 2000, Schutte et al. 1999

Basic physical process on interstellar grains



Accretion

$F_x = \alpha\ \sigma\ v\ N_x\ N_d$

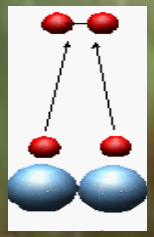
Diffusion

$t_{hop} = \nu_0^{-1} \exp(E_b/KT_d)$ sec

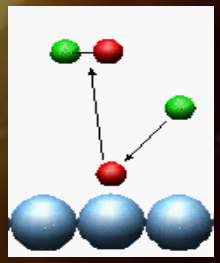
$t_{tun} = \nu_0^{-1}[(4\pi a/h)(2mE_b)^{1/2}]$ sec

Reaction

LH



ER



Evaporation

$k_e = \nu_0 \exp(-E_d/KT_d)\ s^{-1}$

$K_{crd} = f(70K)k_e(i,70K)\ s^{-1}$

Various approaches to handle grain chemistry

Deterministic approach

- Define an effective rate coefficient based on the mobility and mean free path before interaction.

- Need to solve a set of coupled ODEs.

- Much faster and would easily be coupled with the large gas phase network but results are acceptable in some regime of simulation.

- Rate equation, Master equation methods belongs to this category.

Stochastic Approach

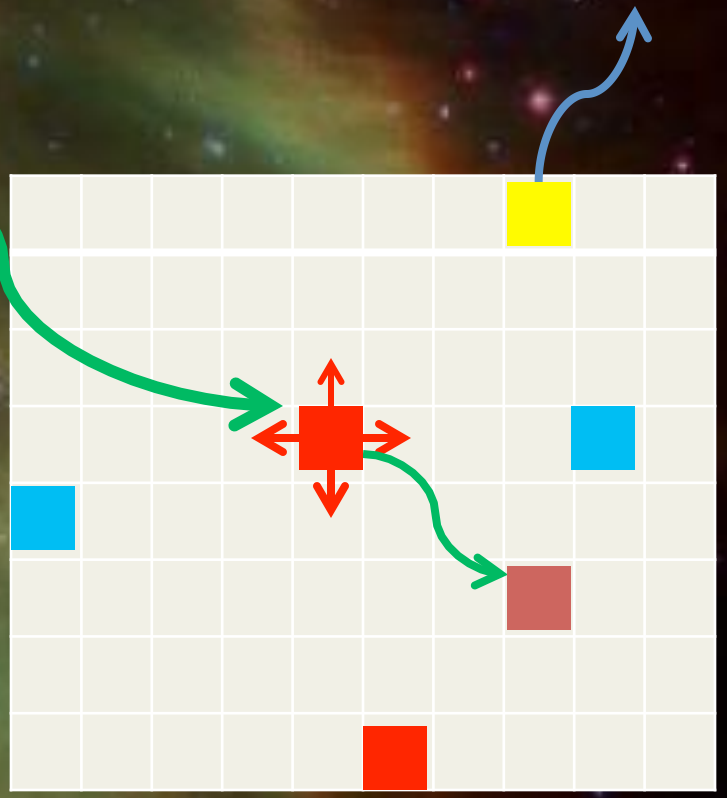
All the possibilities are modeled with the random number generators.

Accretion

Diffusion

Reaction

Evaporation



Monte carlo method belongs to this category. Very slow process. Quite impossible to couple with gas phase chemical network.


Formation of H_2

Formation of most abundant molecule, H_2

Variation of n_H and n_{H2} on grains:

$$\frac{dn_H}{dt} = \phi_H - W_H n_H - 2(A_H/S)n_H^2$$

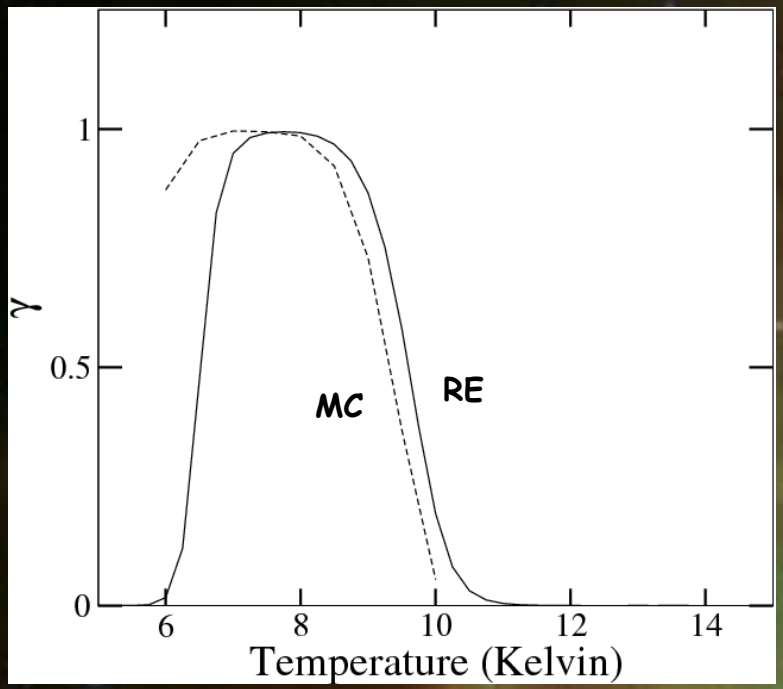
$$\frac{dn_{H2}}{dt} = \mu(A_H/S)n_H^2 - W_{H2}n_{H2}$$

