Water formation through O_2+D pathway on cold silicate, graphite and amorphous water surfaces of interstellar interest

Henda Chaabouni

LERMA-LAMAp, Université de Cergy-Pontoise, FRANCE

UMR 8112 du CNRS, Observatoire de Paris

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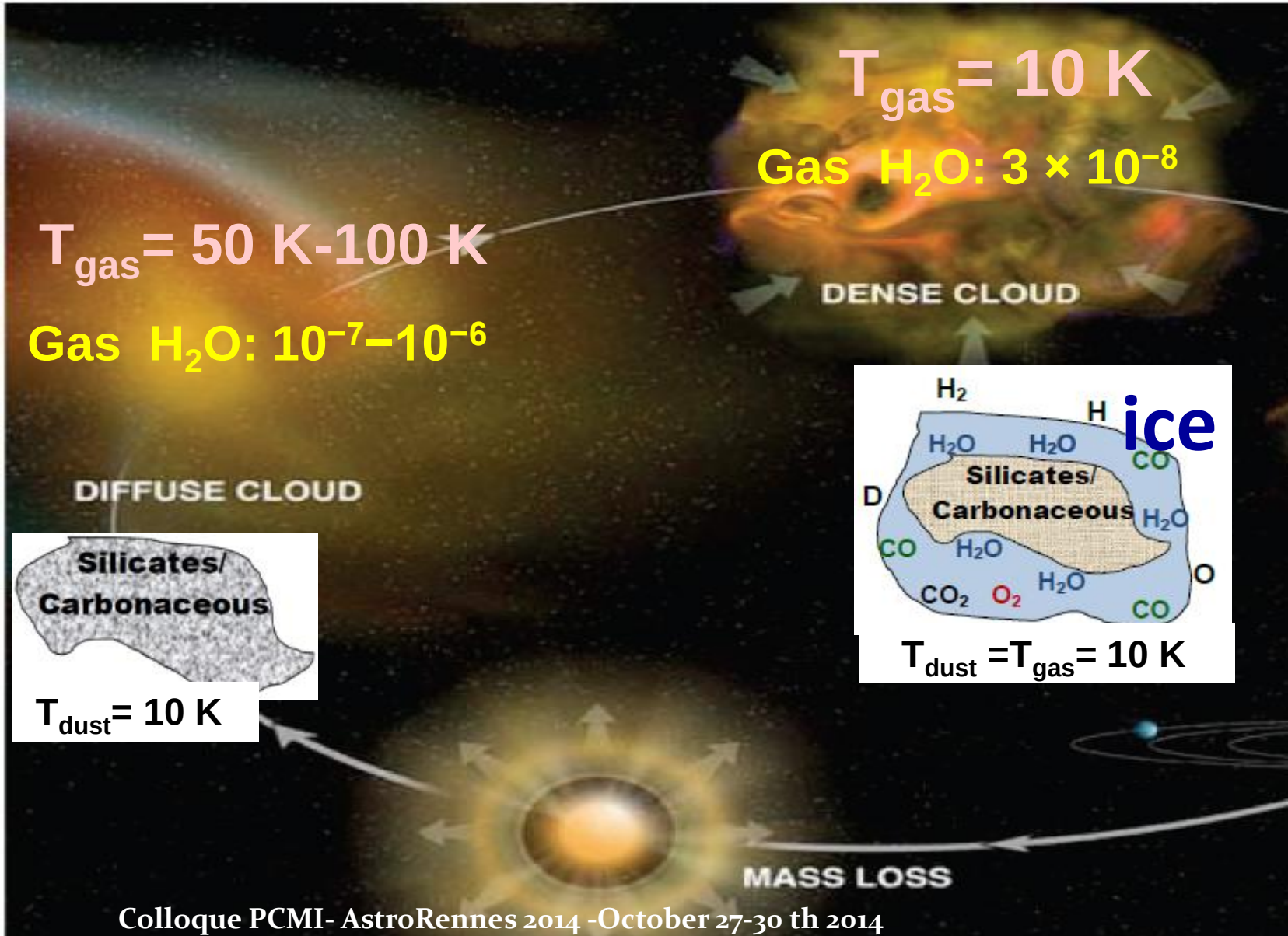
Background

Water is detected in the **ISM** and outside of our Solar System as **Gas,** and **Ice**.



Background

Previous studies

Gas-surface chemistry of water formation in the ISM

$H + O \rightarrow OH$

$H + OH \rightarrow H_2O$

Dulieu et al A&A (2010)

Jing et al, APJL (2013)

$H + O_2 \rightarrow HO_2$

$H + HO_2 \rightarrow H_2O_2$

$H + H_2O_2 \rightarrow H_2O + OH$

$H + OH \rightarrow H_2O$

Miyauchi et al. Chem.Phys.Lett (2008)

Ioppolo et al. APJ (2007), PCCP (2010)

$H + O_3 \rightarrow O_2 + OH$

$H + O_2 \rightarrow HO_2$

$H + HO_2 \rightarrow H_2O_2$

$H + H_2O_2 \rightarrow H_2O + OH$

$H + OH \rightarrow H_2O$

$H_2 + OH \rightarrow H_2O + H$

Mokrane et al APJL(2009)

Romanzin et al , JCP (2011)

