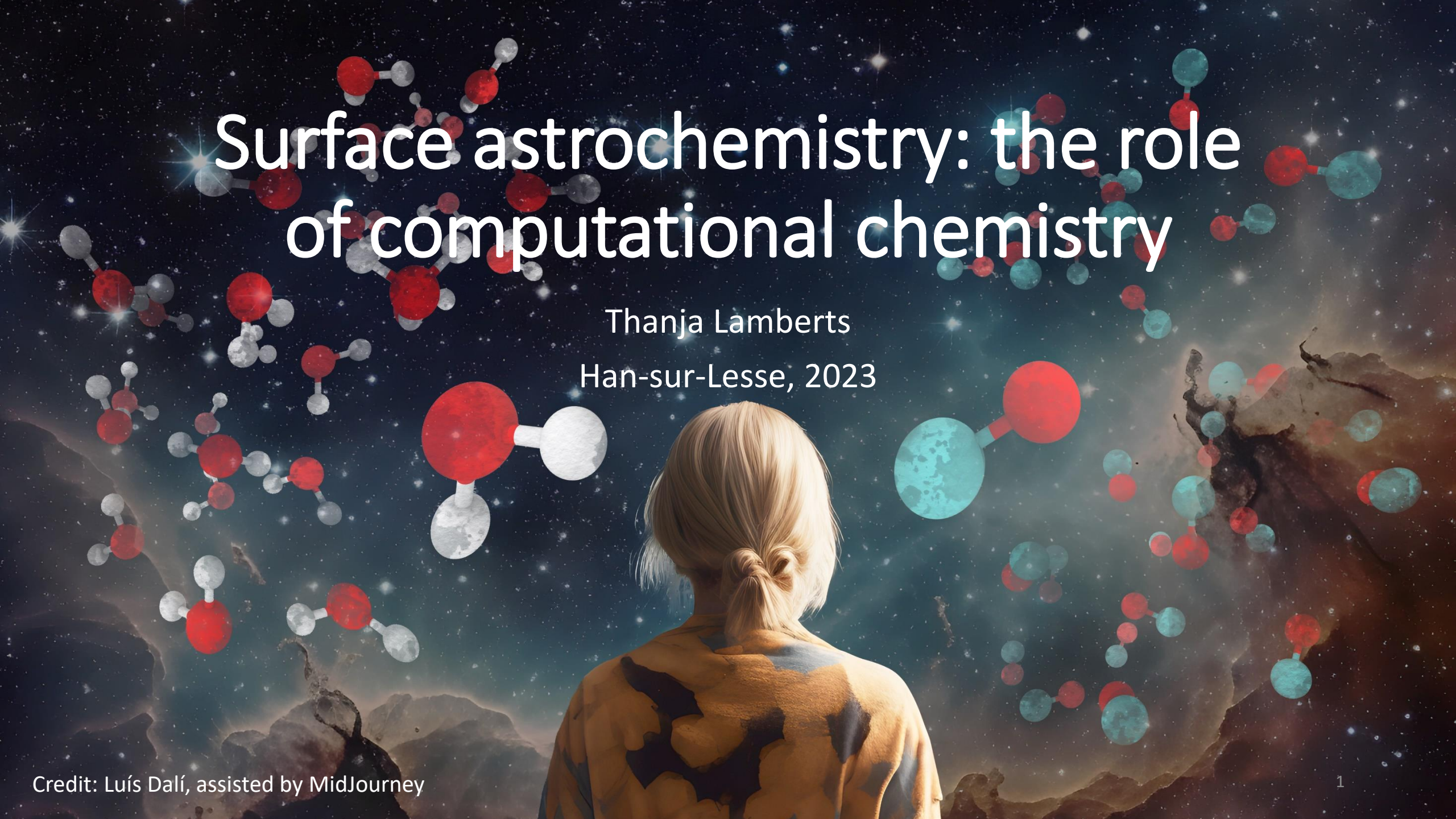
Surface astrochemistry: the role of computational chemistry

Thanja Lamberts

Han-sur-Lesse, 2023

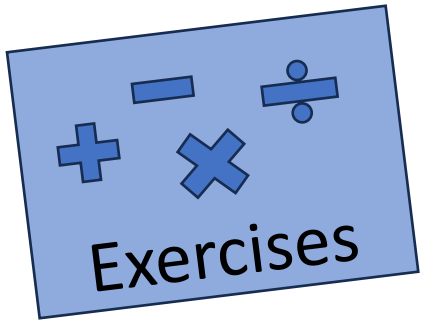


Credit: Luís Dalí, assisted by MidJourney

Lecture Overview

- Introduction Astrochemistry

- Surface processes & Timescales
  - Dissipation (3rd body)
  - Adsorption
  - Desorption
  - Diffusion
  - Reaction
    - Energetics of a chemical reaction
    - Surface reaction mechanisms



- Energetic Processing & Non-thermal Desorption

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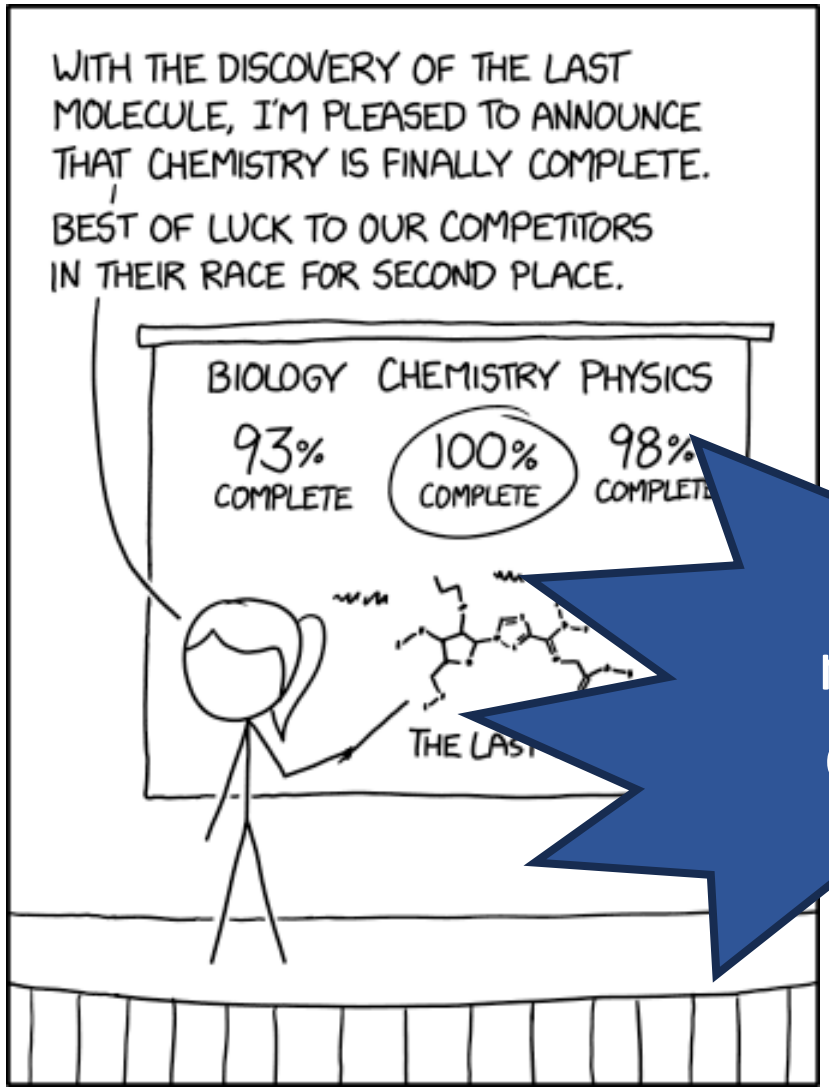
- Energetic Processing & Non-thermal Desorption