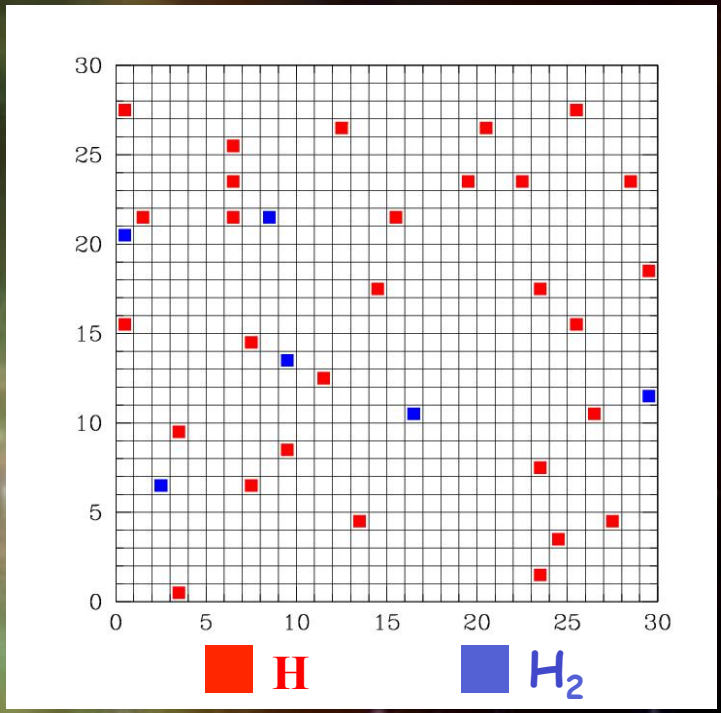
Gas phase production

Recombination Rate

$$R_{H2} = (1-\mu)(A_H/S)n_H^2 + W_{H2}n_{H2}$$

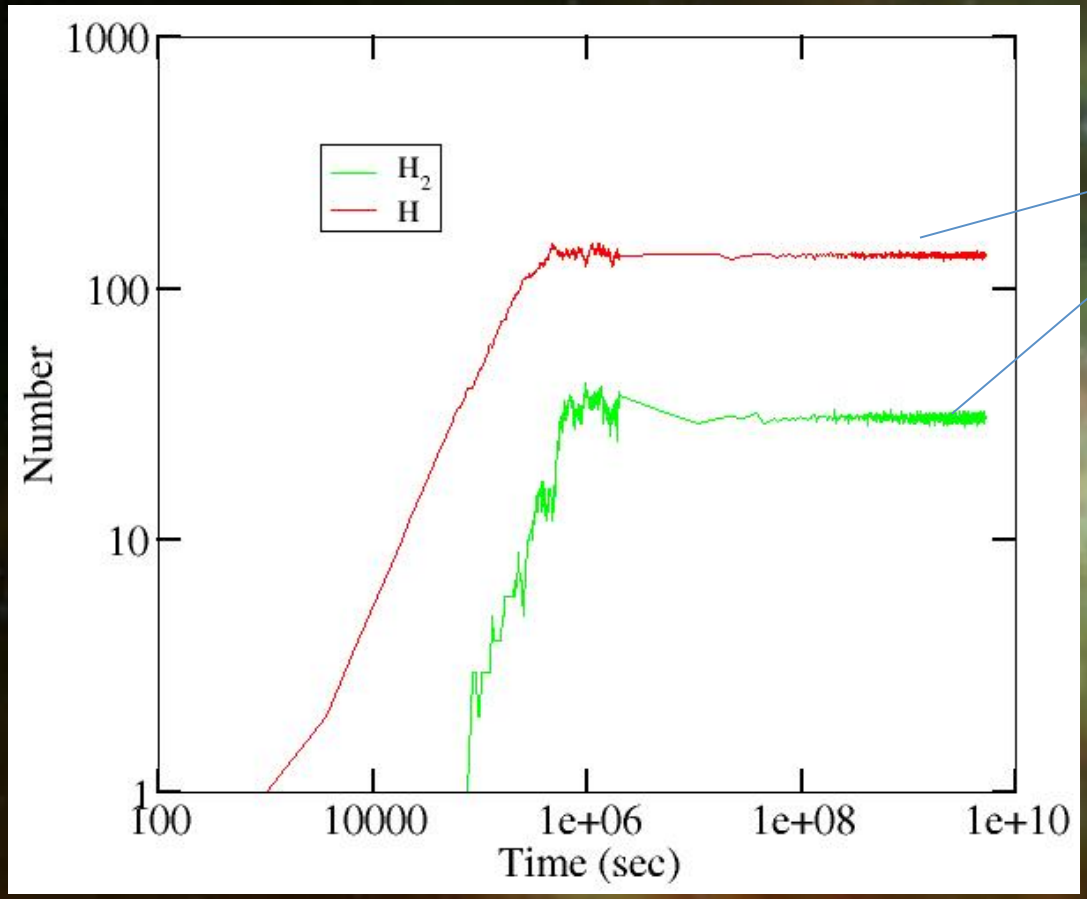
H_2 formation efficiency





Chakrabarti, Das et al. 2006, A&A

Difference between two methods would be attributed due to the assumption of average recombination efficiency ($R_e = A_H/S$) in case of rate equation method. In principle $R_e = A_H/S^{\alpha}$)

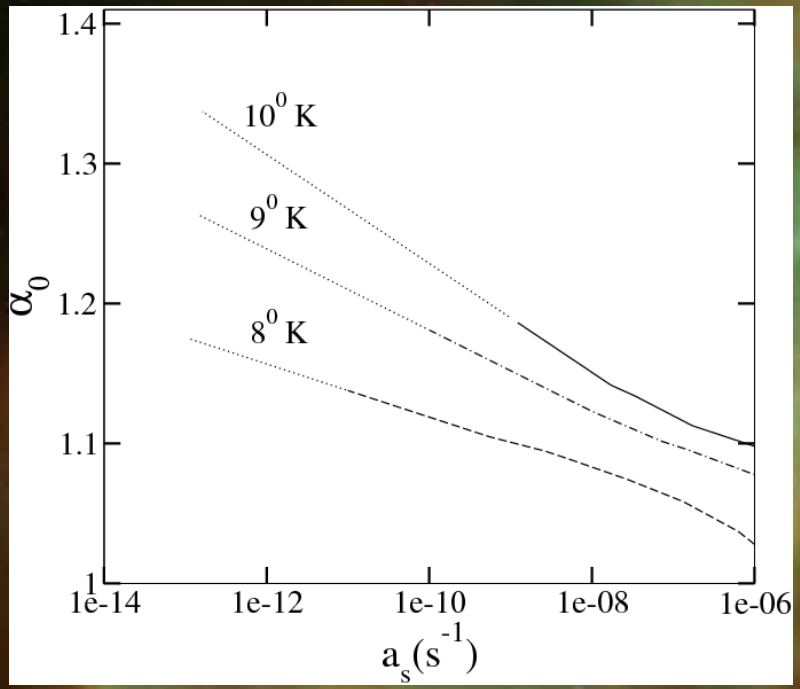


Steady state

In a steady state $\alpha \rightarrow \alpha_0$ and $dn_H/dt=0$ and $dn_{H2}/dt=0$ thus

$\alpha_0 = \log[2A_H n_H^2/(\Phi_H - W_H n_H)]/\log(S)$

Chakrabarti S. K., Das A. et al., A&A, 2006



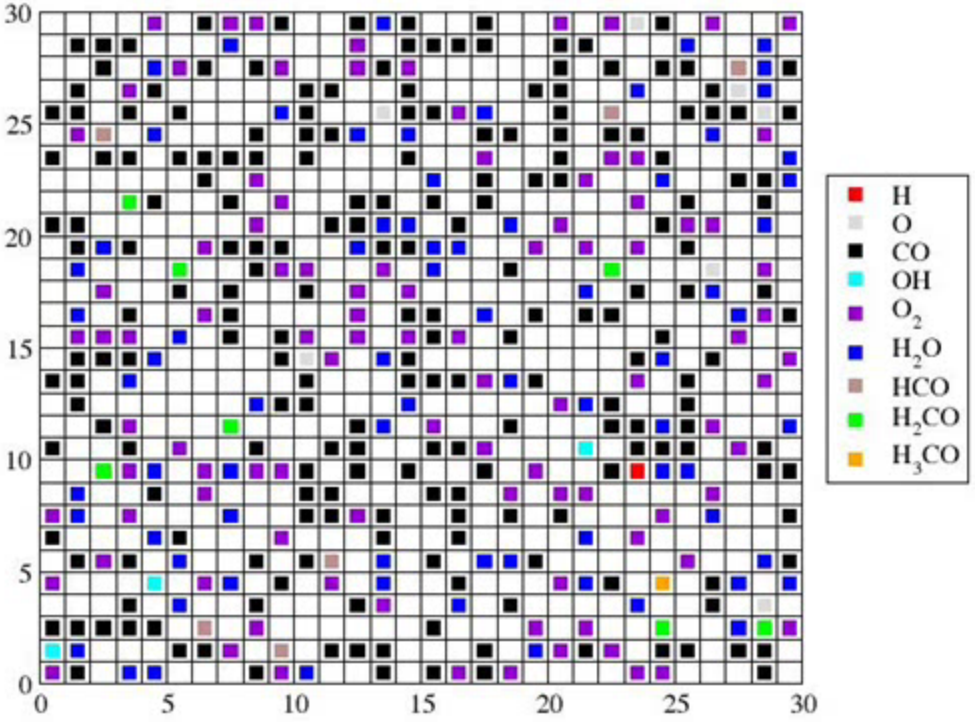
Chakrabarti, Das et al. 2006, A&A

α_0 clearly deviates from 1. Thus it is essential to consider Monte Carlo method to appropriately study the grain chemistry.