Thick film of O_2 (10-30 layers) at 10 K

Efficient formation of H_2O and H_2O_2 in the <u>Multi-layer regime</u>

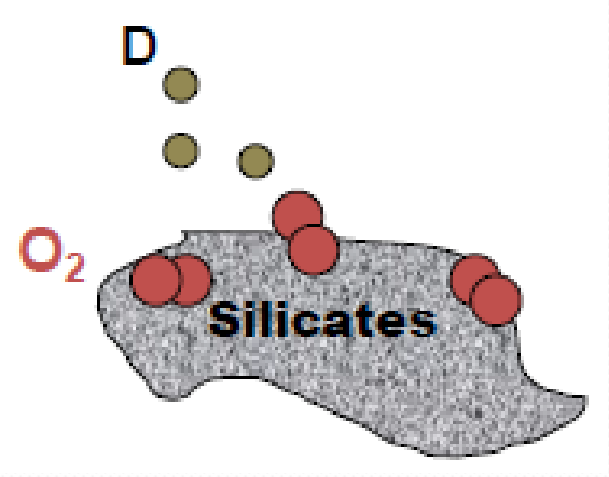
$H_2O_2 > H_2O$

$H + HO_2 \rightarrow OH + OH \rightarrow H_2O_2$

Cuppen et al. PCCP (2010)

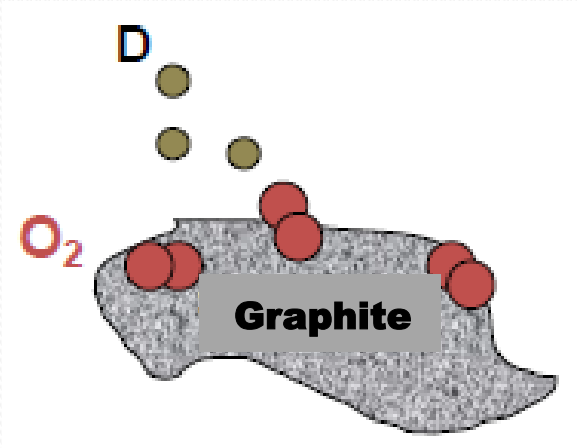
O_2 + D in the sub monolayer regime

SILICATE

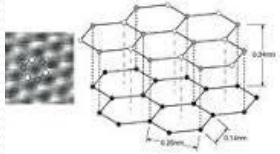


(~100 nm) amorphous
Olivine ($Mg_{1.8}Fe_{0.2}SiO_4$)

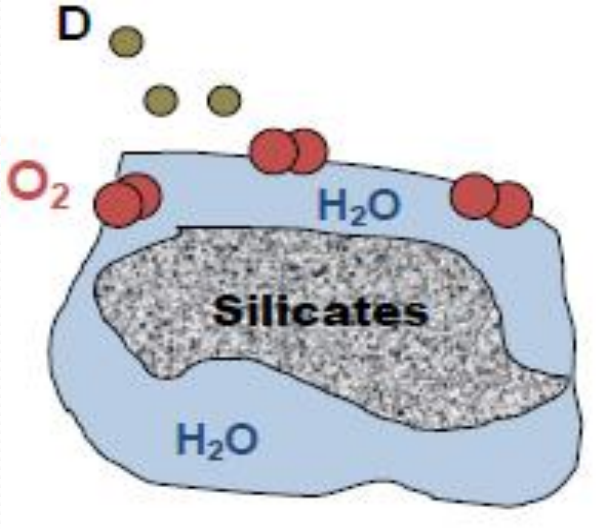
GRAPHITE



HOPG slab
Highly Ordered Pyrolytic Graphite



WATER ice



10-20 ML film
Amorphous Solid Water ices
(H_2O vapor deposition)

Experiments

FORMOLISM setup (LERMA, Cergy)

Qudrupole mass spectrometer **QMS**

(Gas phase detection)