Astrochemistry

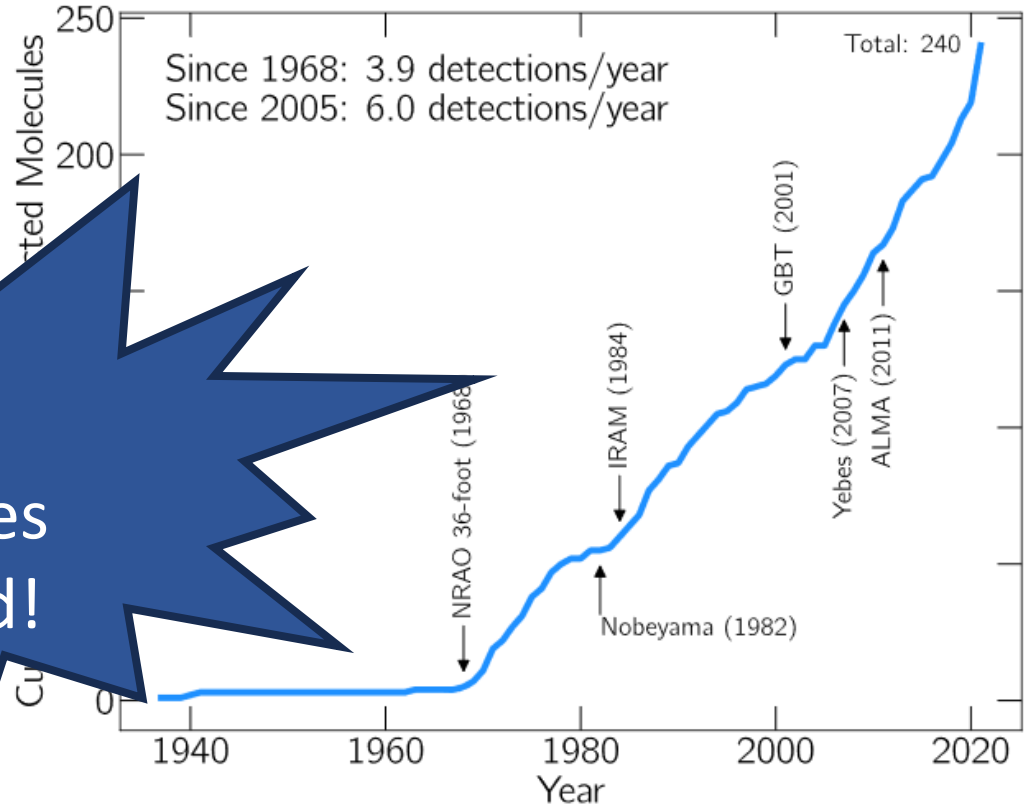
Article Talk

From Wikipedia, the free encyclopedia

Astrochemistry is the study of the abundance and reactions of molecules in the universe, and their interaction with radiation.[1] The discipline is an overlap of astronomy and chemistry. The word "astrochemistry" may be applied to both the Solar System and the interstellar medium. The study of the abundance of elements and isotope ratios in Solar System objects, such as meteorites, is also called cosmochemistry, while the study of interstellar atoms and molecules and their interaction with radiation is sometimes called molecular astrophysics. The formation, atomic and chemical composition, evolution and fate of molecular gas clouds is of special interest, because it is from these clouds that solar systems form.



> 300 molecules detected!



Astrochemistry

- Bridging astronomy, physics, chemistry

- More than a stamp-collection of molecules:
  - Role of molecules in forming the Universe
  - Tracers of physical conditions in different interstellar regions (spectroscopy!)
  - Formation, excitation and destruction

- 1937/1940: CH is the first molecule to be detected

  Radio astronomy is pivotal!

Ices and the star formation process

NASA, ESA, CSA, STScI; Joseph DePasquale (STScI), Anton M. Koekemoer (STScI), Alyssa Pagan (STScI). Bill Saxton, NRAO, L. I. Cleeves

Prestellar Core

n_H ~10^6 cm^{-3}

T ~ 10 K

Dense cloud

n_H ~1-10^4 cm^{-3}

T ~ 20 K

Protostar

n_H ~10^7 cm^{-3}

T ~ 100 K

Protoplanetary disk

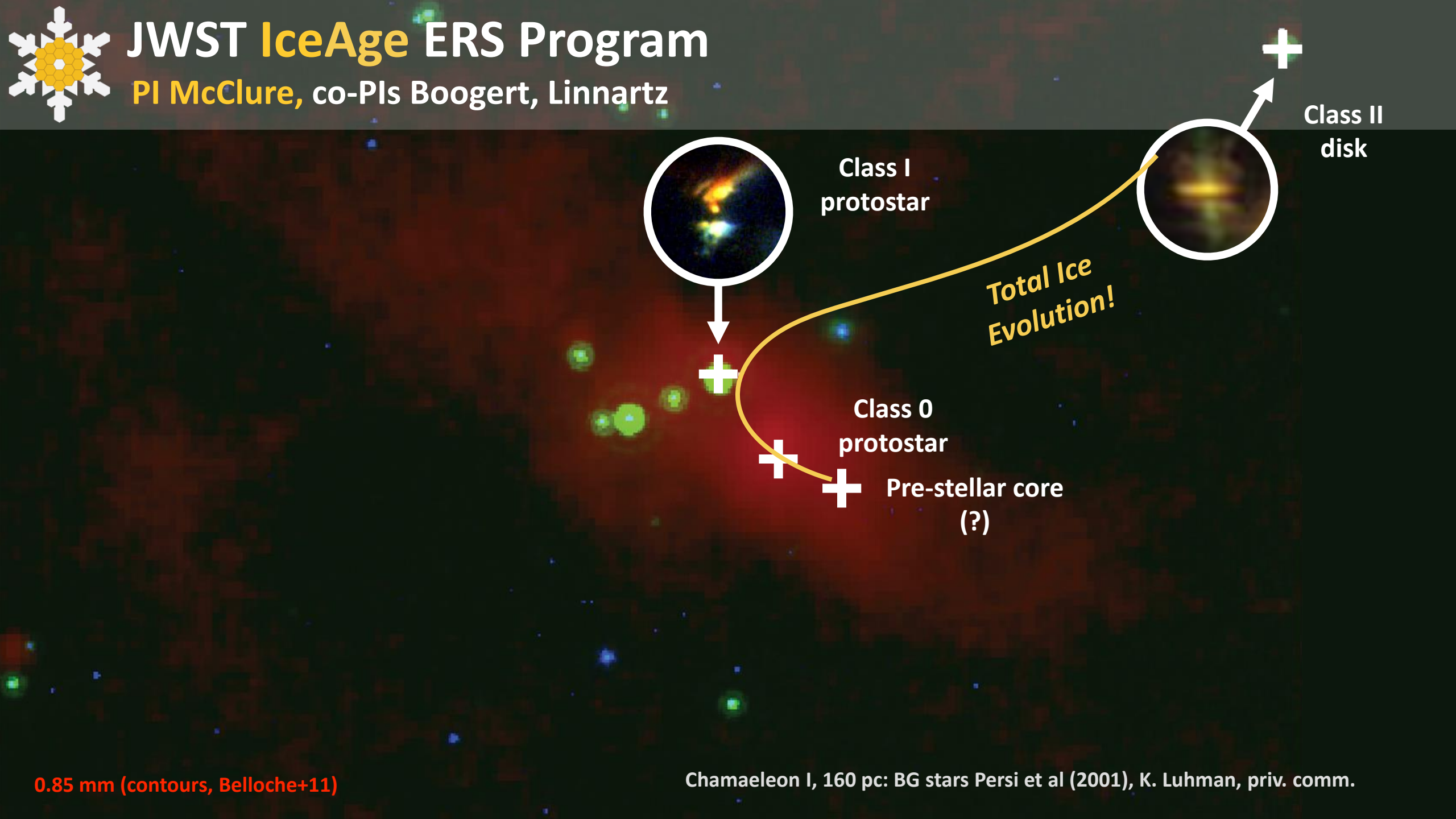
n_H ~10^9 - 10^{15} cm^{-3}

T ~ 10-10,000 K

Solar System

JWST IceAge ERS Program

PI McClure, co-PIs Boogert, Linnartz



0.85 mm (contours, Belloche+11)

Chamaeleon I, 160 pc: BG stars Persi et al (2001), K. Luhman, priv. comm.

Region	n_{H} (cm^{-3})	T (K)
Coronal gas	$< 10^{-2}$	5×10^{5}
HII regions	> 100	1×10^{4}
Diffuse gas	100-300	70
Molecular clouds	10^{4}	10
Pre-stellar cores	10^{5}-10^{6}	10-30
Star Forming Regions	10^{7}-10^{8}	100-300
Protoplanetary disks	10^{4}(outer)-10^{10}(inner)	10(outer)-500(inner)
Envelopes of Evolved stars	10^{10}	2000-3500

