

***Molecular hydrogen in star forming regions***

***Gargi Shaw***

***UM-DAE Centre for excellence in basic sciences  
University of Mumbai***

# OUTLINE

## Hydrogen Molecule & Cloudy

- ➔ Energy diagram of  $H_2$
- ➔ Formation of  $H_2$
- ➔ Destruction of  $H_2$
- ➔ Ortho-Para conversion

## Our results on high redshift Damped Ly $\alpha$ absorbers (DLAs)

# Hydrogen Molecule

## ...Why is it so important ?

- About **90%** of the current Baryonic matter is in the form of **Hydrogen**.
- **Molecular hydrogen plays an important role in astrophysics.**
  - It is the first and the most abundant neutral molecule to be formed in the Universe.
  - As a highly efficient coolant, it increases the rate of formation of galaxies in primordial gas
  - Molecular hydrogen is a major constituent of giant molecular clouds.

# Hydrogen Molecule

- Hydrogen molecule ( $H_2$ ) is the simplest neutral molecule consisting of two protons and two electrons.

## Fermi statistics

- Total (nuclear  $\times$  electronic ) wave function must be anti-symmetric under the exchange of nuclei
- Ortho states : Total spin  $I = 1$ , Degeneracy :  $3 \times (2J+1)$   
Nuclear spin wave function : symmetric  
Spatial wave function : anti-symmetric
- Para states : Total spin  $I=0$ , Degeneracy :  $2J+1$   
Nuclear spin wave function : anti-symmetric  
Spatial wave function : symmetric

### Ground state

Even  $J$  : Para state

Odd  $J$  : Ortho state

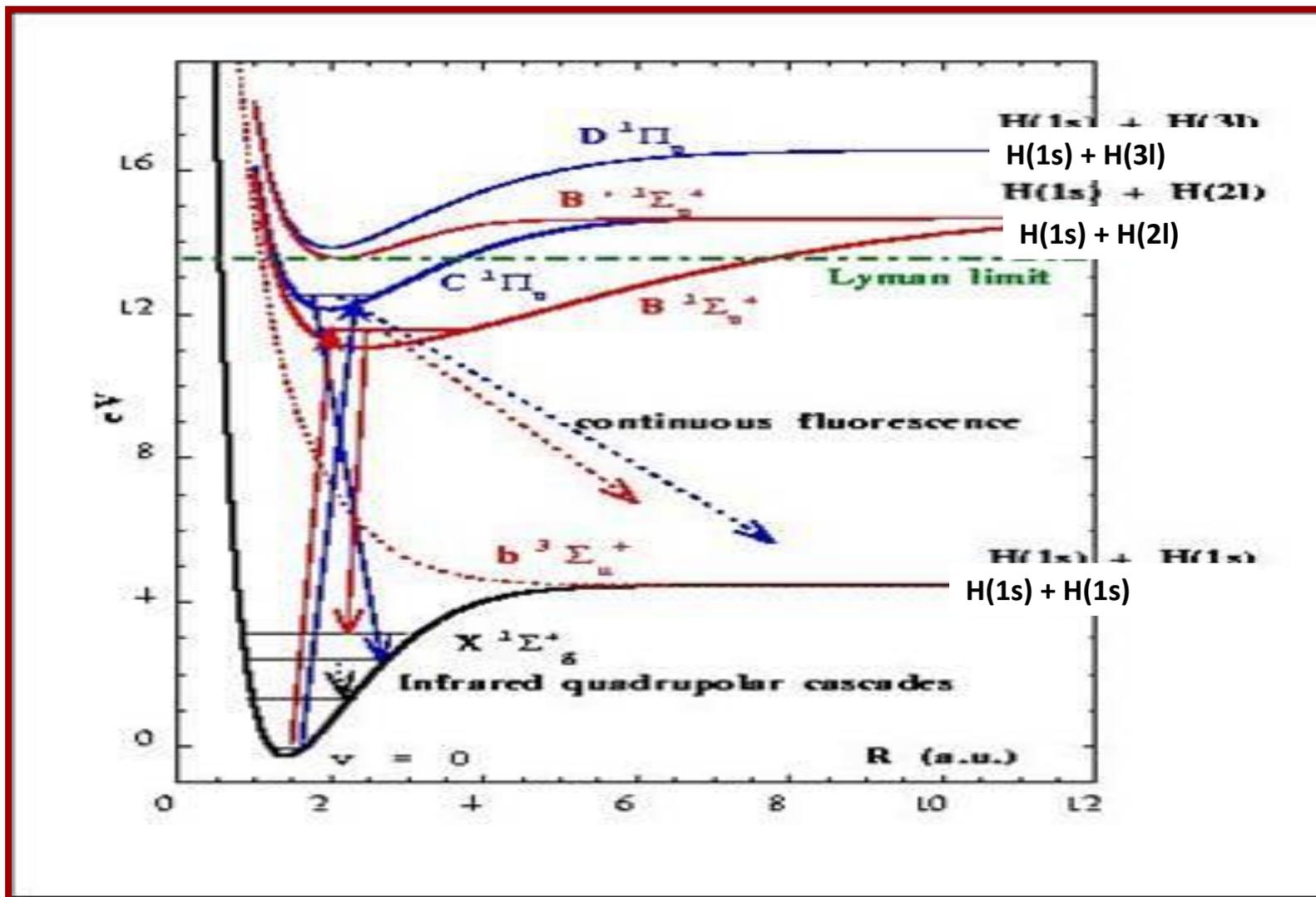
# Hydrogen Molecule

- Hydrogen molecule ( $H_2$ ) is the simplest neutral molecule consisting of two protons and two electrons.
- It is a symmetric molecule and does not have a permanent electric dipole moment.