Hydrogenation network for the formation of water and methanol

	Reactions	E_a(K)	Comments
1	$H+H \rightarrow H_2$		
2	$H+O \rightarrow OH$		
3	$H+OH \rightarrow H_2O$		
4	$H+CO \rightarrow HCO$	2000	390K ± 40K at 12K (Fuchs et al., 2009)
5	$H+HCO \rightarrow H_2CO$		
6	$H+H_2CO \rightarrow H_3CO$	2000	415K ± 40K at 12K (Fuchs et al., 2009)
7	$H+H_3CO \rightarrow CH_3OH$		
8	$O+O \rightarrow O_2$		
9	$O+CO \rightarrow CO_2$	1000	2970K (Talbi et al. 2002), 2500K (Goumans & Andersson 2010)
10	$O+HCO \rightarrow CO_2+H$		
11	$O+O_2 \rightarrow O_3$		
12	$H+O_2 \rightarrow HO_2$	1200	barrier less (Ioppolo et al., 2008)
13	$H+HO_2 \rightarrow H_2O_2$		
14	$H+H_2O_2 \rightarrow H_2O+OH$	1400	barrier less (Cazaux et al., 2010)
15	$H+O_3 \rightarrow O_2+OH$	450	
16	$H2+OH \rightarrow H_2O+H$	2600	