Drivers of chemistry

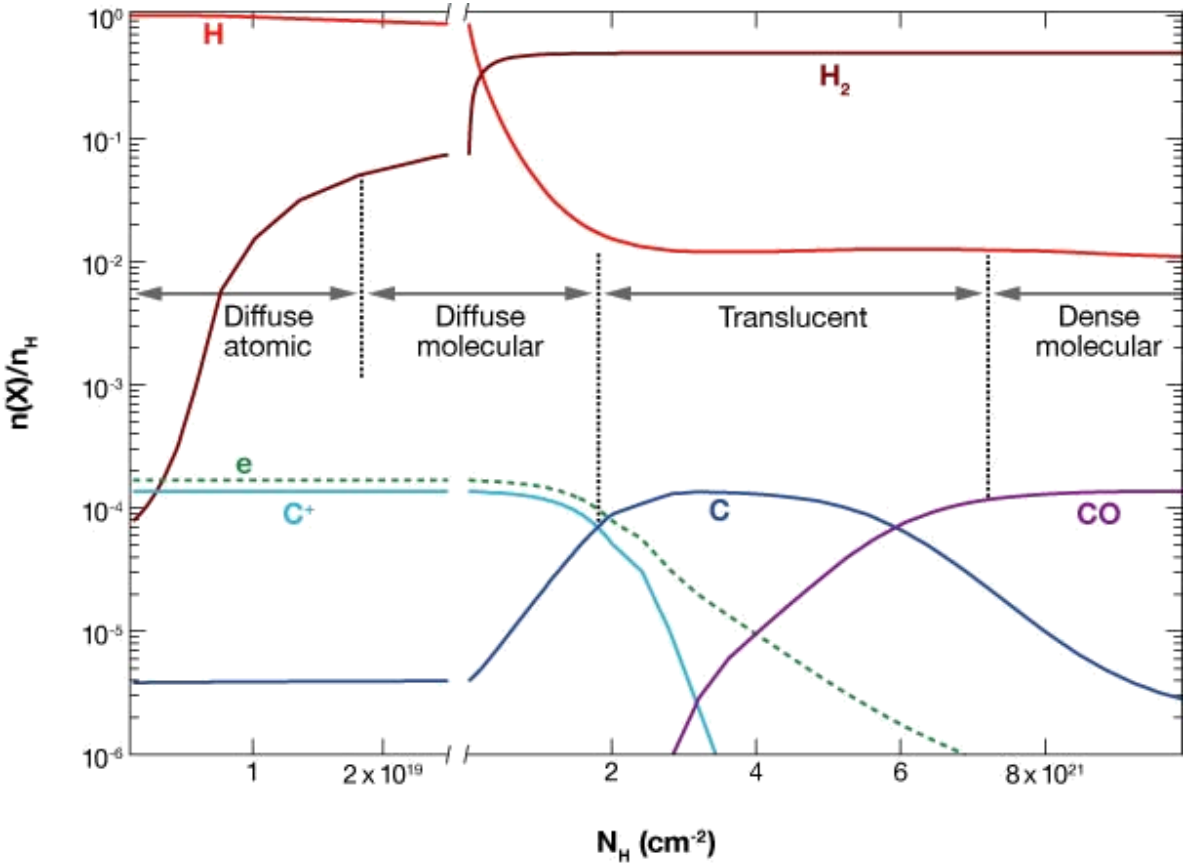
- Not in thermodynamic equilibrium

- Low density & low temperature: chemistry needs to be driven
  - Starlight
  - Cosmic rays
  - (Exothermic) grain chemistry
  - Gas hydrodynamics

Ingredients: **Radiation**, Gas, and Dust

Different sources of radiation:

- UV (dense clouds are shielded)
- X-Rays
- Cosmic Rays (= high energy nuclei)

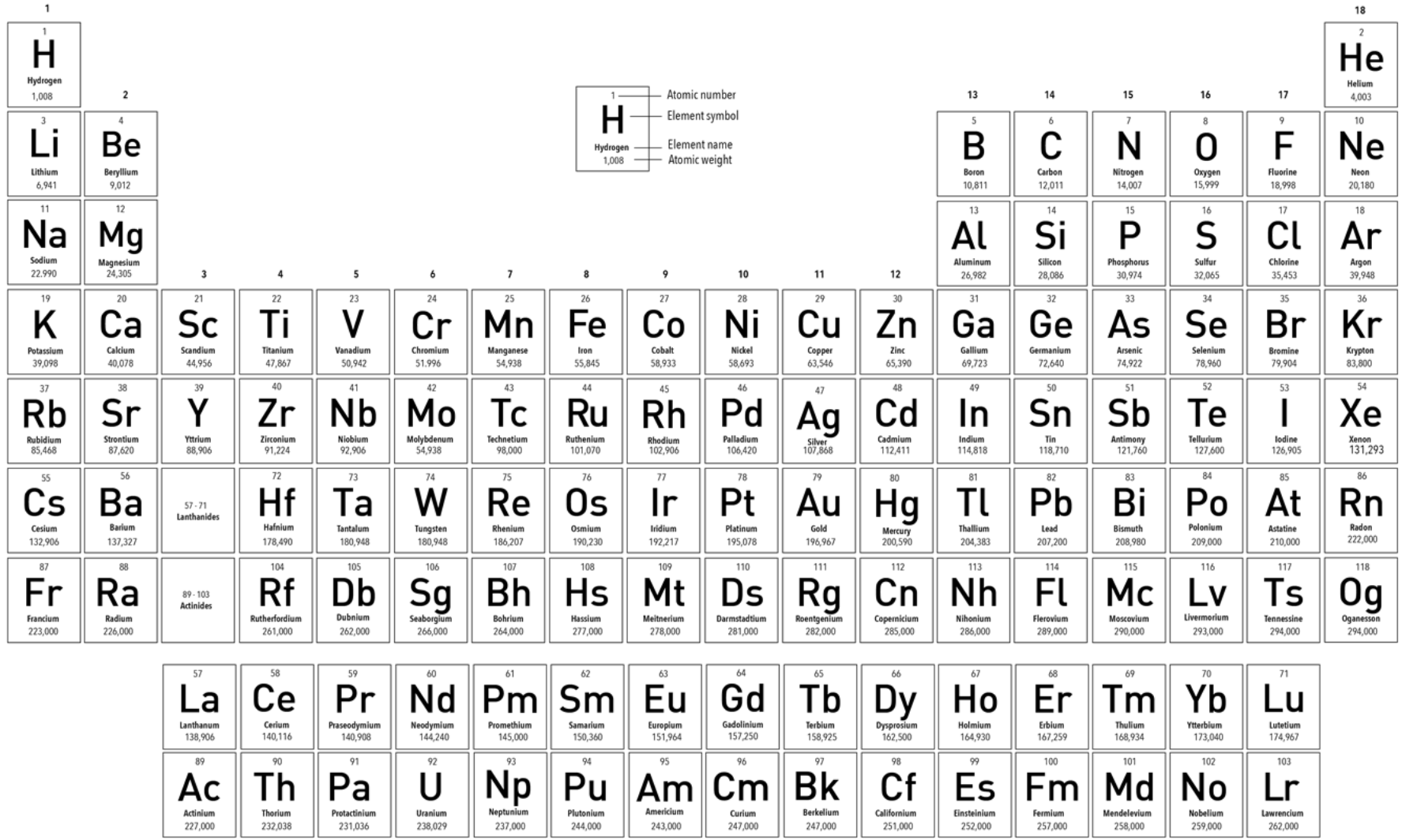


Snow & McCall ARAA 44, 367 (2006)

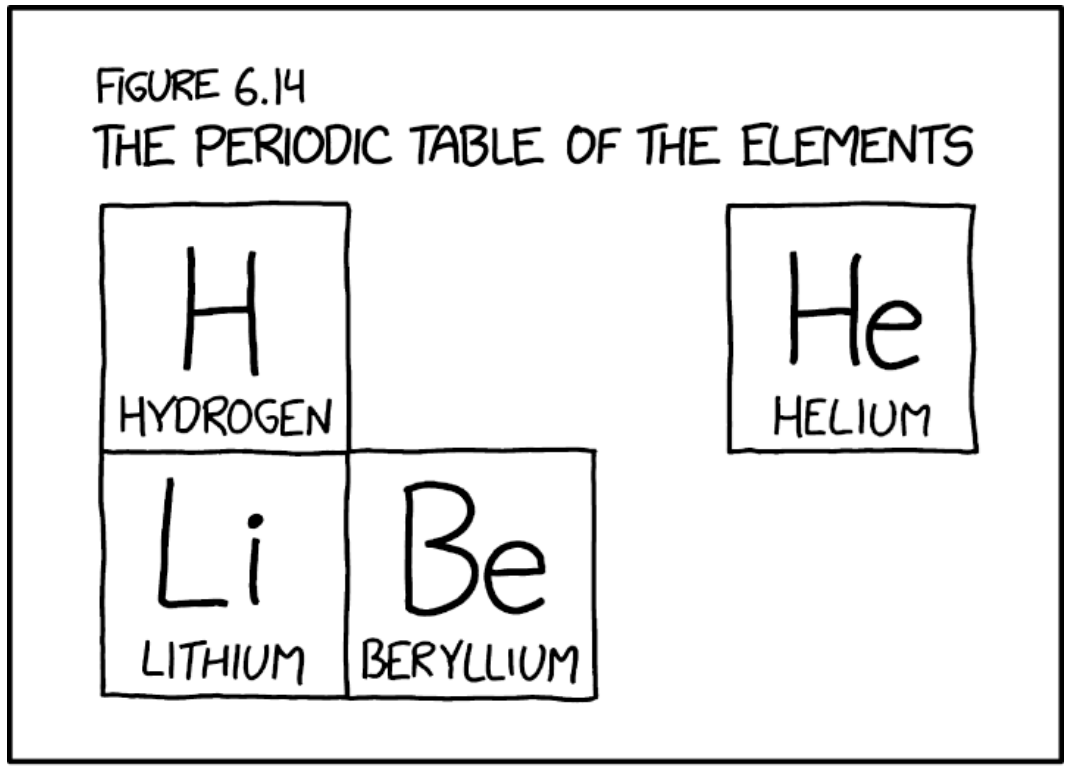
Ingredients: Radiation, **Gas**, and Dust

- Gas: H, He + other elements
  - formed in stellar nucleosynthesis
  - distributed by novae, supernovae, and stellar winds
- Relative elemental abundances vary within a galaxy and from galaxy to galaxy
- Solar abundances used as a conventional reference level

PERIODIC TABLE OF THE ELEMENTS



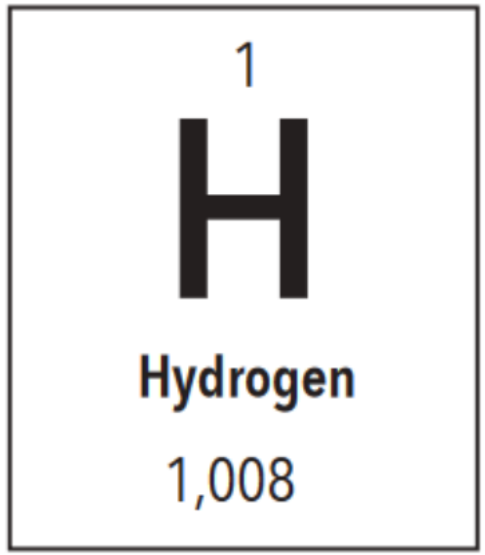
www.periodictable.co.za | Designed by Mia Viljoen

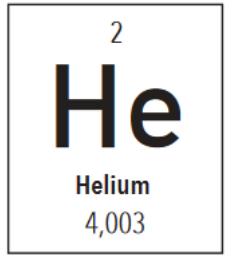


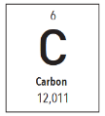
YOU CAN SPOT AN OUTDATED SCIENCE TEXTBOOK BY CHECKING THE BOTTOM OF THE PERIODIC TABLE FOR MISSING ELEMENTS. FOR EXAMPLE, MINE WAS PUBLISHED HALF AN HOUR AFTER THE BIG BANG.