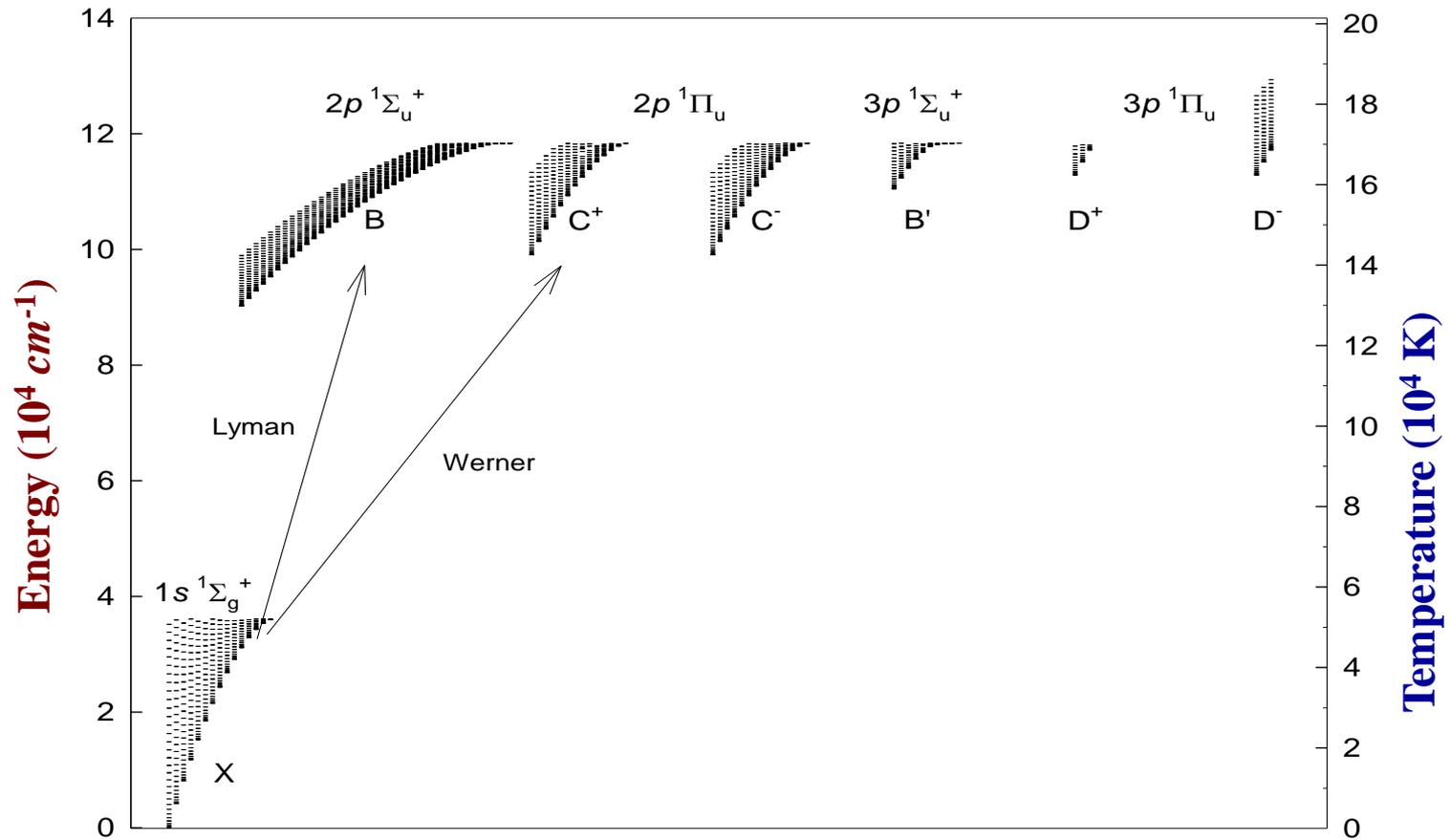
In ground state rovibrational transitions can occur only via

quadrupole transitions with  $\Delta J=0, \pm 2$ .

# Potential curves involved in the Lyman and Werner bands (Roueff 00)



# Energy levels of H<sub>2</sub>



# Molecular Hydrogen lines

## “Atom H2”

### Branch Notation

Branch  $J_{\text{up}} - J_{\text{lo}}$

O..... -2

P .....-1

Q..... 0

R.....+1

S ..... +2

### Spectroscopic notation

H2 17.03m 0-0 S(1)

H2 12.28m 0-0 S(2)

H2 9.665m 0-0 S(3)

H2 8.025m 0-0 S(4)

H2 6.909m 0-0 S(5)

H2 2.12099m 1-0 S(1)

H2 2.22269m 1-0 S(0)

H2 2.41307m 1-0 Q(2)

H2 2.42307m 1-0 Q(3)

H2 2.43683m 1-0 Q(4)

# Micro-physics of $H_2$

Formation of $H_2$	Destruction of $H_2$
<ul style="list-style-type: none"><li data-bbox="73 525 911 582">• Catalysis on the grain surface <math>H + H + \text{grain} \rightarrow H_2 + \text{grain}</math></li><li data-bbox="73 753 935 811">• Radiative association processes<ul style="list-style-type: none"><li data-bbox="227 825 877 882">i. <math>H^- + H \rightarrow H_2 + e^-</math></li><li data-bbox="208 902 819 959">ii. <math>H_2^+ + H \rightarrow H_2 + H^+</math></li></ul></li></ul>	<ul style="list-style-type: none"><li data-bbox="989 525 1460 582">• Solomon process</li><li data-bbox="989 674 1696 731">• Direct photo-dissociation</li><li data-bbox="989 822 1607 879">• Collisional dissociation</li></ul>

Shaw et al. 2005

# DESTRUCTION OF H<sub>2</sub>

## ✚ Collisional dissociation

Collisional dissociation by H, He, H<sub>2</sub> and e<sup>-</sup> are also possible from higher vib-rotational state

## ✚ Pumping via X-ray electrons

Molecular hydrogen is excited to B<sup>1</sup>Σ<sub>u</sub><sup>+</sup> or C<sup>1</sup>Π<sub>u</sub><sup>±</sup> state by secondary electrons.