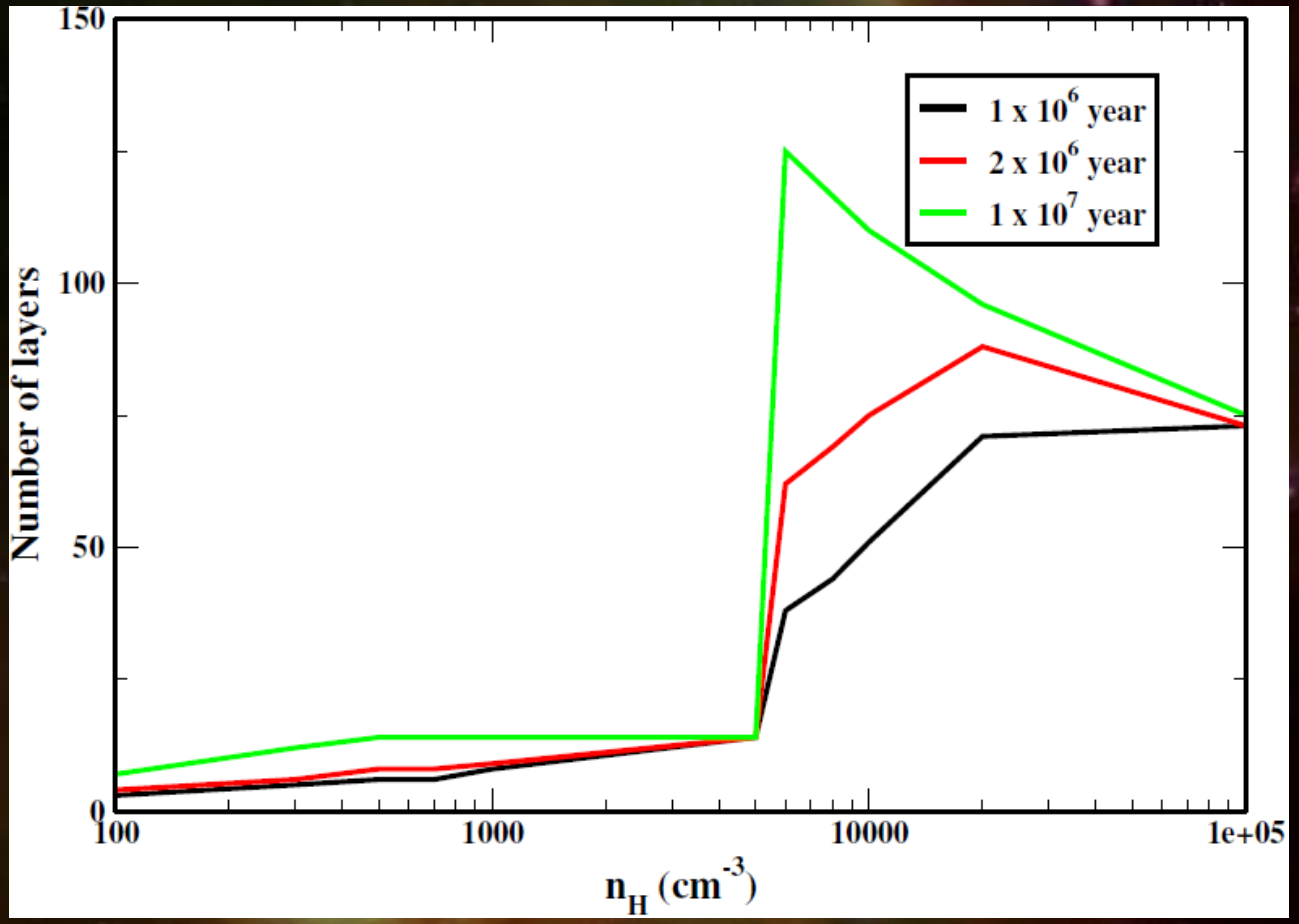
Simulation in mono-layer regime



Das et al. , 2008, A&A

Recombination efficiency strongly depends on surface coverage

Simulation in the multi-layer regime



Observed abundance of ice phase species with respect to H2O

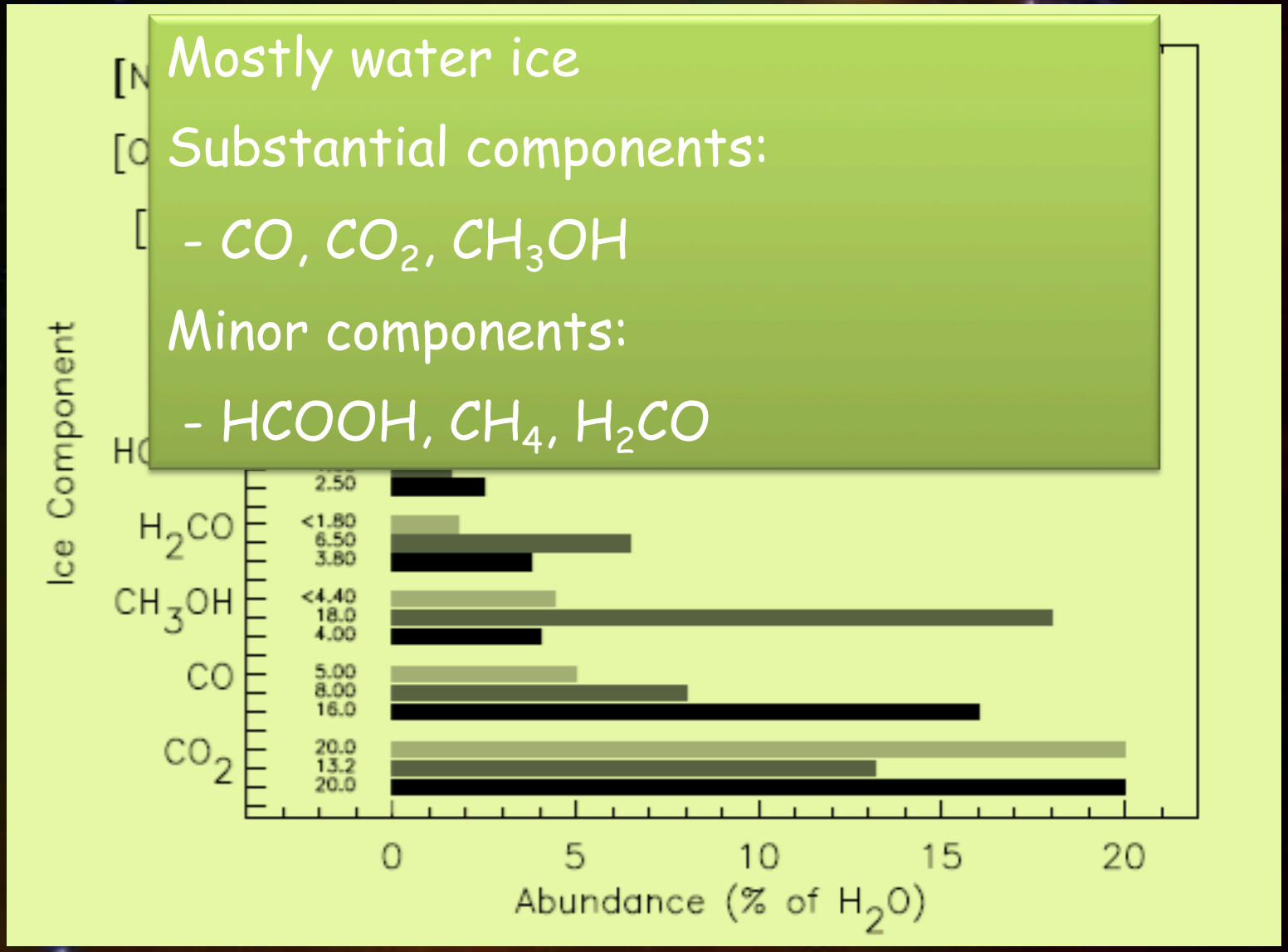
Mostly water ice

Substantial components:

- CO, CO_2, CH_3OH

Minor components:

- $HCOOH$, CH_4, H_2CO



Boogert et al., 2004

Composition of grain mantle

Observational evidences along dense cloud

No. of maximum layer ~ 100

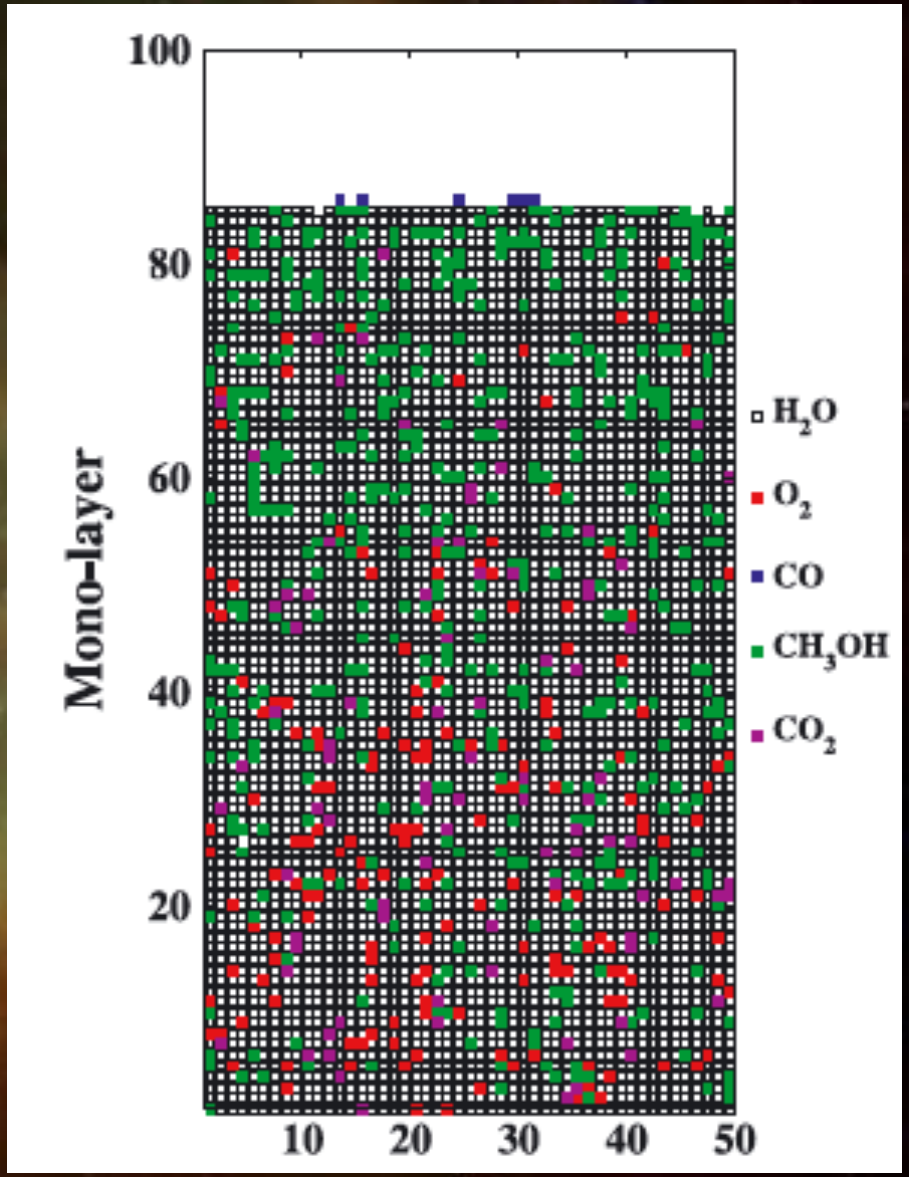
Surface Coverage of H_2O >60%~abundance 10^{-4}