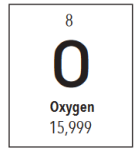
Astronomers'

PERIODIC TABLE OF THE ELEMENTS









Molecular complexity ?!

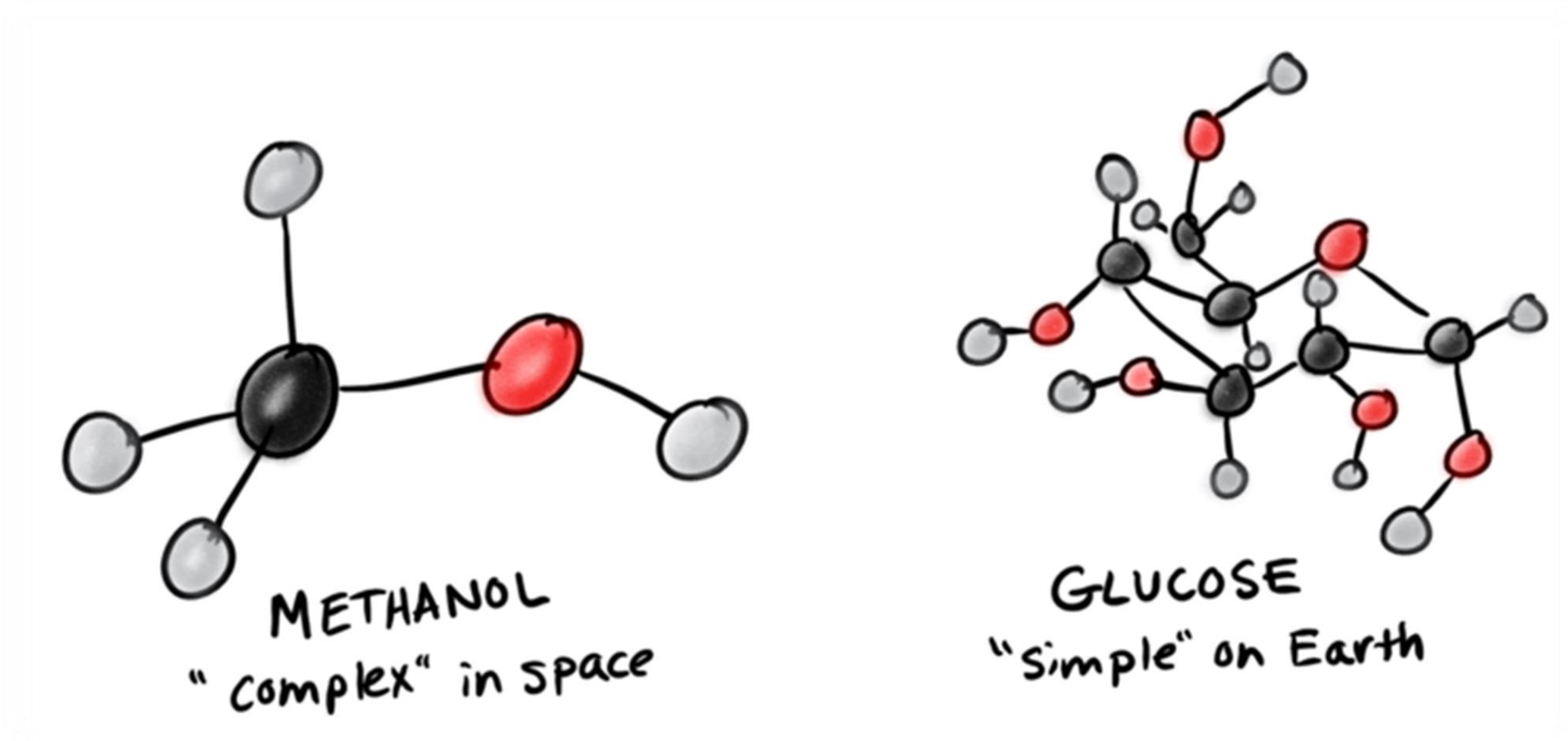


Figure courtesy: Olivia Harper Wilkins

Types of important gas-phase reactions

Two-body reactions with “two-body” products

Associative detachment

UV photoreactions

Dissociative recombination

Cosmic Ray ionization

Collisional dissociation

Cosmic Ray induced photoreactions

Ion-molecule reactions

Radiative association

Neutral-neutral reactions

Charge-transfer reactions

Different types of molecules are observed, why?

- N_2H+ ($N{\equiv}N\text{-}H^+$)
- HC_3N ($H\text{-}C{\equiv}C\text{-}C{\equiv}N$)
- C_2H
- $C{\equiv}O$
- H_2

- H_2O
- CH_4
- NH_3
- CH_3OH
- CO_2 ($O{=}C{=}O$)
- $C{\equiv}O$

High hydrogen content = saturation

$H + X \rightarrow HX$

Ingredients: Radiation, Gas, and **Dust**

- Nucleates in the envelopes of cool stars, in novae and in supernovae
- The dust-to-gas ratio in our own Galaxy is ~ 1:100
- Size ranges from nm to μm
- Silicates and carbonaceous material (incl. metals, Mg, Fe, Si)
- Grains allow reactions of the form $A_{ads} + B_{ads} \rightarrow C_{ads}$ (e.g., H_2)

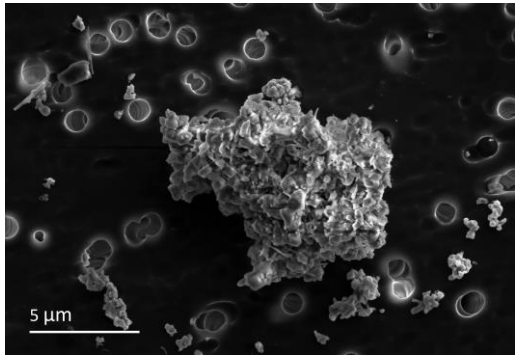
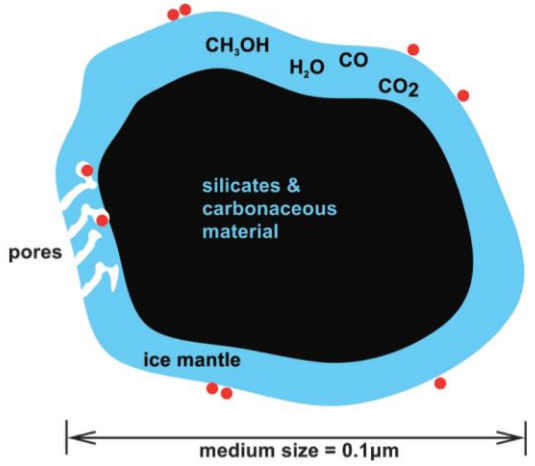


Figure courtesy:
Hope Ishii, University of Hawai'i



Karssemeijer et al. (2012)

Which (physical) conditions are important for surface chemistry to efficiently occur?