## ✚ Excitation to the triplet b state

Molecular hydrogen is excited to triplet b state by energetic secondary electrons and is dissociated

## ✚ Cosmic ray ionization

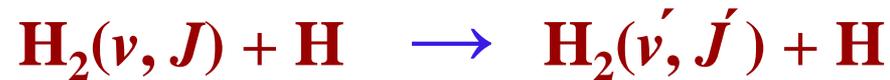


# Collisional cross-sections

Rate coefficient fits for collisional de-excitation processes:

Le Bourlot et al. (1999; <http://ccp7.dur.ac.uk>)

**Nonreactive transitions**



**Gerlich 1990**



Shaw et.al 2005

# Ortho-Para conversion

❖ No Radiative decay

❖ Exchange collisions between  $\text{H}_2$  and  $\text{H}$ ,  $\text{H}^+$  and  $\text{H}_3^+$



➤ On grain surfaces (below critical temperature)

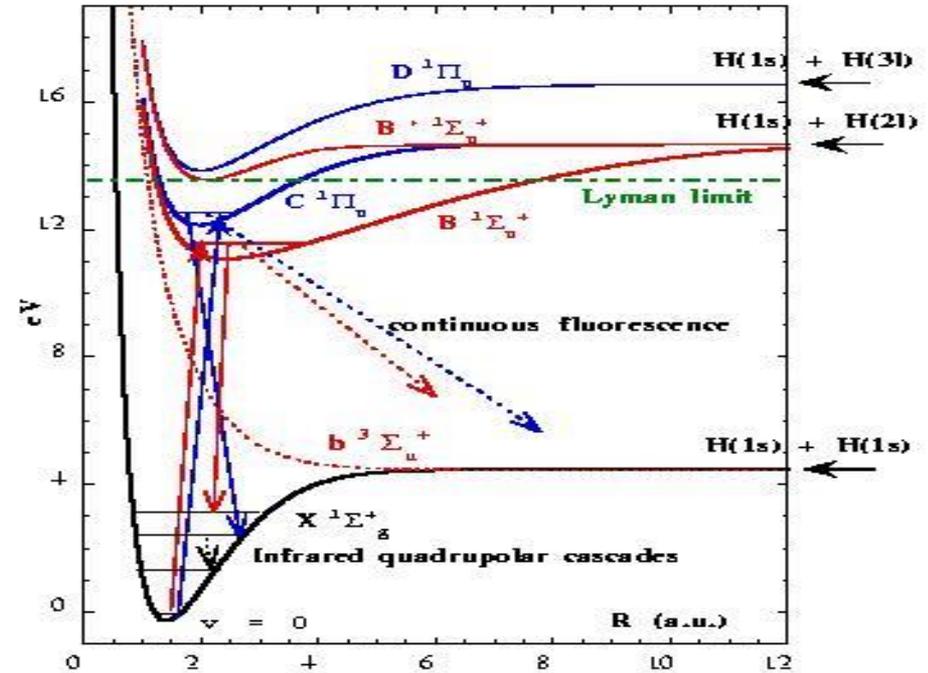
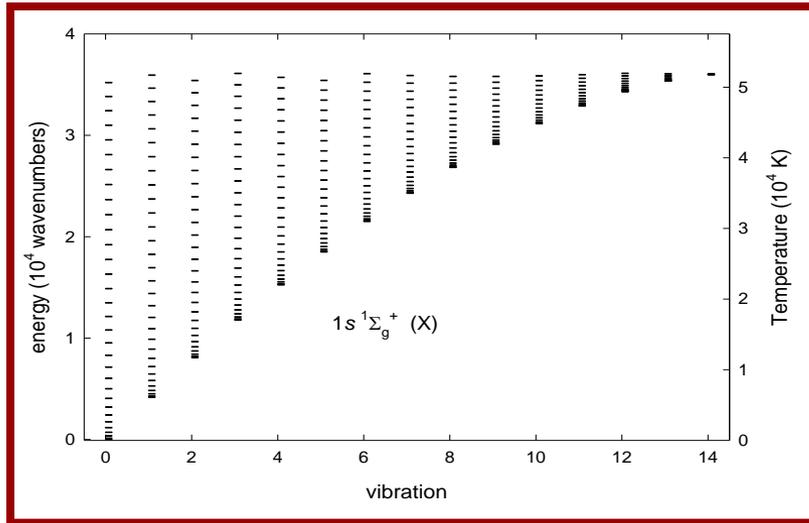
# Some important reactions

$H_2$  helps to form other molecules in PDRs.



# FUV and formation pumping of Molecular Hydrogen

- ❖  $H_2$  has small moment of inertia.
- ❖  $H_2$  energy levels are widely spaced.
- FUV pumping can excite higher levels.