TPD *Temperature Programmed Desorption*

Heating rate: β =0.04 K/s

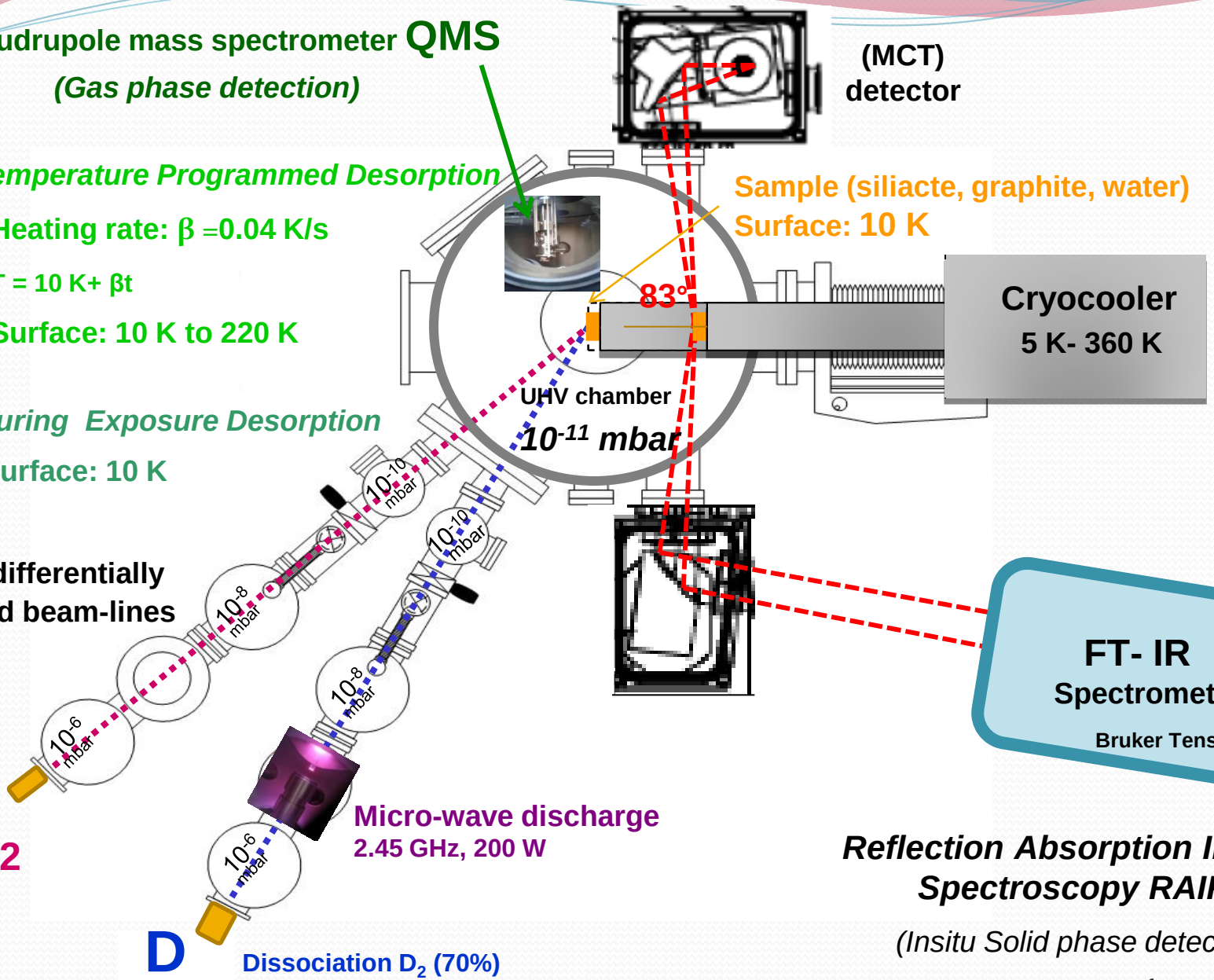
T = 10 K+ βt

Surface: 10 K to 220 K

DED *During Exposure Desorption*

Surface: 10 K

Triply differentially pumped beam-lines

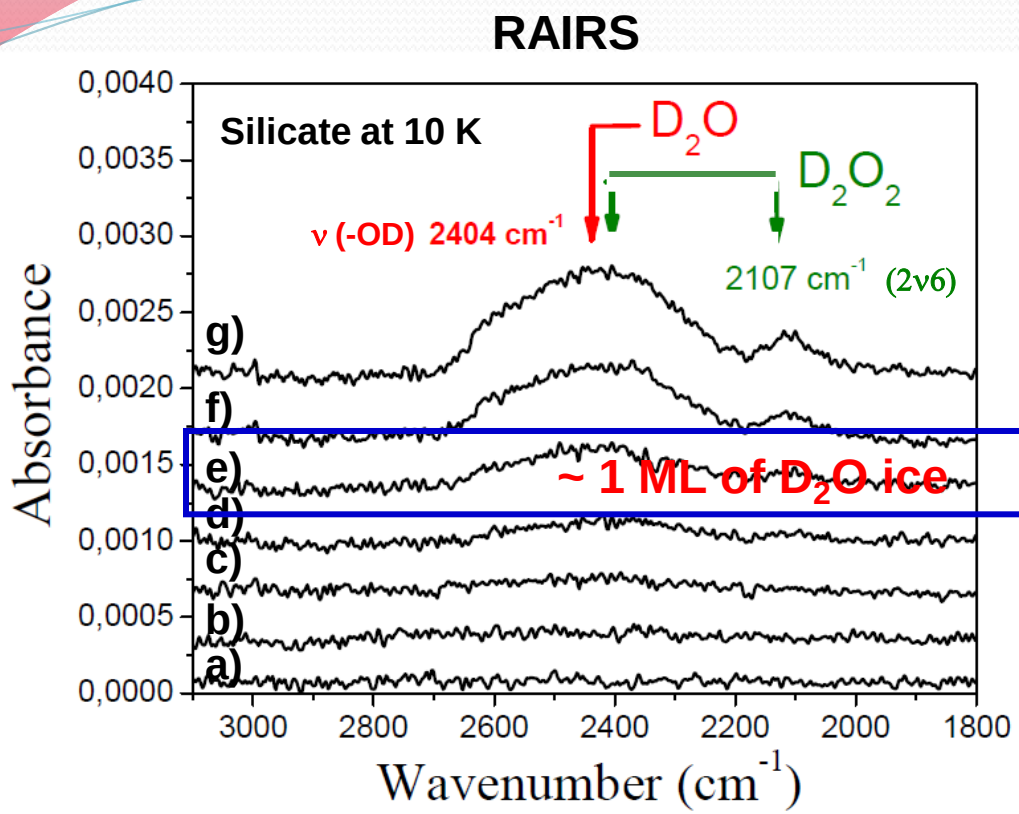


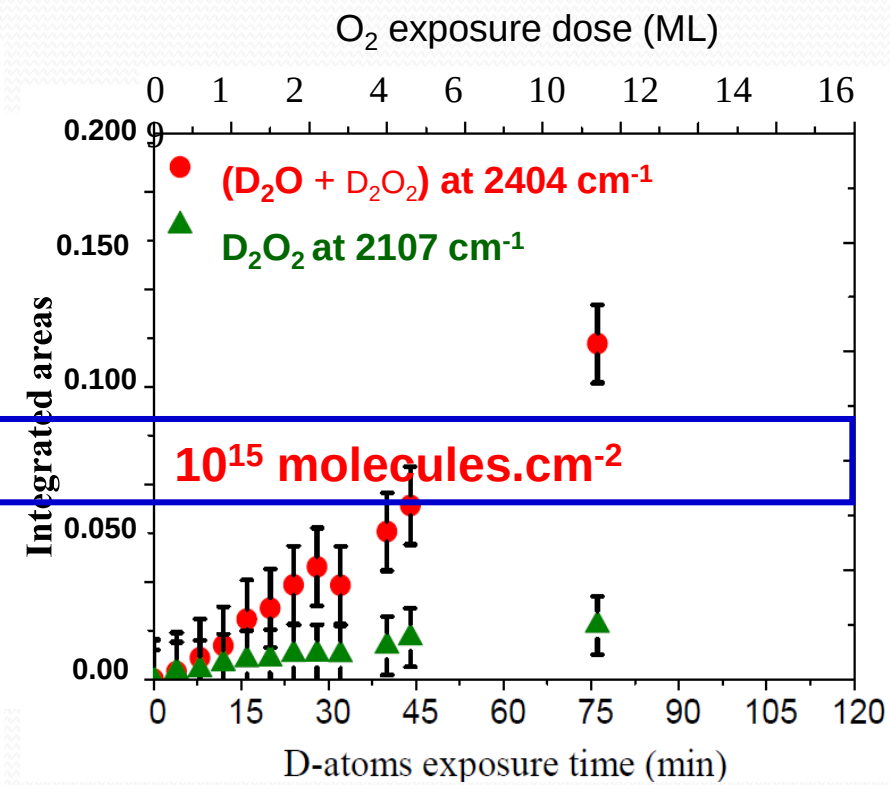
Reflection Absorption Infra-Red Spectroscopy RAIRS