- Low temperature
- High density (H/H_2 <<1)
- UV-shielded ("high Av")

Region	n_H (cm^{-3})	T (K)
Coronal gas	$< 10^{-2}$	5×10^5
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Strong lines at mm wavelengths, so-called low-J transitions

Spectroscopy for astronomers

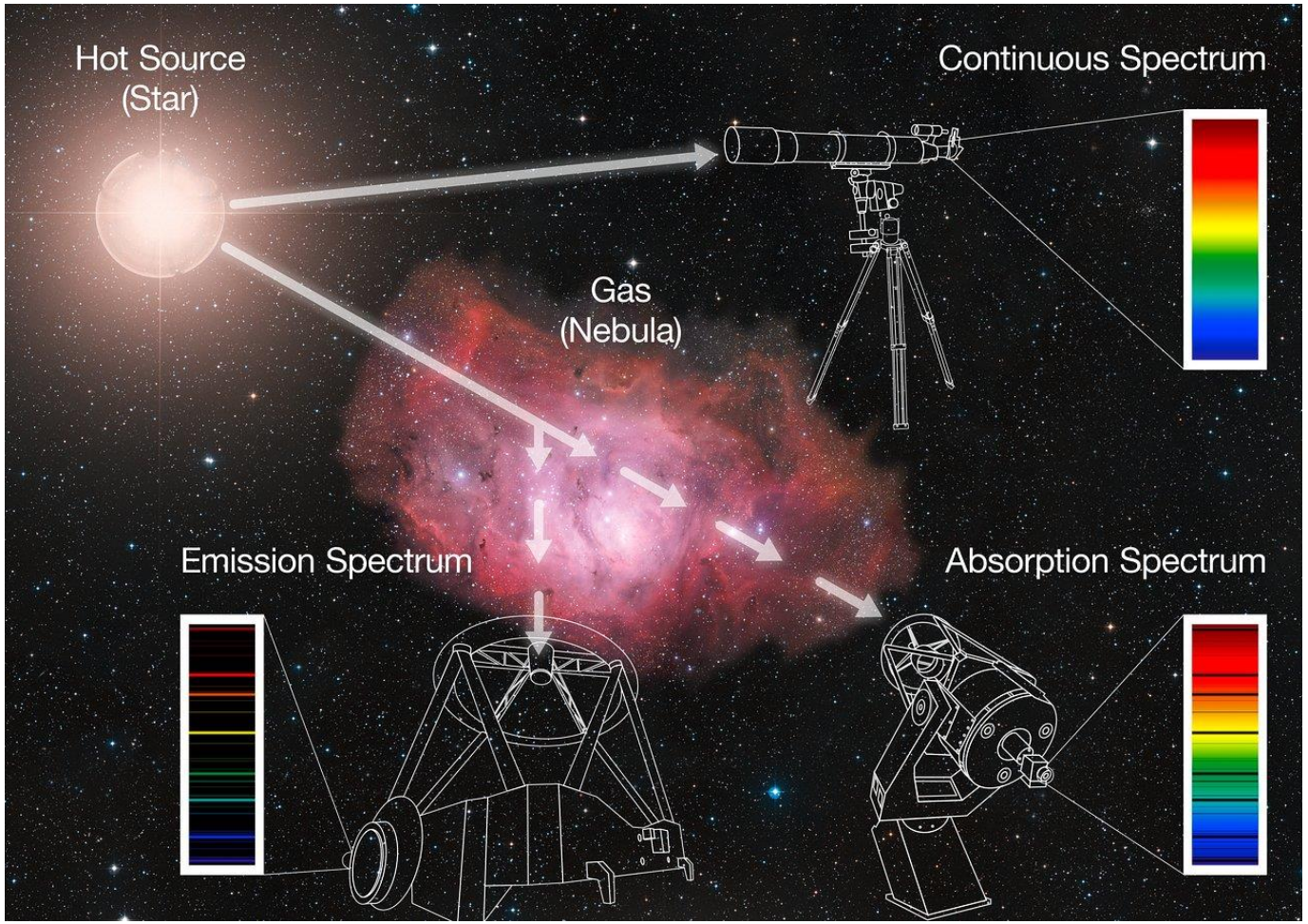
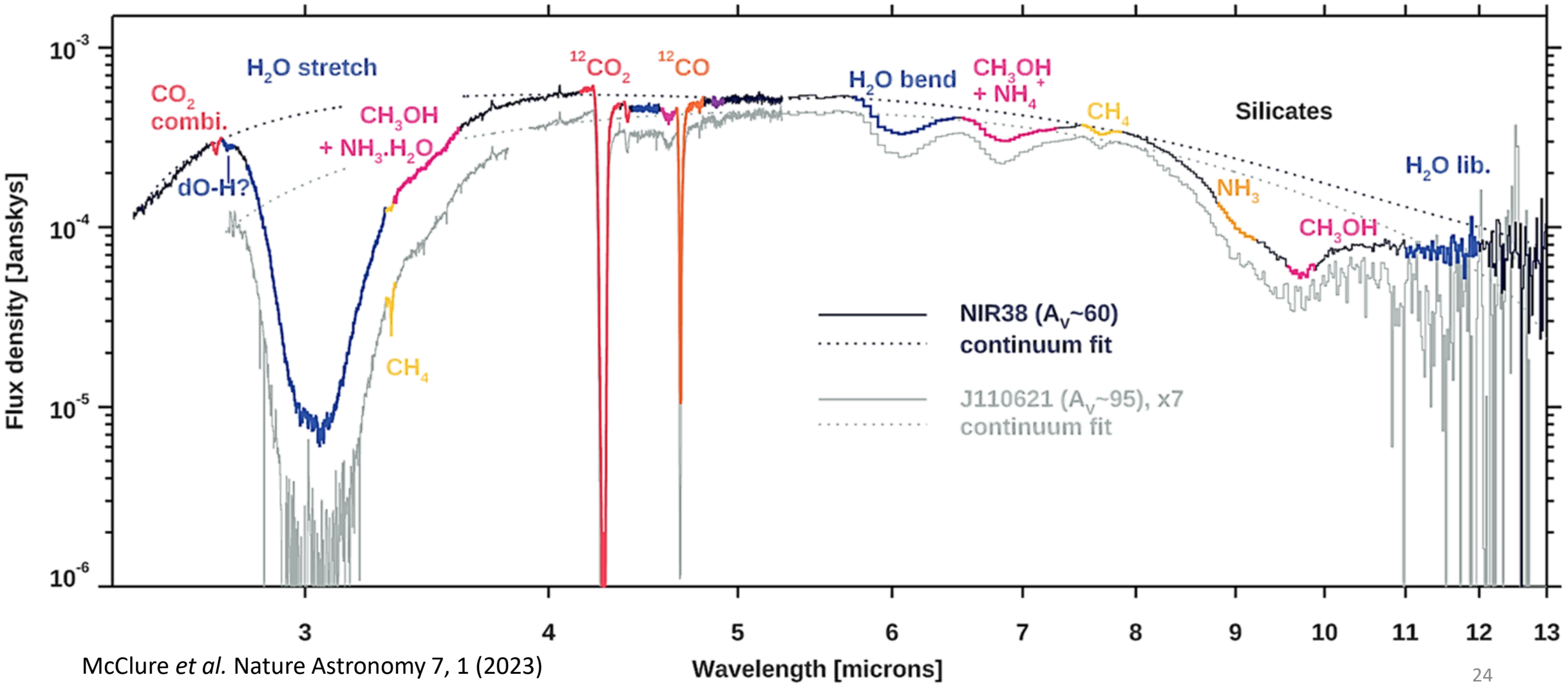


Figure courtesy: ESO

Figure courtesy: NASA, ESA, CSA, and M. Zamani (ESA/Webb);
Science: F. Sun (Steward Observatory), Z. Smith (Open University), and the Ice Age ERS Team

IceAge: JWST IR spectroscopy of ices



McClure *et al.* Nature Astronomy 7, 1 (2023)

Spectroscopy calculations?

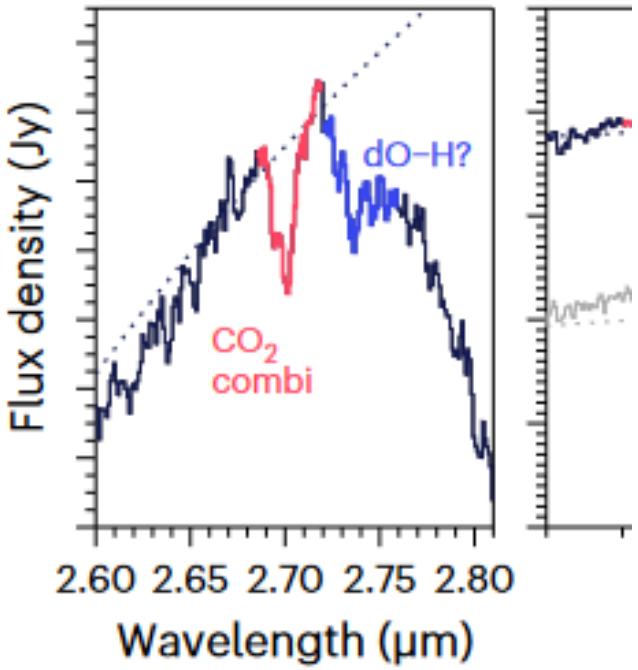
Measure spectra in the laboratory and compare to observations