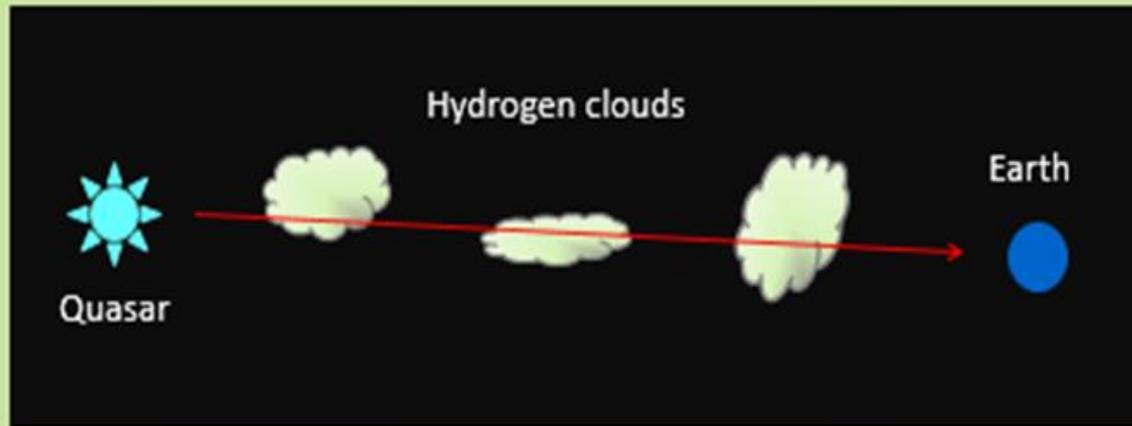
➤ Formation pumping

$H_2$  formation on dust grain surfaces is exothermic process and can excite higher levels.

Shaw et al. 2005

# Damped Ly $\alpha$ Absorbers (DLAs)

*DLAs are defined as absorption-line systems having large neutral hydrogen column density  $N(\text{HI}) \geq 2 \times 10^{20} \text{ cm}^{-2}$  when seen against the emission of background QSOs.*



*Fig. 1: Schematic representation of absorbers at different redshifts along the line-of-sight to a quasar*

# Damped Ly $\alpha$ Absorbers (DLAs)

- *DLAs are believed to be the progenitors of present day disk galaxies.*
- *Study of DLAs at high redshift provides information about :*
  - *early evolution of galaxies,*
  - *intergalactic medium,*
  - *early star formation,*
  - *evolution of chemical elements.*

# UVES Observations at VLT

- ***DLA at  $z_{abs} = 2.3377$  observed in absorption along the sightline towards the quasars LBQS 1232+0815***
- ***DLA at  $z_{abs} = 2.41837$  observed in absorption along the sightline SDSS J143912.04+111740.5***

***$H_2$  has been detected in both DLAs, and CO has also been observed in the DLA at  $z_{abs} = 2.41837$ .***

# OUR MODEL

***We perform our simulation using the spectral synthesis code CLOUDY.***

## **Model assumptions**

- ***A plane parallel slab of gas irradiated from both sides.***
- ***We included,***
  - ***Haardt-Mada metagalactic radiation of background galaxies and QSOs***
  - ***CMB***
  - ***cosmic ray ionization***
  - ***radiation from in-situ star formation.***

# Results for DLA at $z = 2.3$ towards LBQS

## 1232+0815

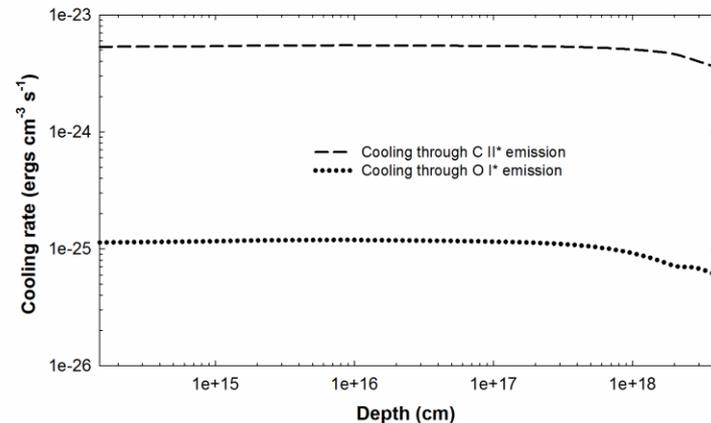
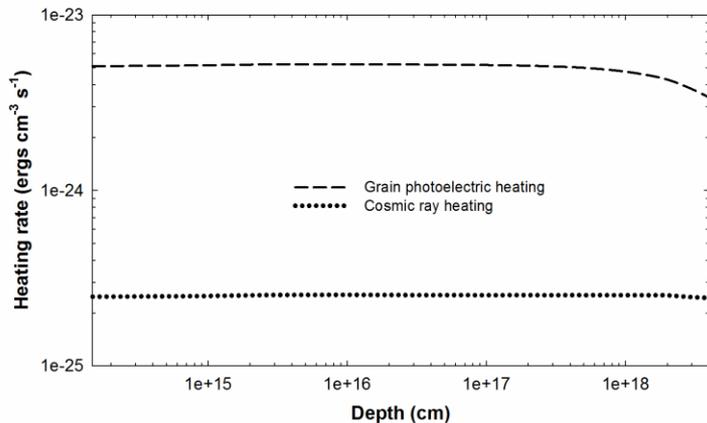
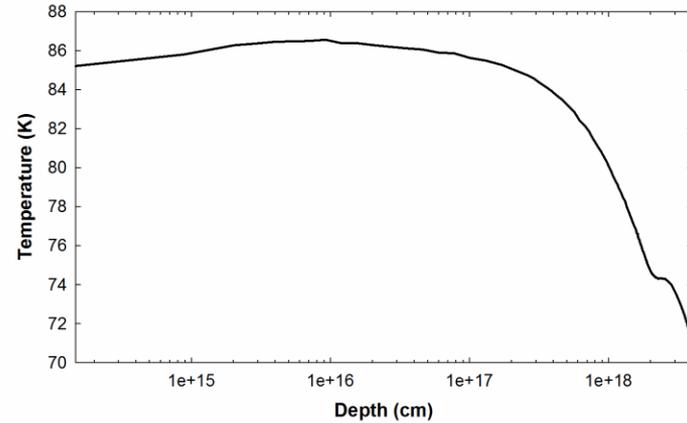
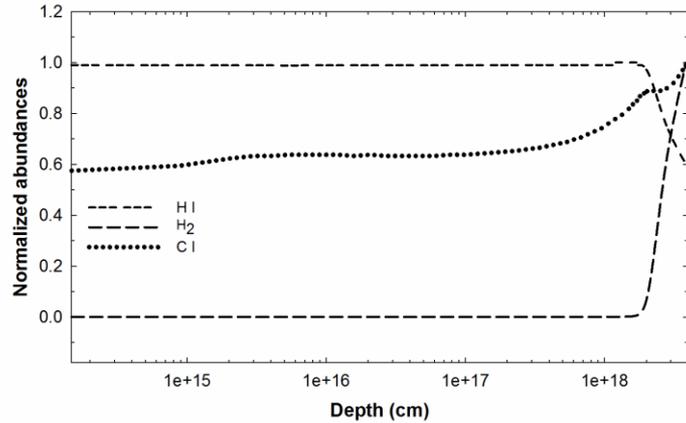
Model parameter	Value
Hydrogen density	$100 \text{ cm}^{-3}$
Intensity of radiation field	$2.5 \times 10^{-3} \text{ erg cm}^{-2} \text{ s}^{-1}$ (between 6 and 13.6 eV)
Cosmic ray ionisation rate of H I	$2 \times 10^{-16} \text{ s}^{-1}$
Metallicity	0.3 ISM
Turbulence	4 km/s
Grain size	0.5 ISM