2%<CH_3OH <30% w.r.t. H_2O

2<CO2<20% w.r.t. H_2O

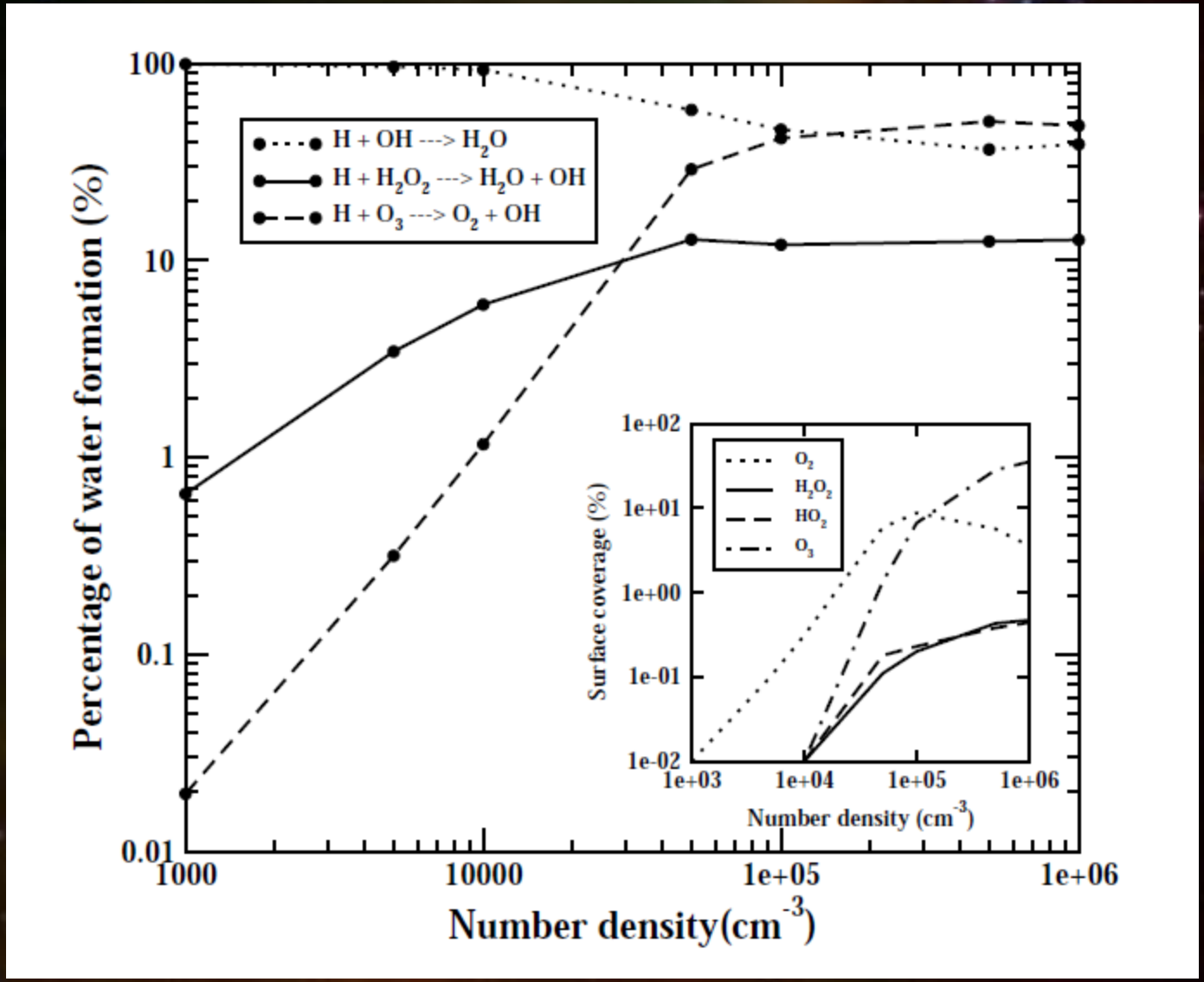
Our Results

Dominated by H_2O, CH_3OH, CO_2 and CO



Das et al., 2010, MNRAS

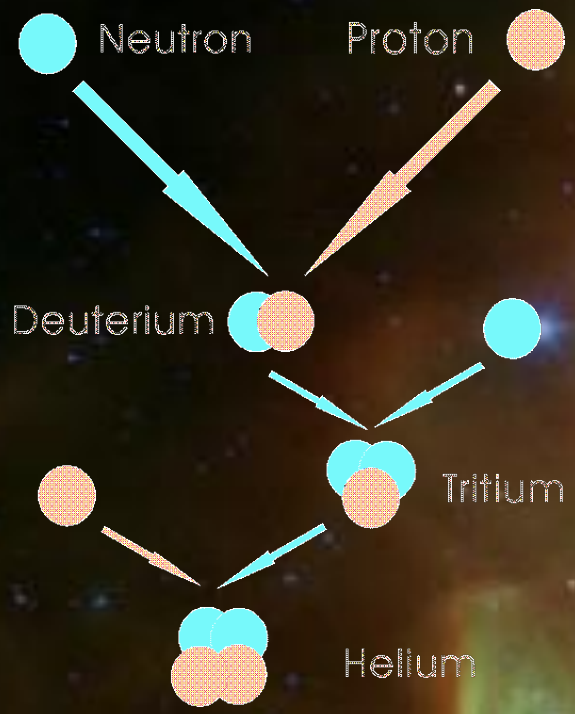
Various routes to the formation of H_2O



Das et al., 2011, MNRAS


Why Deuterium fractionation is important?

Sources of deuterium



Deuterium is destroyed in the interior of stars faster than it produced

Measurement of D/H ratio

Earth's Oceans – 1.5×10^{-4}

Neptune, Uranus, Titan – $1\text{-}2 \times 10^{-4}$

Comet Halley – 4×10^{-4}

Jupiter, Saturn – 2×10^{-5}

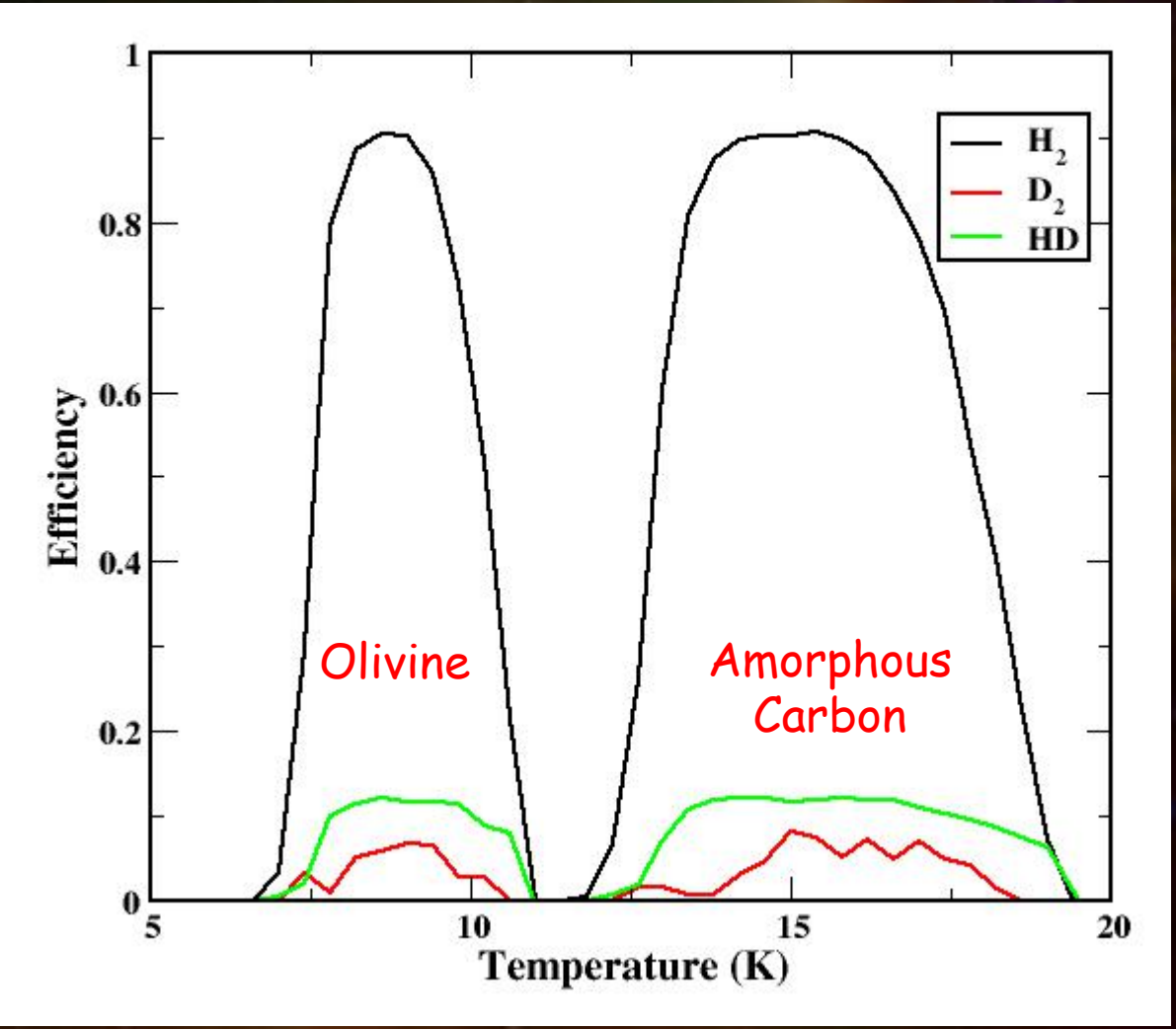
Nearby Interstellar Medium – $1\text{-}3 \times 10^{-5}$