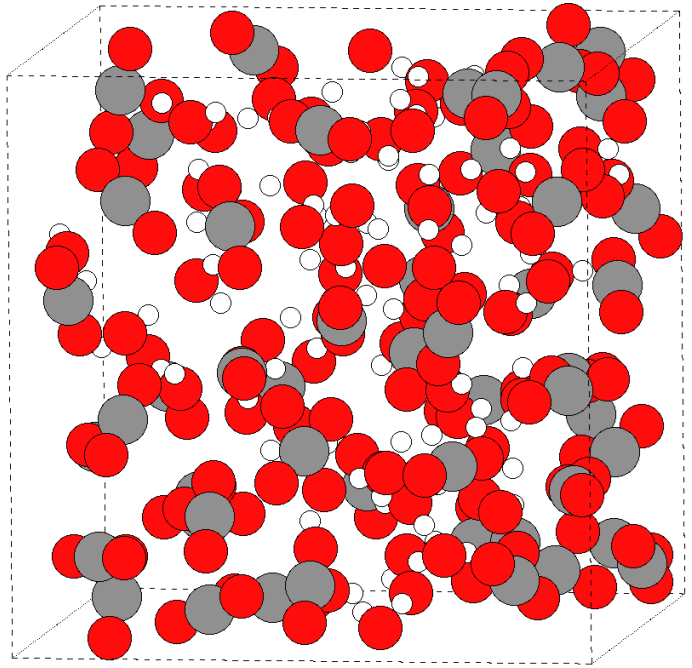
Leiden Ice Database for Astrochemistry

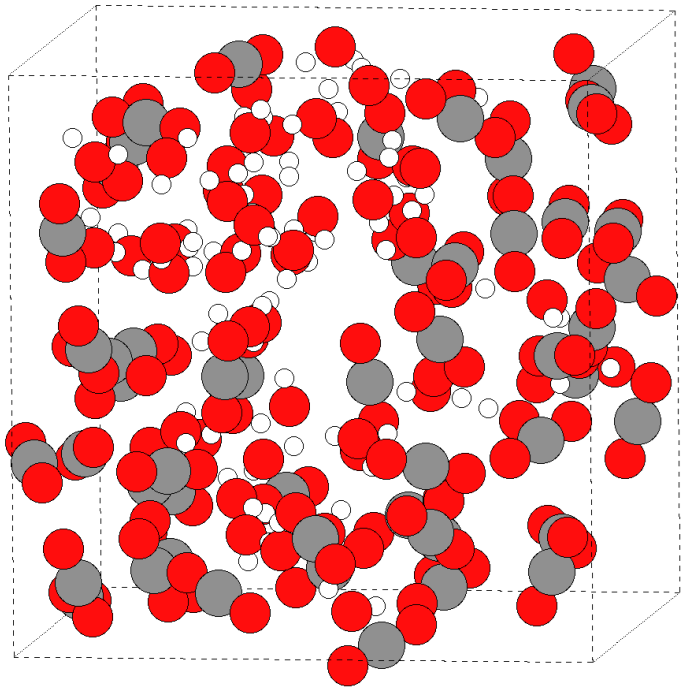
IR spectra and optical constants measured in the Leiden Laboratory for Astrophysics

Spectroscopy calculations: atomistic insight

Does the OH dangling mode shift as a result of different coordination with bulk H_2O or due to being covered by an adsorbed molecule?







McClure *et al.* Nature Astronomy 7 (2023) 431

Spectroscopy calculations: H_2O:CO_2

Need: description of energies, forces and dipole moments

Solution: parametrized force field MB-nrg (*)

based on ωB97M-V, CCSD(T) and CCSD(T)-F12b+CP data

$$V^{MB} = V_{perm.} + V_{polar.} + V_{short} + V_{disp}$$

Structures: Global optimisation vs. Random generation

(*) a machine-learned potential would ofc also be possible

Riera *et al.* JCTC 16 (2020) 2246

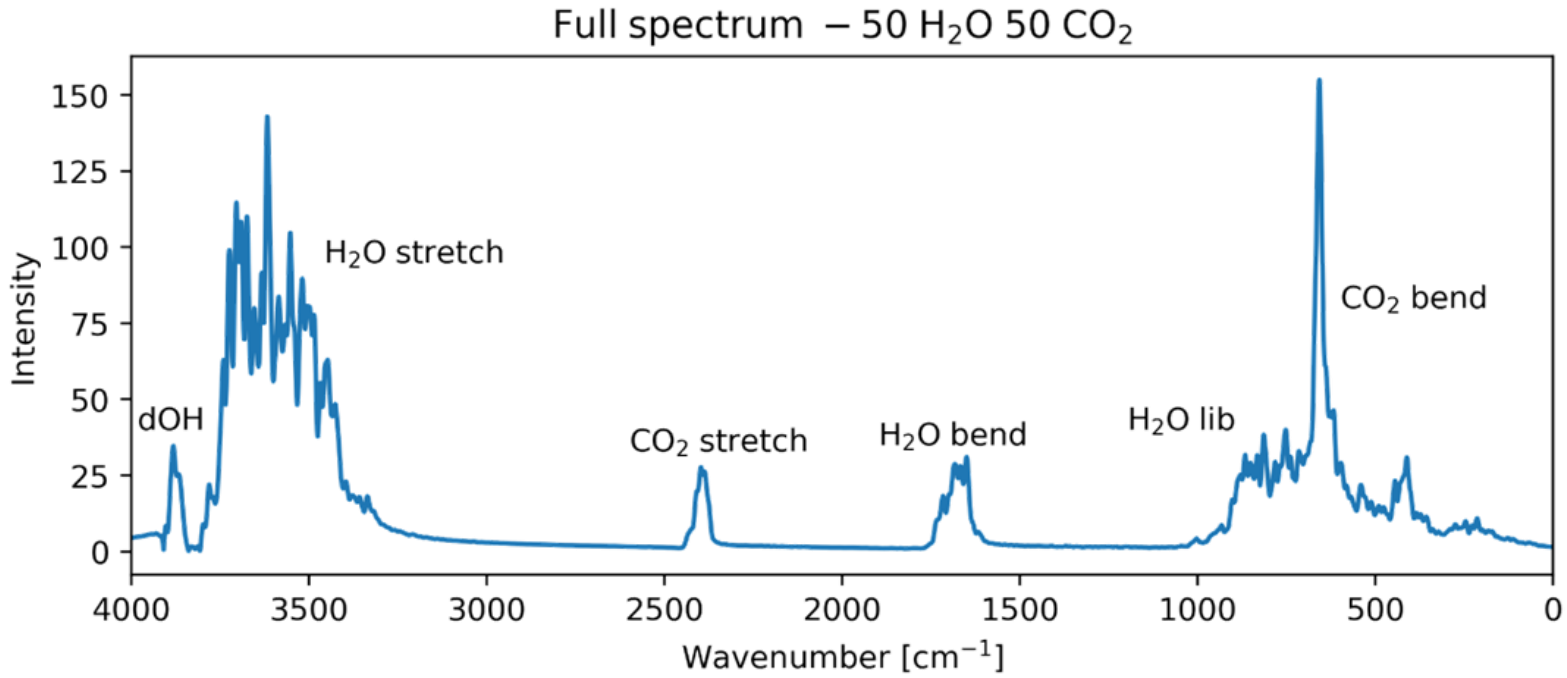
Spectroscopy calculations: MD simulations