Species (X)	Column density from observation $\log N(X) \text{ cm}^{-2}$	Column density predicted by model $\log N(X) \text{ cm}^{-2}$
H I	$20.90 \pm 0.08^a$	20.84
H <sub>2</sub>	$19.68^{+0.08}_{-0.10}^a$	19.70
H <sub>2</sub> (0, 0)	$19.45 \pm 0.10^a$	19.43
H <sub>2</sub> (0, 1)	$19.29 \pm 0.15^a$	19.37
H <sub>2</sub> (0, 2)	$16.78 \pm 0.24^a$	16.99
H <sub>2</sub> (0, 3)	$16.36 \pm 0.10^a$	15.70
H <sub>2</sub> (0, 4)	$14.70 \pm 0.06^a$	14.63
H <sub>2</sub> (0, 5)	$14.36 \pm 0.07^a$	14.33
CO	$< 12.6^b$	12.54
C I*	$13.87 \pm 0.05^c$	13.86
C I**	$13.56 \pm 0.04^c$	13.72
C I***	$12.82 \pm 0.07^c$	13.02
N I	$14.54 \pm 0.22^b$	14.52
Mg II	$15.33 \pm 0.24^b$	15.29
Si II	$15.06 \pm 0.05^b$	15.02
P II	$12.86 \pm 0.24^b$	12.81
S II	$14.81 \pm 0.09^b$	14.76
Cl I	$12.97 \pm 0.14^b$	12.66
Ar I	$13.86 \pm 0.22^b$	13.81
Mn II	$12.22 \pm 0.08^b$	12.19
Fe II	$14.44 \pm 0.08^b$	14.40
Ni II	$12.81 \pm 0.04^b$	12.82