(Insitu Solid phase detection)

(4000- 600) cm^{-1}

RESULT 1: Water formation on Silicate surface





Successive deposition of O_2 and D atoms

(0.2 ML) **O_2** + 4 min **D-atoms**

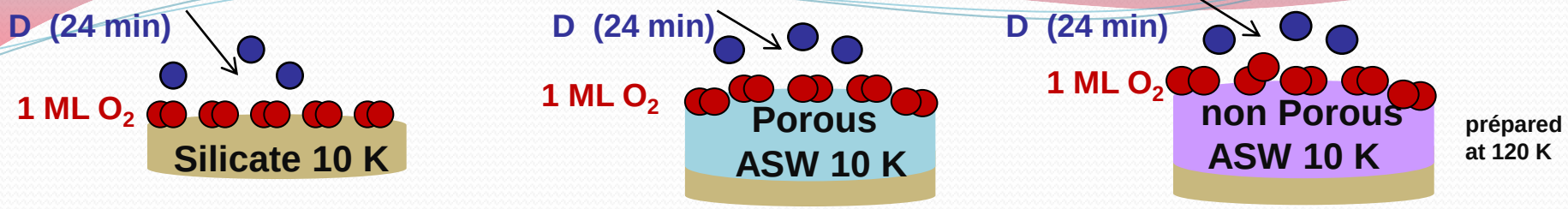
Low surface coverage

$D_2O > D_2O_2$

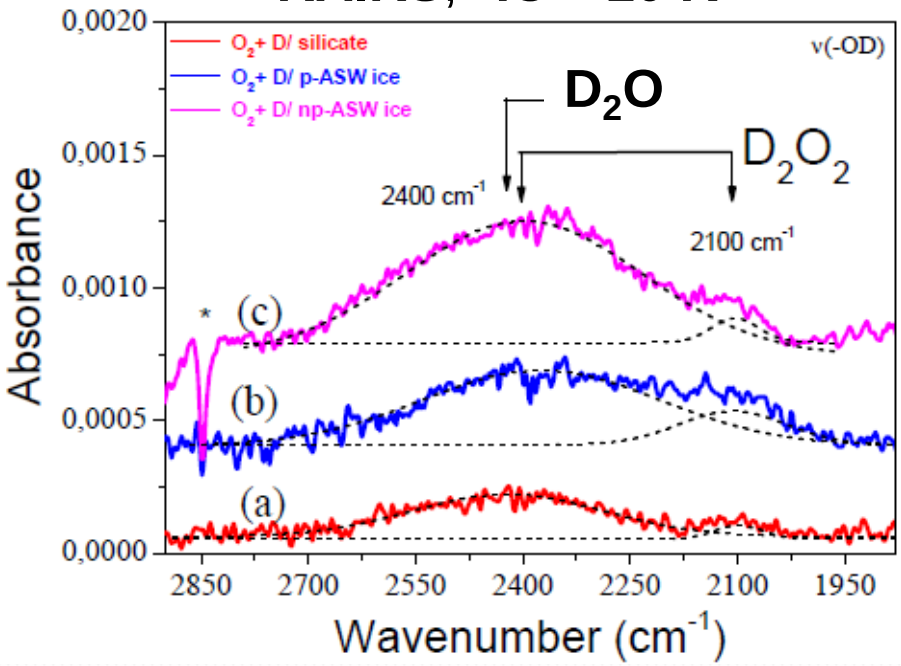
Sub-monolayer regime

Chaabouni et al. J. Chem. Phys (2012)

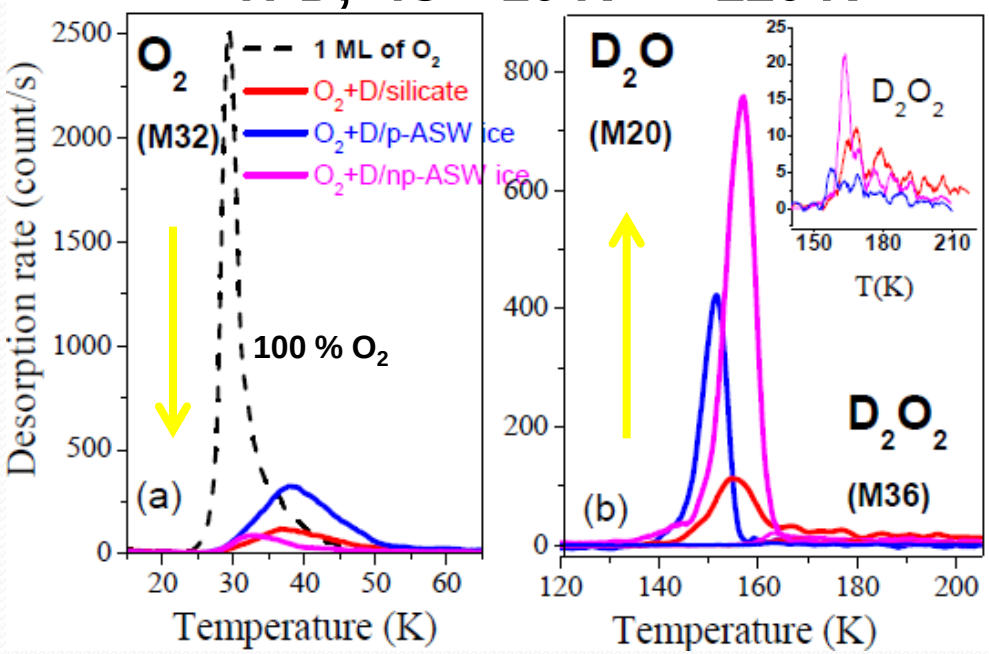
RESULT 2: Effect of the substrate on O_2 +D