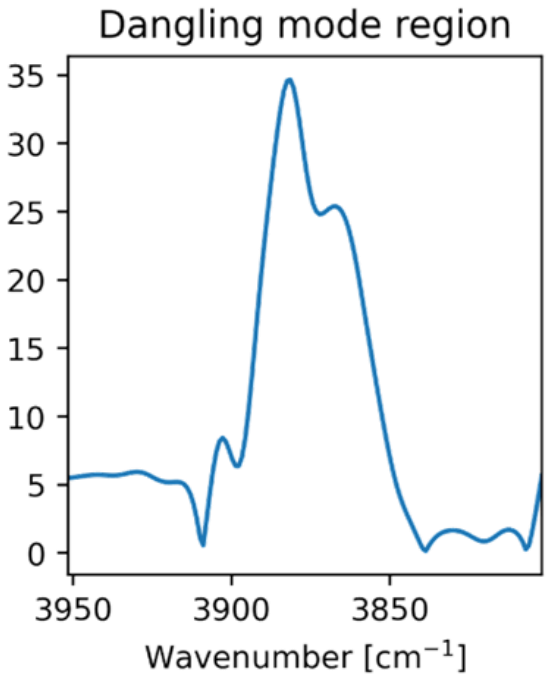
Autocorrelation

$$\langle \dot{\mu}(\tau)\dot{\mu}(t+\tau)\rangle_\tau \longrightarrow$$

Infrared spectrum

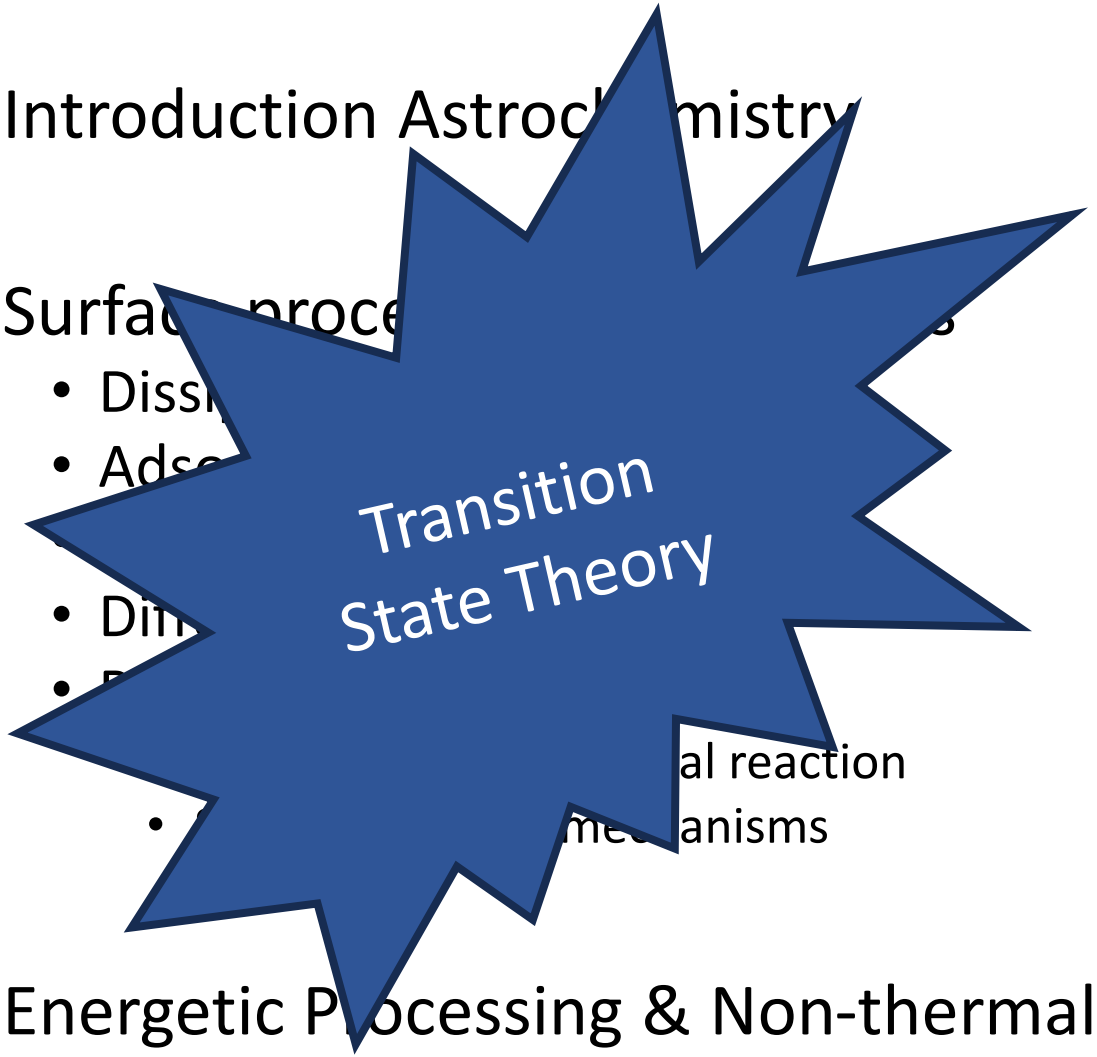
$$I(\omega) \propto \int \langle \dot{\mu}(\tau)\dot{\mu}(t+\tau)\rangle_\tau \, e^{-i\omega t} dt$$





Sneak-peak at the molecular scales

- Introduction Astroch mistry
- Surfac proce s
  - Diss
  - Ads
  - Di
  - al reaction
    - anisms
- Energetic P ocessing & Non-thermal Desorption



Reminder: TST

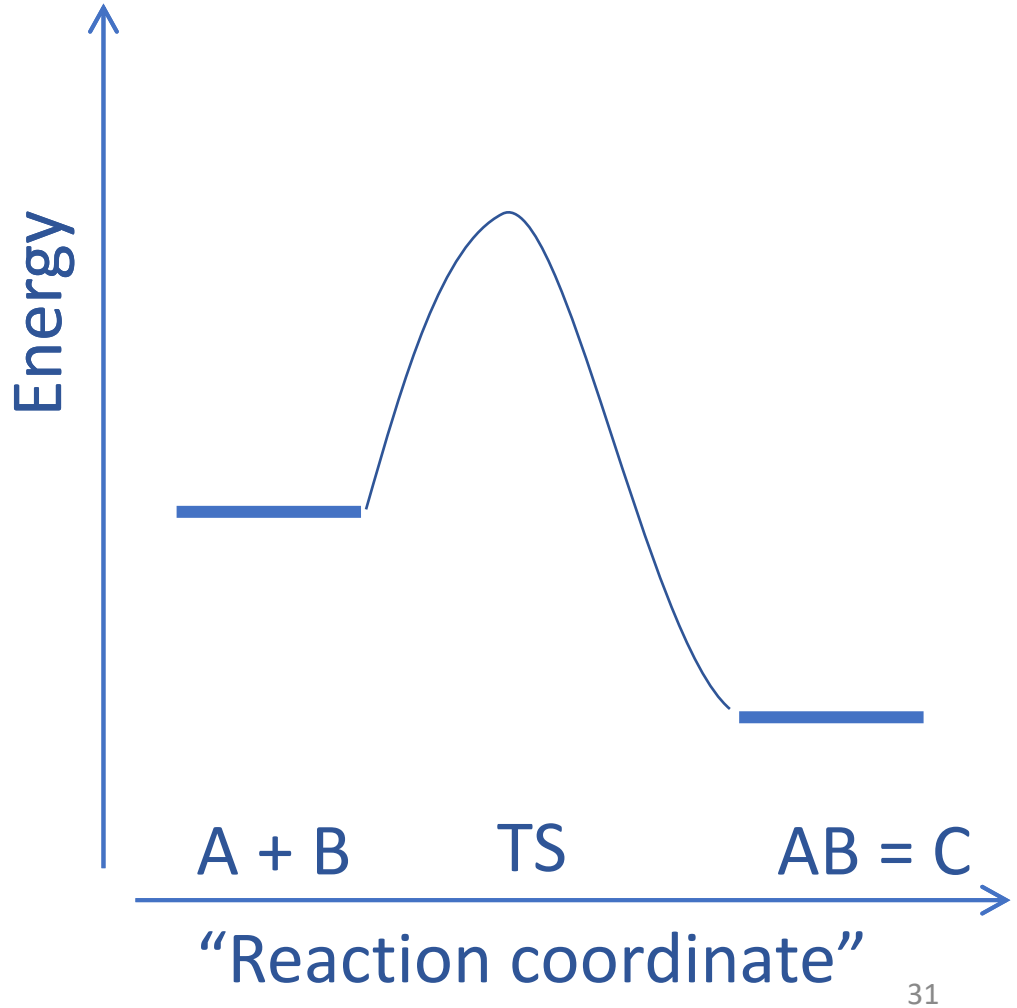
Reaction rate = $v\ [\mathrm{TS}]$

$= k\ [\mathrm{A}][\mathrm{B}]$

therefore $k = v \cdot \frac{[\mathrm{TS}]}{[\mathrm{A}][\mathrm{B}]} = v\mathrm{K}$

with (stat. therm.) $\mathrm{K} = \frac{z'_{\mathrm{TS}}}{z'_{\mathrm{A}} z'_{\mathrm{B}}}$