Ivanchik et al. 2010; Balashev et al. 2011

# The physical conditions of the DLA at

$$z_{abs} = 2.3377$$



# Results for DLA at $z = 2.4$ towards SDSS

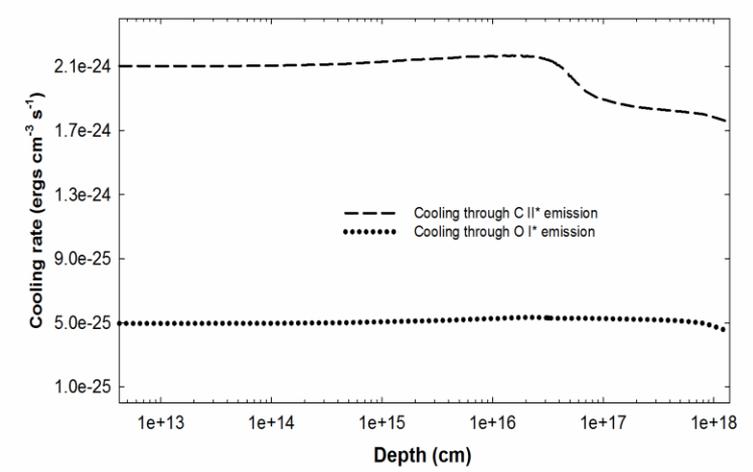
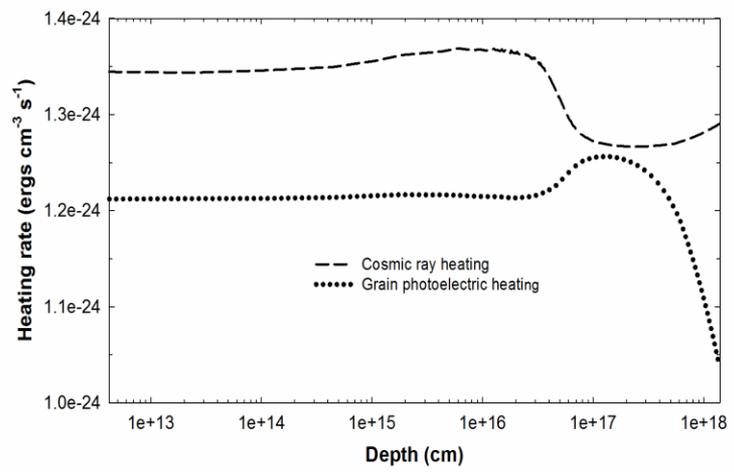
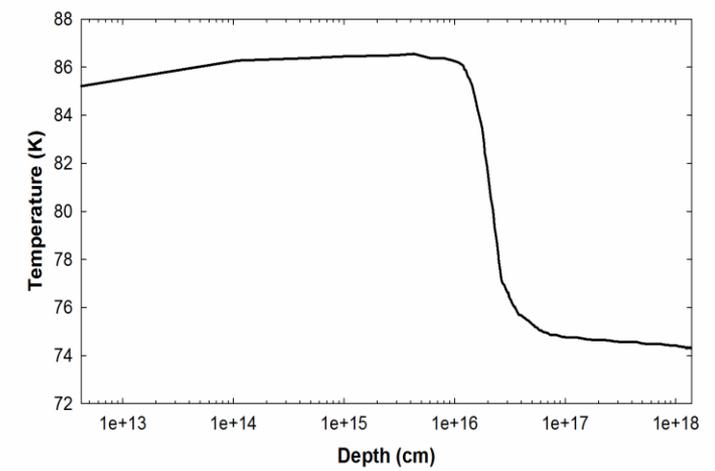
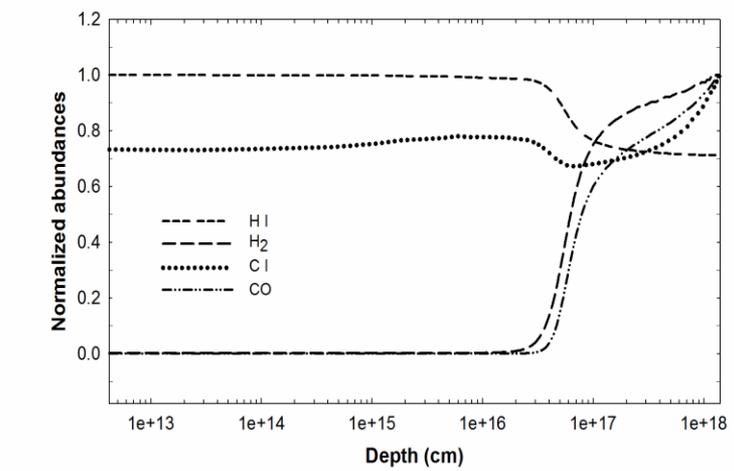
## J143912.04+111740.5

Model parameter	Value
Hydrogen density	$60 \text{ cm}^{-3}$
Intensity of radiation field (between 6 and 13.6 eV)	$10^{-4} \text{ erg cm}^{-2} \text{ s}^{-1}$
Cosmic ray ionisation rate of H I	$1.4 \times 10^{-15} \text{ s}^{-1}$
Metallicity	0.5 ISM
Turbulence	1.5 km/s
Grain size	0.5 ISM

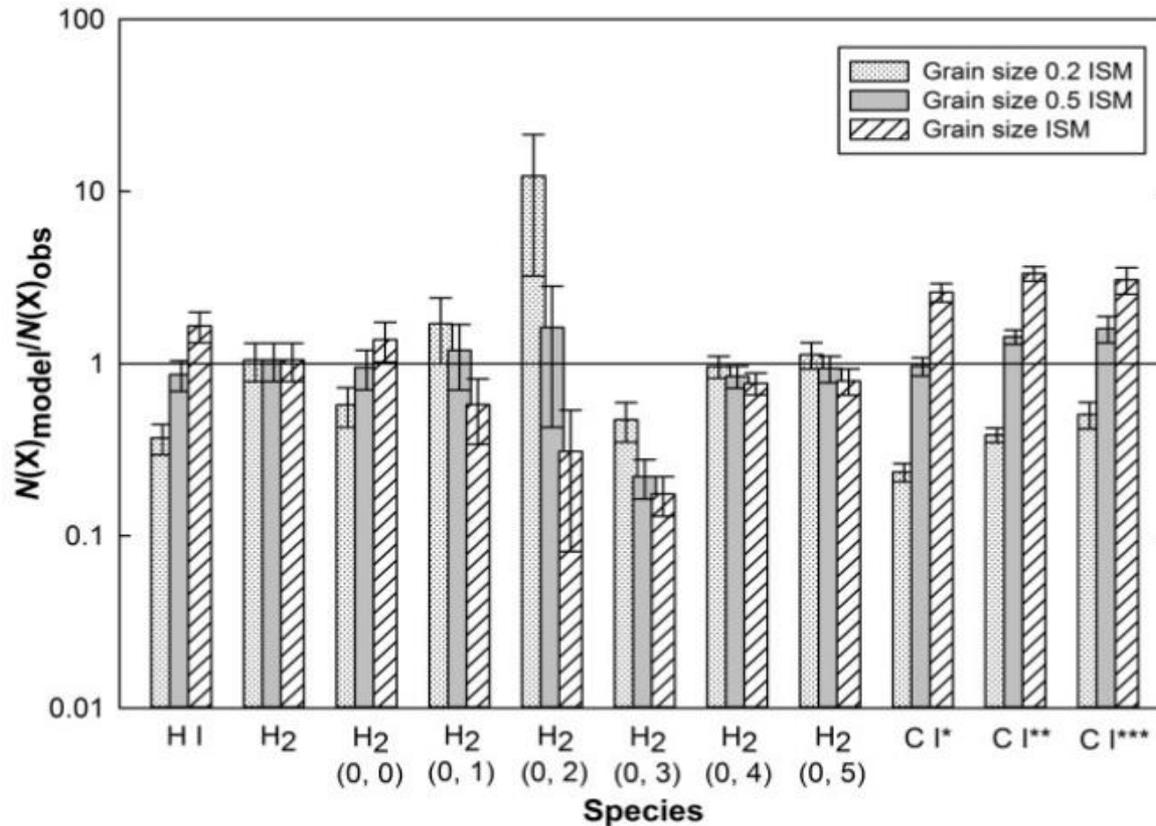
Srianand et al. 2008;  
Noterdaeme et al. 2008b