Mostly Observed deuterated species around the ISM

HD	H_2D^+	D_2H^+	DCN	DNC
N_2D^+	CCD	C_3HD	DC_3N	DC_5N
HDO	HDCS	HDCO	D_2CO	DCO^+
CH_3OD	CH_2DOH	CHD_2OH	CD_3OH	CH_2DCN
NH_2D	NHD_2	ND_3	C_4D	D_2CS
CH_2DCCH	CH_3CCD	HDS	D_2S	

Surprisingly some molecular fractionation ratio found to be $>10^{-5}$ or even sometimes close to 1

Deuterium enrichment of most simplest & abundant species H2 @ low temperatures



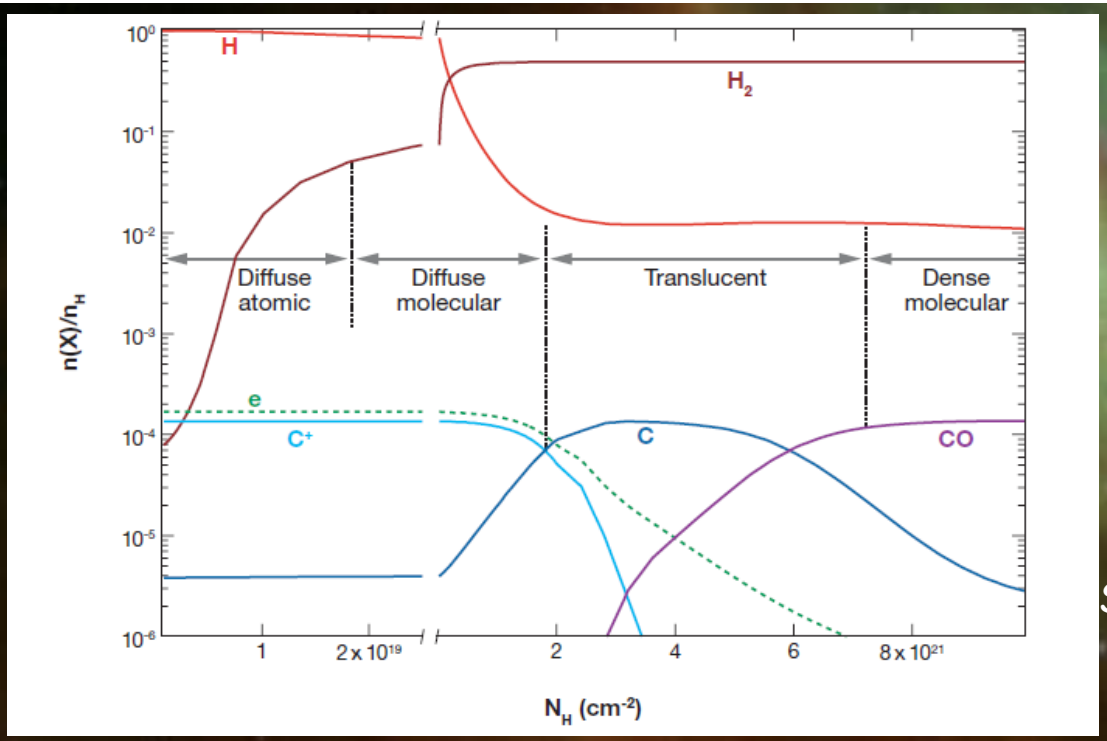
Sahu, Das, Majumdar, Chakrabarti, 2015, New Astronomy

Deuterated network

	Reactions	E_a(K)
1	$H + H \rightarrow H_2$	
2	$H + O \rightarrow OH$	
3	$H + OH \rightarrow H_2O$	
4	$H + CO \rightarrow HCO$	390
5	$H + HCO \rightarrow H_2CO$	
6	$H + H_2CO \rightarrow H_3CO$	415
7	$H + H_3CO \rightarrow CH_3OH$	
8	$O + O \rightarrow O_2$	
9	$O + CO \rightarrow CO_2$	1000
10	$O + HCO \rightarrow CO_2 + H$	
11	$O + O_2 \rightarrow O_3$	
12	$H + O_2 \rightarrow HO_2$	
13	$H + HO_2 \rightarrow H_2O_2$	
14	$H + H_2O_2 \rightarrow H_2O + OH$	
15	$H + O_3 \rightarrow O_2 + OH$	450
16	$H_2 + OH \rightarrow H_2O + H$	2600
17	$H + D \rightarrow HD$	
18	$D + D \rightarrow D_2$	
19	$D + O \rightarrow OD$	
20	$D + OH \rightarrow HDO$	
21	$H + OD \rightarrow HDO$	
22	$D + OD \rightarrow D_2O$	
23	$D + CO \rightarrow DCO$	320
24	$H + DCO \rightarrow HDCO$	
25	$D + HCO \rightarrow HDCO$	
26	$D + H_2CO \rightarrow H_2DCO$	214
27	$D + HDCO \rightarrow HD_2CO$	173
28	$D + D_2CO \rightarrow D_3CO$	128
29	$H + HDCO \rightarrow H_2DCO$	380
30	$H + D_2CO \rightarrow HD_2CO$	340
31	$D + H_3CO \rightarrow CH_3OD$	
32	$D + H_2DCO \rightarrow CH_2DOD$	
33	$D + HD_2CO \rightarrow CHD_2OD$	
34	$D + D_3CO \rightarrow CD_3OD$	
35	$H + H_2DCO \rightarrow CH_3OD$	
36	$H + HD_2CO \rightarrow CH_2DOD$	
37	$H + D_3CO \rightarrow CHD_2OD$	
38	$O + DCO \rightarrow CO_2 + D$	
39	$D + O_2 \rightarrow DO_2$	
40	$D + HO_2 \rightarrow HDO_2$	
41	$D + DO_2 \rightarrow D_2O_2$	
42	$H + DO_2 \rightarrow HDO_2$	
43	$D + O_3 \rightarrow O_2 + OD$	450
44	$H_2 + OD \rightarrow HDO + H$	2600
45	$HD + OD \rightarrow HDO + D$	2600
46	$HD + OD \rightarrow D_2O + H$	2600
47	$HD + OH \rightarrow H_2O + D$	2600
48	$D_2 + OD \rightarrow D_2O + D$	2600