RAIRS, Ts = 10 K



TPD, Ts = 10 K → 220 K



5 % O_2 — 17 % D_2O

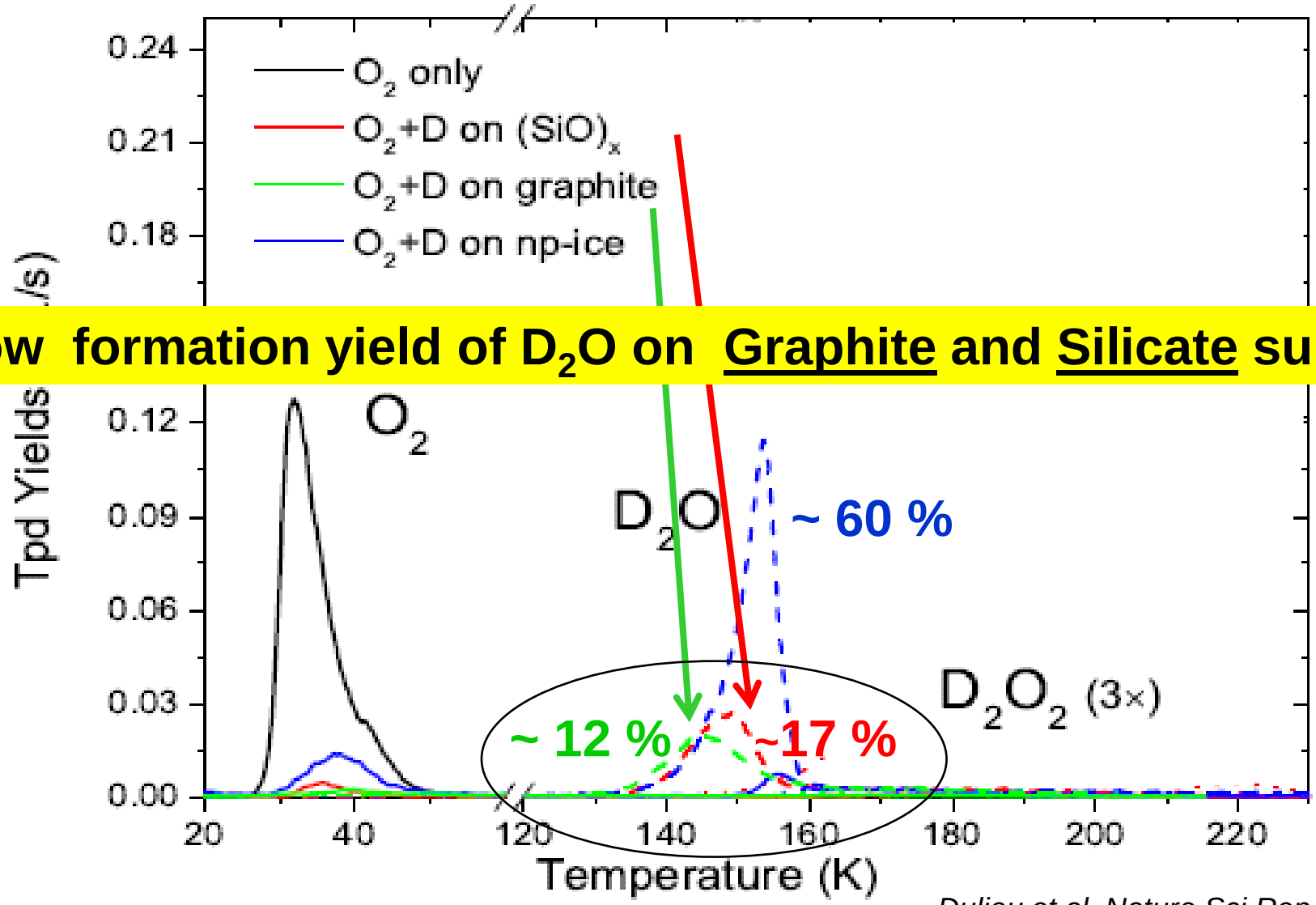
15 % O_2 — 50 % D_2O

2 % O_2 — 60 % D_2O

Low formation yield of D_2O water ice on the <u>Silicate surface</u> at 10K

Chaabouni et al. J. Chem. Phys (2012)