Species (X)	Column density from observation $\log N(X) \text{ cm}^{-2}$	Column density predicted by model $\log N(X) \text{ cm}^{-2}$
H I	$20.10^{+0.10}_{-0.08}^a$	20.08
H <sub>2</sub>	$19.38 \pm 0.10^a$	19.45
H <sub>2</sub> (0, 0)	$18.90 \pm 0.10^a$	19.06
H <sub>2</sub> (0, 1)	$19.18 \pm 0.10^a$	19.22
CO	$13.89 \pm 0.02^a$	13.88
CO (0, 0)	$13.27 \pm 0.03^a$	13.28
CO (0, 1)	$13.48 \pm 0.02^a$	13.53
CO (0, 2)	$13.18 \pm 0.06^a$	13.26
C I*	$14.26 \pm 0.01^a$	14.23
C I**	$14.02 \pm 0.02^a$	13.99
C I***	$13.10 \pm 0.02^a$	13.21
N I	$\geq 15.71^b$	15.86
Si II	$14.80 \pm 0.04^b$	14.84
S II	$15.27 \pm 0.06^b$	15.30
Fe II	$14.28 \pm 0.05^b$	14.35
Zn II	$12.93 \pm 0.04^b$	12.85

# The physical conditions of the DLA at $z_{abs} = 2.41837$



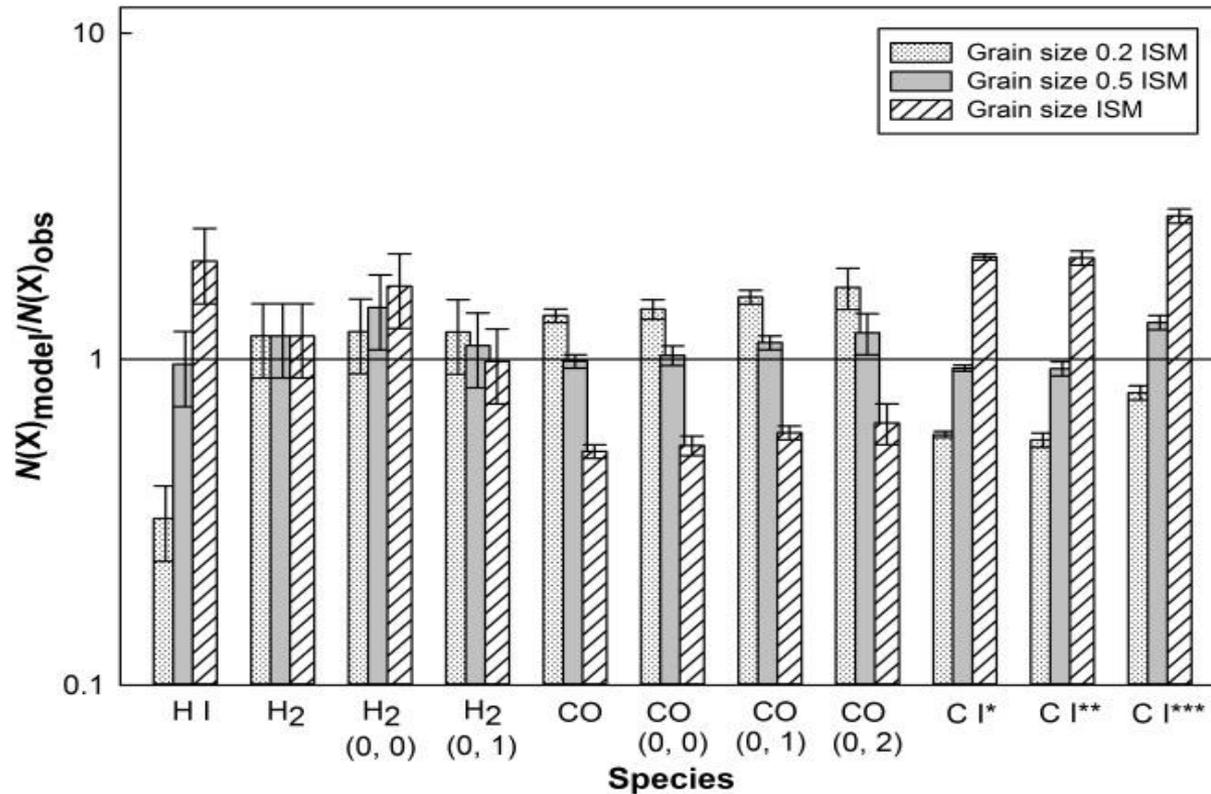
# Effect of grain size on predicted column densities



The ratio of model-to-observed column densities for H I, C I and H<sub>2</sub> for the DLA at  $z_{\text{abs}} = 2.3377$ . The best-fitting model is clearly the one with grains of size 0.5 times the ISM grain size.