Classification of clouds

	Diffuse Atomic	Diffuse Molecular	Translucent	Dense Molecular
Defining Characteristic	$f^n_{H_2} < 0.1$	$f^n_{H_2} > 0.1$ $f^n_{C+} > 0.5$	$f^n_{C+} < 0.5$ $f^n_{CO} < 0.9$	$f^n_{CO} > 0.9$
A_V (min.)	0	~0.2	~1–2	~5–10
Typ. n_H (cm^{-3})	10–100	100–500	500–5000?	$>10^4$
Typ. T (K)	30–100	30–100	15–50?	10–50
Observational Techniques	UV/Vis H I 21-cm	UV/Vis IR abs mm abs	Vis (UV?) IR abs mm abs/em	IR abs mm em

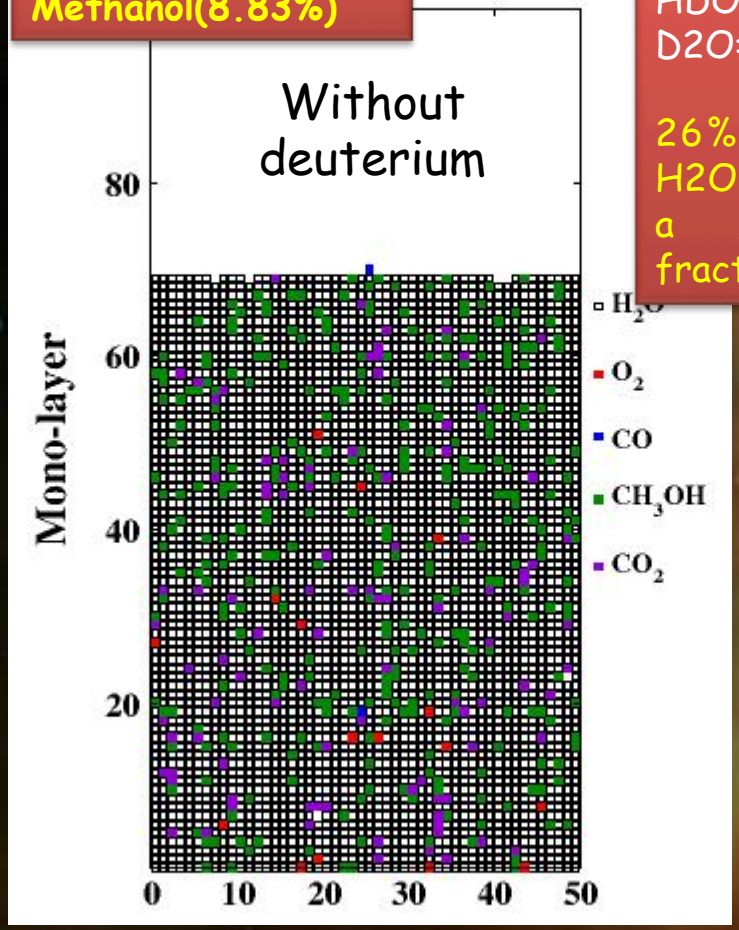


Snow, McCall, 2006, ARAA, 44, 367

Our multi layer model strictly applies to 10K-15K. Thus we are defining cloud parameters based on the hydrogen number density and A_V.

Deuterium enrichment of the grain mantle

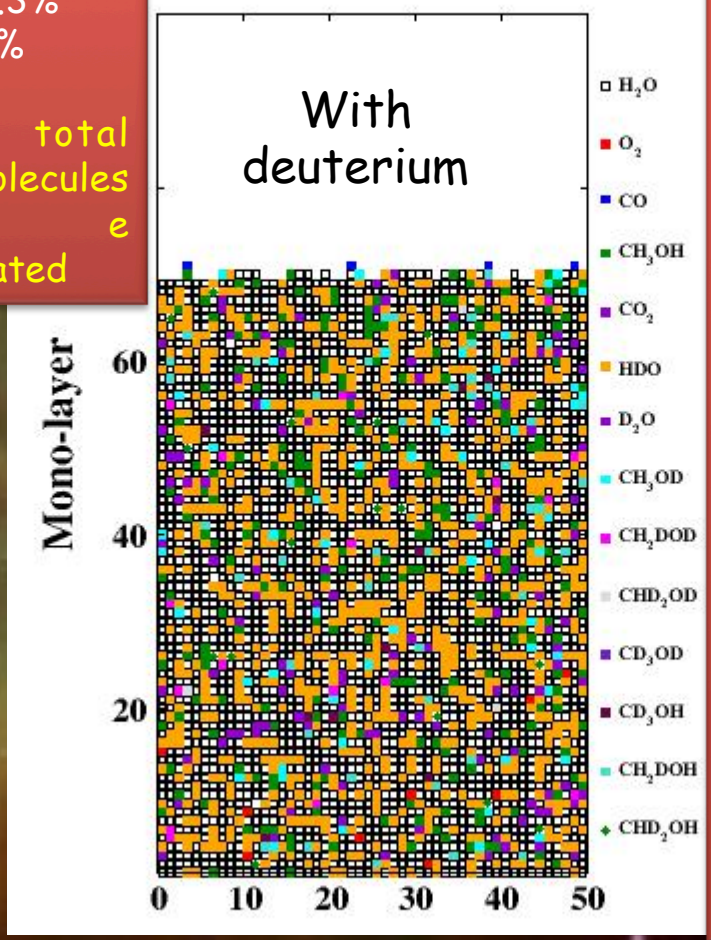
Water(88.17%) & Methanol(8.83%)



Water(88.17%)
H2O= 64.7%

HDO=22.3%
D2O=1.2%

26% of total H2O molecules are fractionated



Methanol(9.377%)