RESULT 2: Effect of the substrate on O_2 +D

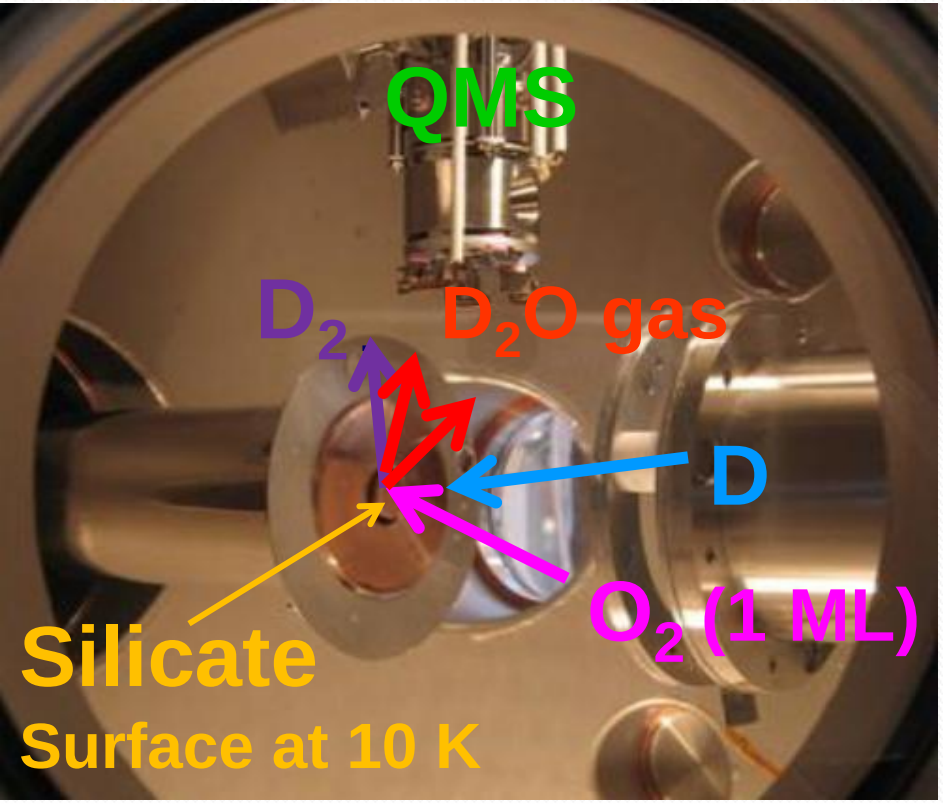


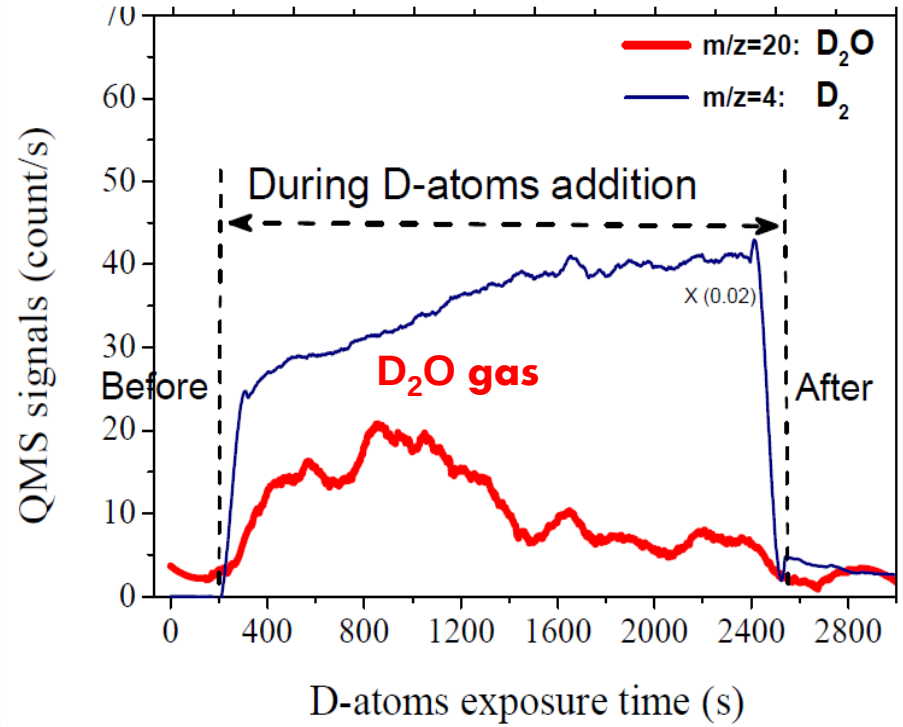
Low formation yield of D_2O on <u>Graphite</u> and <u>Silicate</u> surfaces

Dulieu et al, Nature.Sci.Rep (2013)

RESULT 3: Chemical desorption

DED





Monitoring with the QMS the species desorbing into the gas phase during the exposure of D-atoms on 1 ML (O_2) ice at 10 K.