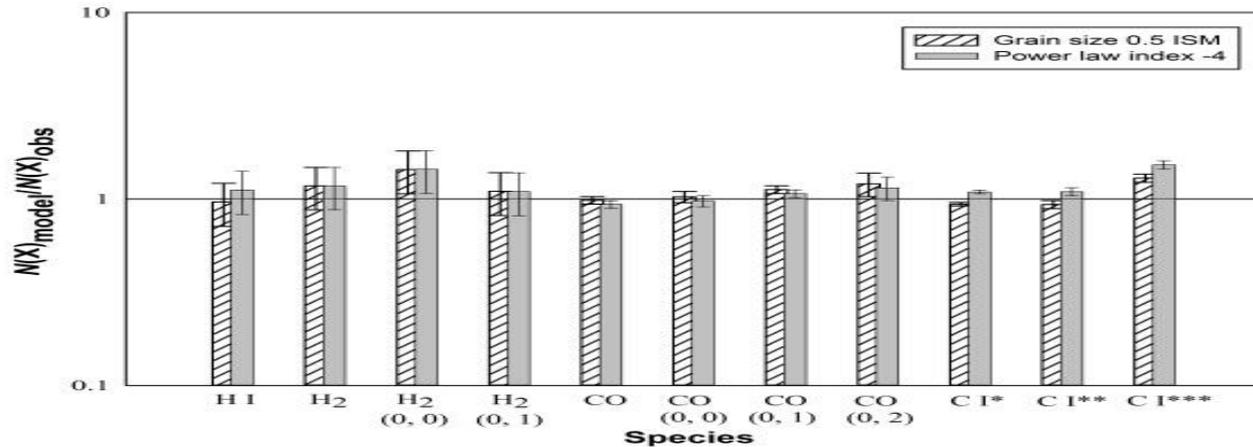
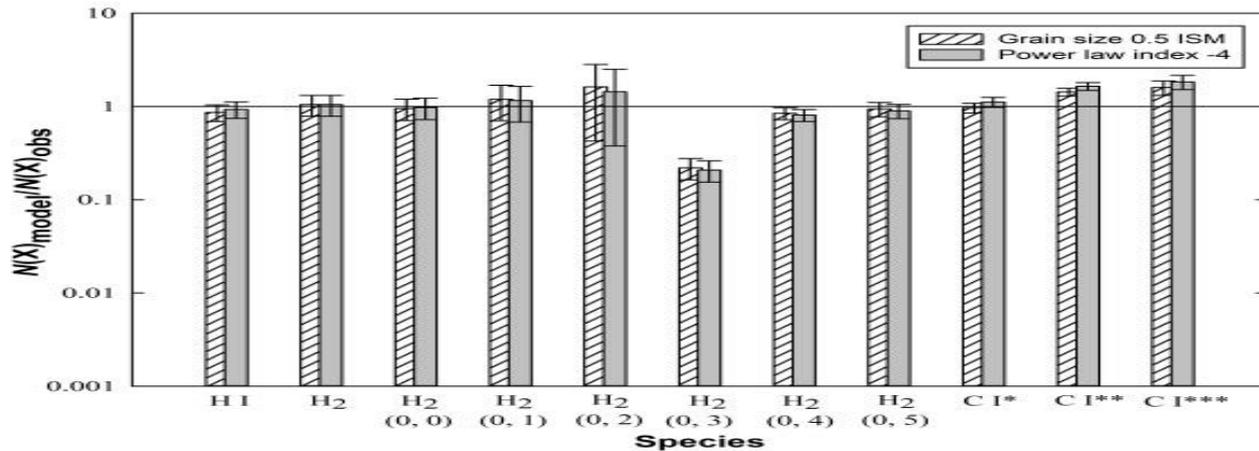
Katherine et al. 2015

# Effect of grain size on predicted column densities



The ratio of model-to-observed column densities for H I, H<sub>2</sub>, CO and C I for the DLA at  $z_{\text{abs}} = 2.41837$ . The best-fitting model is clearly the one with grains of size 0.5 times the ISM grain size.

Katherine et al. 2015



Ratio of model-to-observed column densities of C I and H<sub>2</sub> for the 2 DLAs for two different models – one, with grain sizes in the range 0.0025–0.125 μm following the MRN size distribution with exponent -3.5; and two, with grain sizes in the range 0.005–0.250 μm, following a power-law distribution with exponent -4.

# Conclusions

- *We have performed detailed numerical simulation of 2 DLAs: at  $z_{abs} = 2.3377$  towards Q 1232 + 082, at  $z_{abs} = 2.41837$  towards SDSS J143912.04+111740.5 We have reproduced most of the observed column densities satisfactorily.*
- *DLAs with  $H_2$  have high density ( $n_H > 10 \text{ cm}^{-3}$ ) and stars are forming there.*
- *The two DLAs are constant-pressure clouds with in-situ star formation.*
- *We find that grains in the high-redshift DLAs that we have modelled are smaller in size than in the local ISM.*

# Conclusions

*The smaller grains can be due to,*

- *smaller grains distributed by the MRN size distribution*
- *ISM-sized grains following a power-law distribution with an index lower than the MRN distribution.*

*The two scenarios produce almost identical column densities for various species and hence it is not possible to single out one of them as the more likely case.*

*The cosmic ray ionization rates in the 2 systems we have modelled span a range  $> 1.5$  dex. This clearly indicates that the ionization produced by cosmic rays is not uniform everywhere, and encourages further probing of cosmic ray ionization along various sightlines.*

*Thank you*