CH3OH=5.56%

Singly deuterated
CH3OD=1.3%
CH2DOH=1.26%

Doubly deuterated

CH2DOD=0.447%
CHD2OH=0.45%

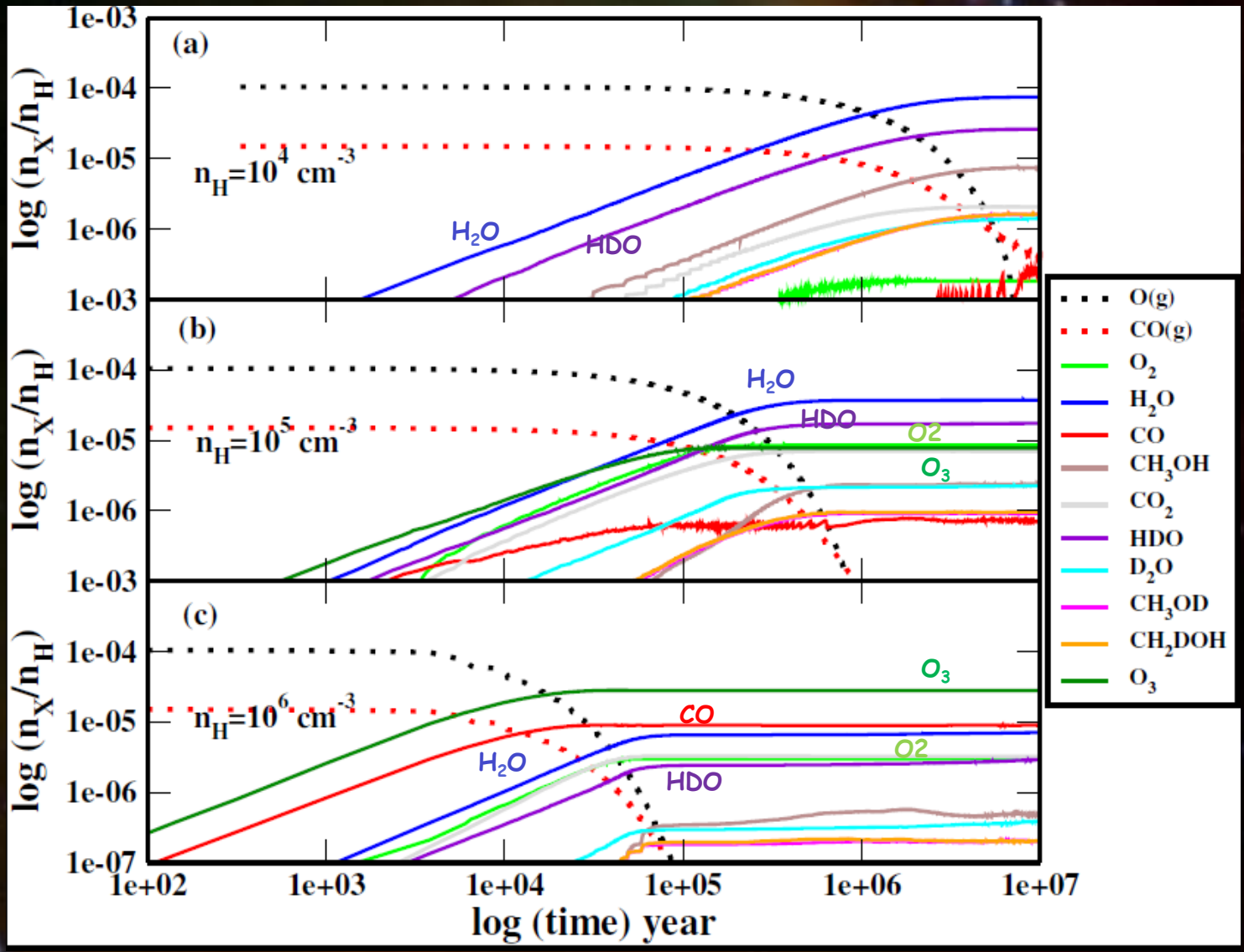
Triply deuterated
CD3OH=0.16%
CHD2OD=0.15%

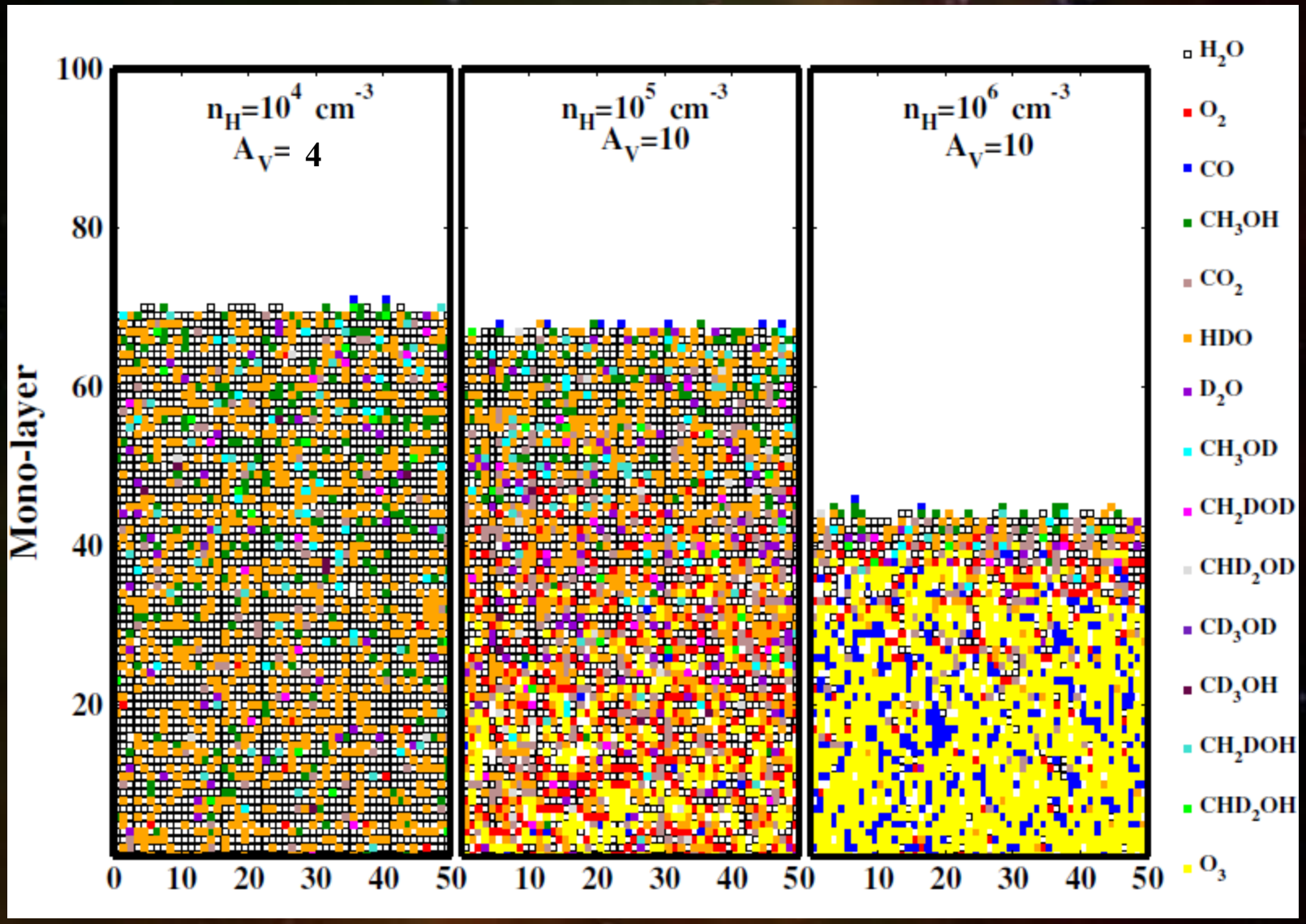
Tetra deuterated
CD3OD=0.05%

40% of total CH3OH molecules are fractionated

Das et al., 2015, MNRAS (communicated)

Chemical evolution of gas-grain species




$n_H=10^4$ cm^{-3}
A_V= 4
$n_H=10^5$ cm^{-3}
A_V=10
$n_H=10^6$ cm^{-3}
A_V=10
Mono-layer
100
80
60
40
20
0
10
20
30
40
50
H_2O
O_2
CO
CH_3OH
CO_2
HDO
D_2O
CH_3OD
CH_2DOD
CHD_2OD
CD_3OD
CD_3OH
CH_2DOH
CHD_2OH
O_3

Conclusions

- Monte carlo simulations are carried out for the formation of simple to complex molecules on interstellar grains.

- Recombination efficiency is dependent upon the grain parameters like accretion rate, grain size, surface coverage, temperature etc.

- Composition of grain mantle is heavily dependent upon surrounding physical conditions. Interstellar radiation field plays a crucial role towards the chemical composition.

- Grain mantles are found to be heavily fractionated around some regions. Around the dense cloud region O_3 formation significantly enhanced.

Acknowledgement

- Liton Majumdar
- Sandip K. Chakrabarti
- Dipen Sahu