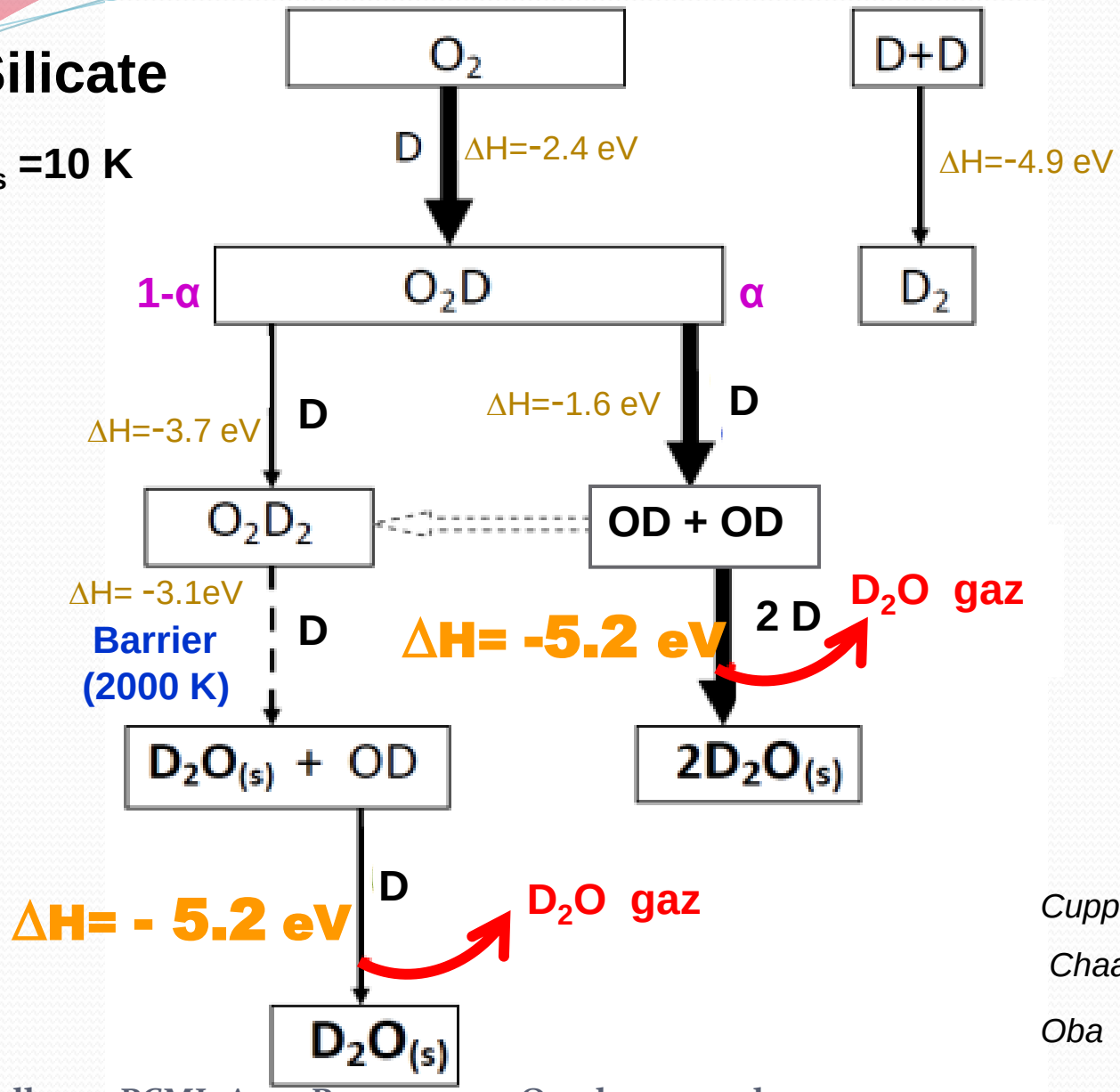
Non thermal desorption of D_2O upon formation on the surface at 10 K

Chemical desorption of D_2O

Reaction routes for water formation

Silicate

T_s =10 K



Eley Rideal mechanism

Barrierless reaction

$$D + OD \longrightarrow D_2O$$

Chemical desorption of D_2O by the **exothermic** reaction

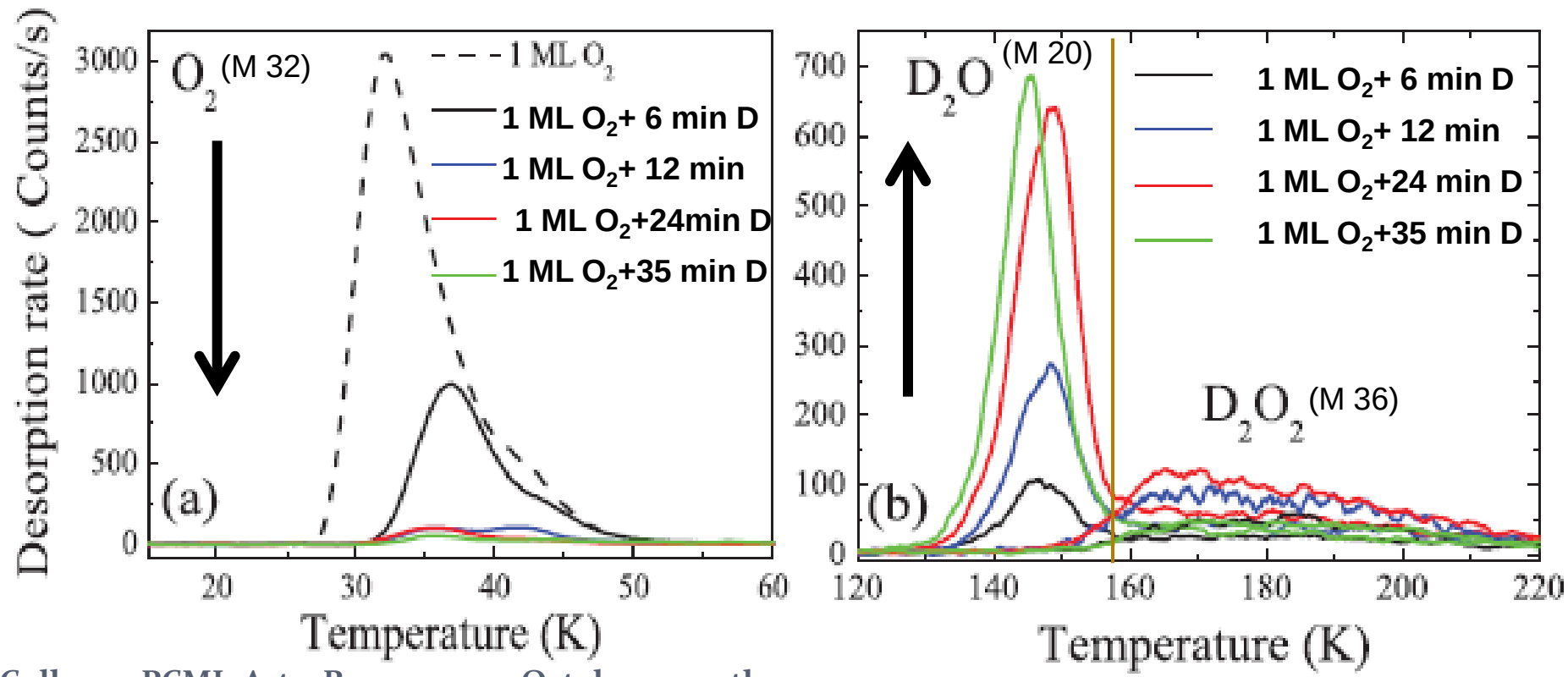
$$D + OD \longrightarrow D_2O$$

Cuppen et al. PCCP (2010)

Chaabouni et al. J.Chem.Phys (2012)

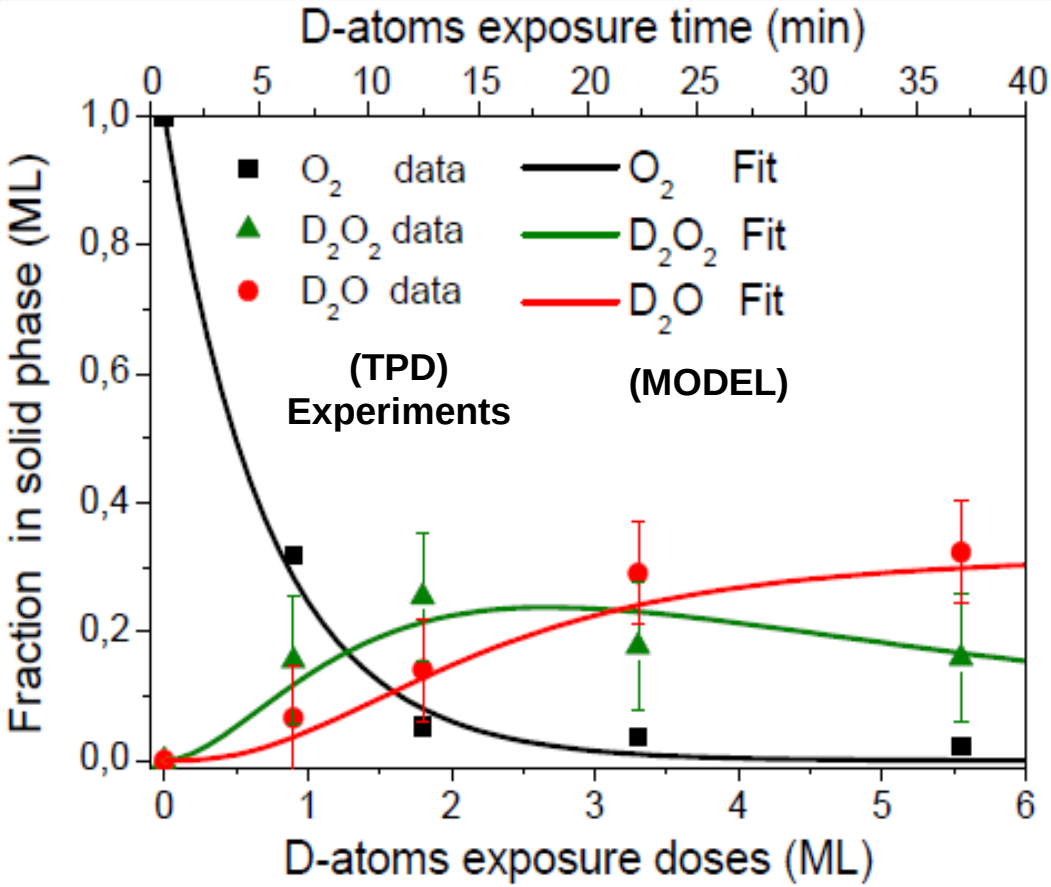
Oba et al. ApJ (2013)

Kinetic O_2+D reaction on Silicates



Kinetic O_2+D reaction on Silicate

Modeling



$O_2 + D \xrightarrow{k} O_2D$

$O_2D + D \xrightarrow{k} OD + OD$ $\alpha = 0,7$

$\xrightarrow{k} D_2O_2$ $1-\alpha=0,3$

$D_2O_2 + D \xrightarrow{k_1} D_2O_{(solid)} + OD$

$OD + D \xrightarrow{k} D_2O_{(solid)}$ (Cd → (gas))

Rate constante of reactions without Barrier **k =1**

Rate constant of reaction with a Barrier **k_1=0.09**

Branching ratio of the reaction **α=0,7**

Chemical desorption rate of D_2O Cd= 80 %

Conclusions

- The formation of water through O_2+D is **efficient** in the **sub-monolayer regime.**
- The **formation yield** of D_2O water ice **depends** on **dust grain surfaces.**

SILICATE and GRAPHITE

$$O_2 + D \longrightarrow DO_2 + D \longrightarrow \begin{array}{l} OD + D \longrightarrow D_2O \\ + \\ OD + D \longrightarrow D_2O \end{array} \quad (gas)$$

The heat of the exothermic reaction desorbe water into the gas phase

High chemical desorption rate (~ 80 %)

WATER ICE

$$O_2 + D \longrightarrow DO_2 + D \longrightarrow OD + OD \longrightarrow D_2O_2 \xrightarrow{D} D_2O\ (solid) + OD$$

WATER ICE dissipate the excess energy released from exothermic reactions

chemical desorption rate (~ 40 %) .

- ***Astrophysical implications:*** *The **chemical desorption** of **water** has an impact on the **gas phase composition** of astrophysical environment, and can affect Stars and Planets formation.*

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