and $\mathrm{z}' = \sum_i e^{-\epsilon_i / k_{\mathrm{B}} T}$



Sneak-peak at the molecular scales

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  - Adsorption
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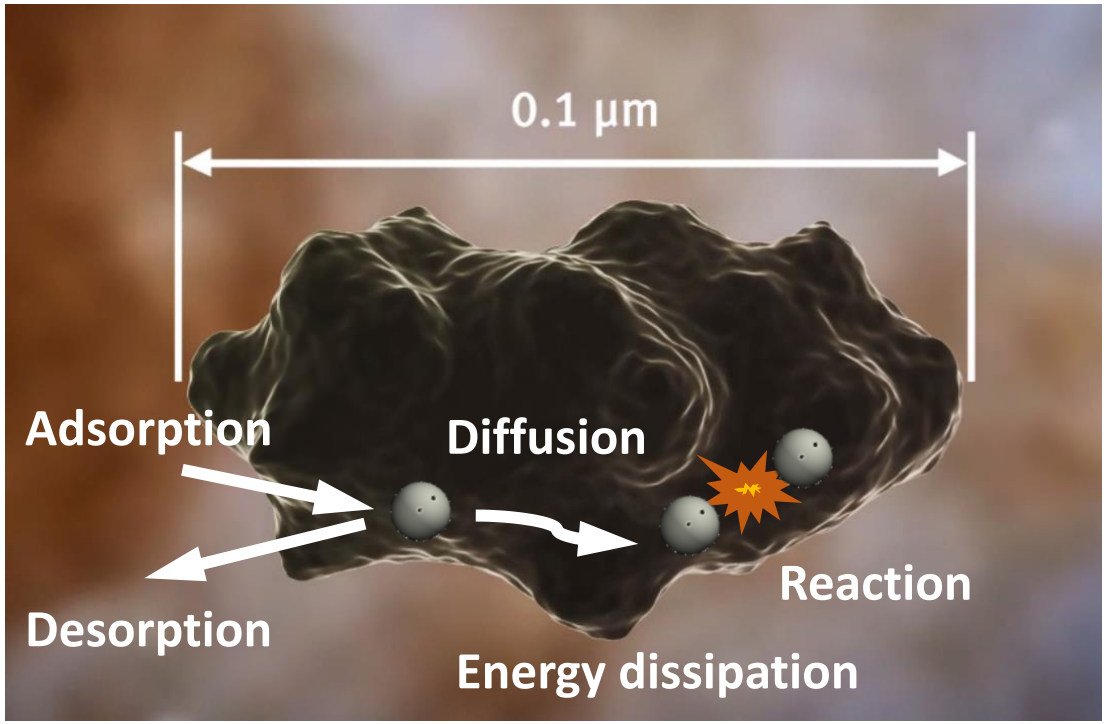
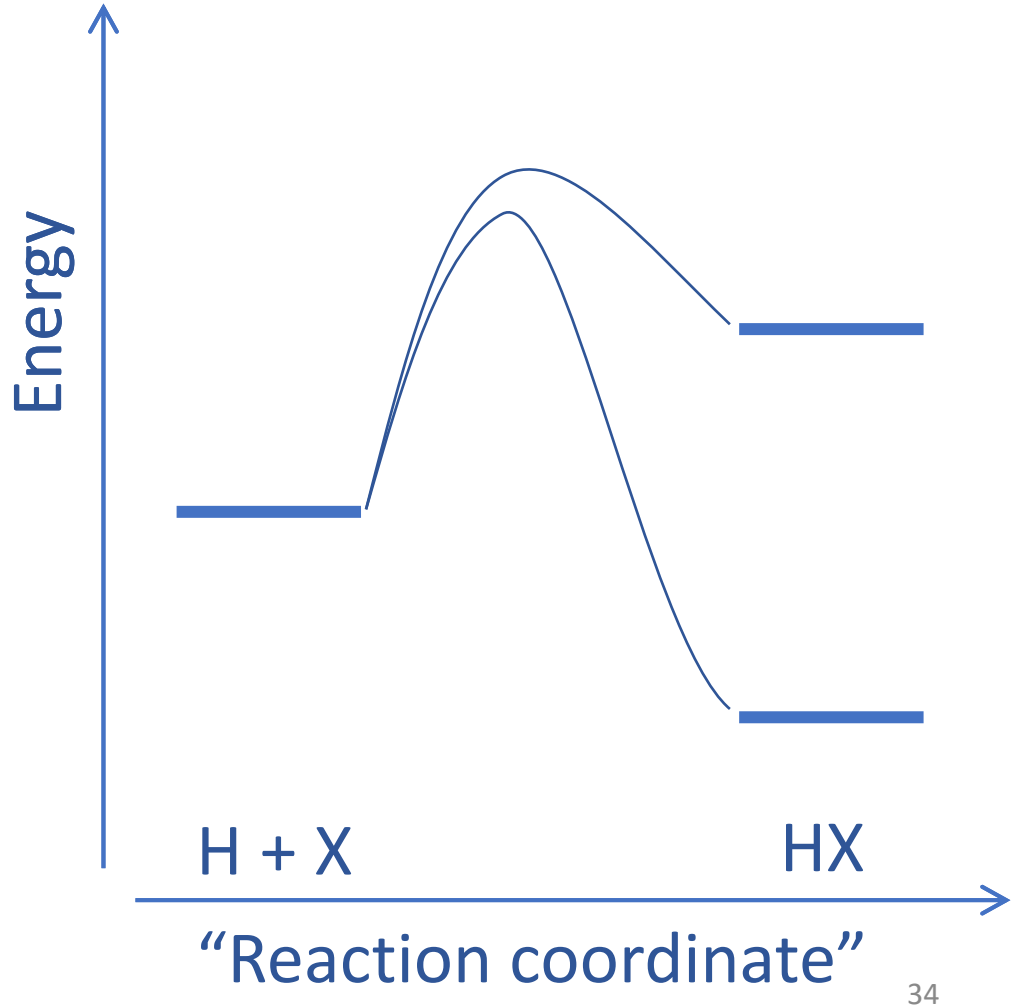
Overview of surface processes



Dissipation: excess energy

- At low T, a reaction should generate energy (exothermic, instead of endothermic)
- This needs to be dissipated: 3rd body = grain/ice
- Otherwise: radiative attachment = a slow process



Example: Do reaction products evaporate?

How do vibrationally excited molecules dissipate their energy?

$H_{ads} + HS_{ads} \rightarrow H_2S_{gas}$?

LETTERS
https://doi.org/10.1038/s41550-018-0380-9
nature astronomy

An infrared measurement of chemical desorption from interstellar ice analogues

Y. Oba[1*], T. Tomaru[1], T. Lamberts[2], A. Kouchi[1] and N. Watanabe[1]

Example: Do reaction products evaporate?

How do vibrationally excited molecules dissipate their energy?

The Astrophysical Journal, 897:56 (13pp), 2020 July 1

https://doi.org/10.3847/1538-4357/ab8a4b

CrossMark

namics

Chemical Desorption versus Energy Dissipation: Insights from Ab Initio Molecular Dynamics of HCO● Formation

Stefano Pantaleone[1], Joan Enrique-Romero[1,2], Cecilia Ceccarelli[1], Piero Ugliengo[3], Nadia Balucani[1,4,5], and Albert Rimola[2]

- Excitation by fixe
- Excitation into a
- Quantum effects

SPACE CHEMISTRY

http://pubs.acs.org/journal/aesccq

Article

Molecular Dynamics Simulations of Energy Dissipation on Amorphous Solid Water: Testing the Validity of Equipartition

Adrien Fredon, Gerrit C. Groenenboom, and Herma M. Cuppen*

Cite This: *ACS Earth Space Chem.* 2021, 5, 2032–2041

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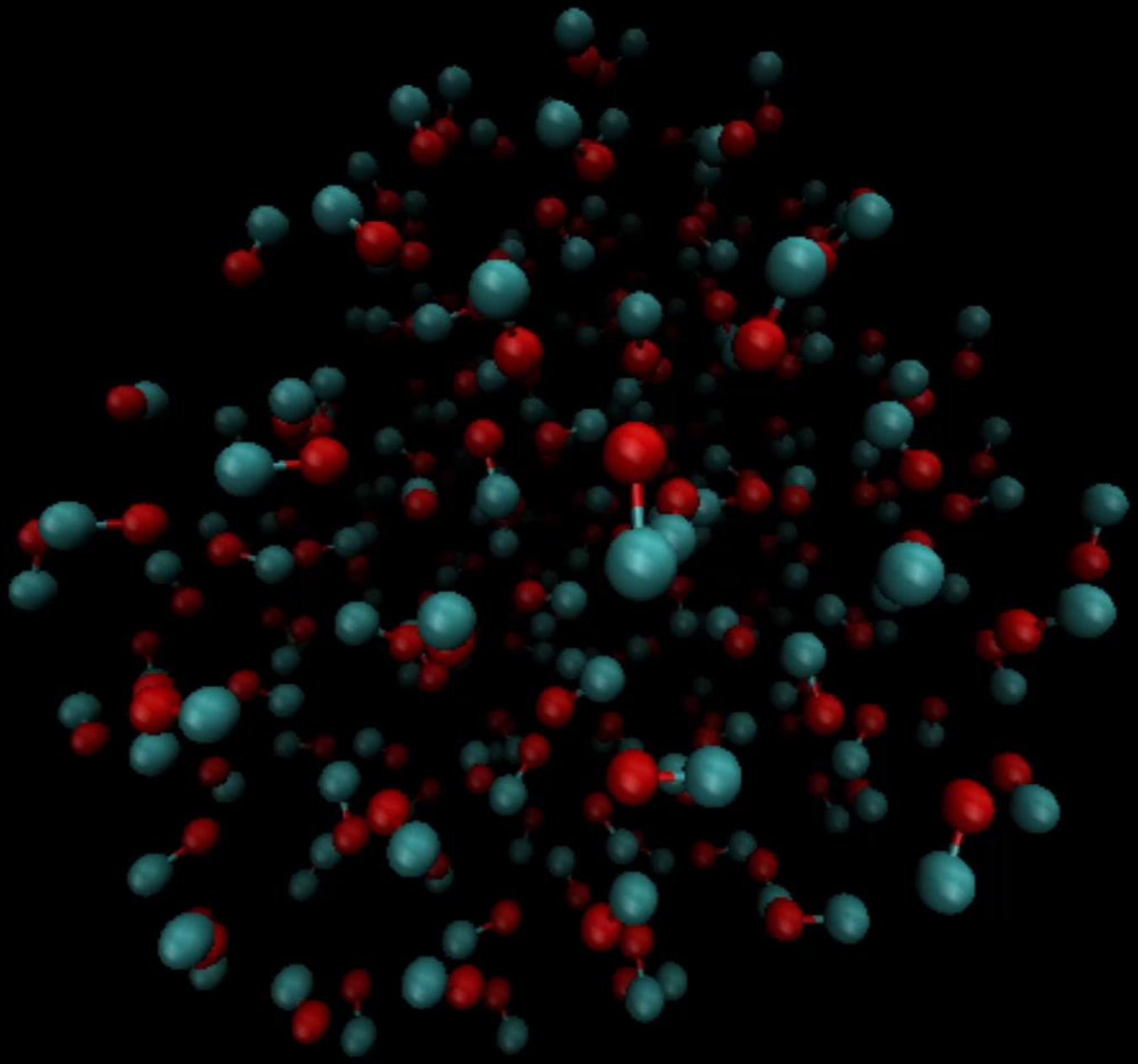


Figure courtesy: Brian C. Ferrari

Adsorption

When an atom or molecule collides with a grain it “can” adsorb:

$$f_{acc,X} = S_X v_X n_{grain} \pi r^2 n_g(X) \quad \text{with} \quad v_X = \sqrt{\frac{8 k_B T_{gas}}{\pi m_X}}$$

Sticking coefficient

Gas-phase thermal velocity

Grain number density

Average grain cross section

X number density

Boltzmann constant

Gas-phase temperature

Mass of X

Different ways of binding

Physisorption vs. chemisorption.

Van der Waals

Hydrogen bonded

Hemibonded

Covalently bonded

Ionic

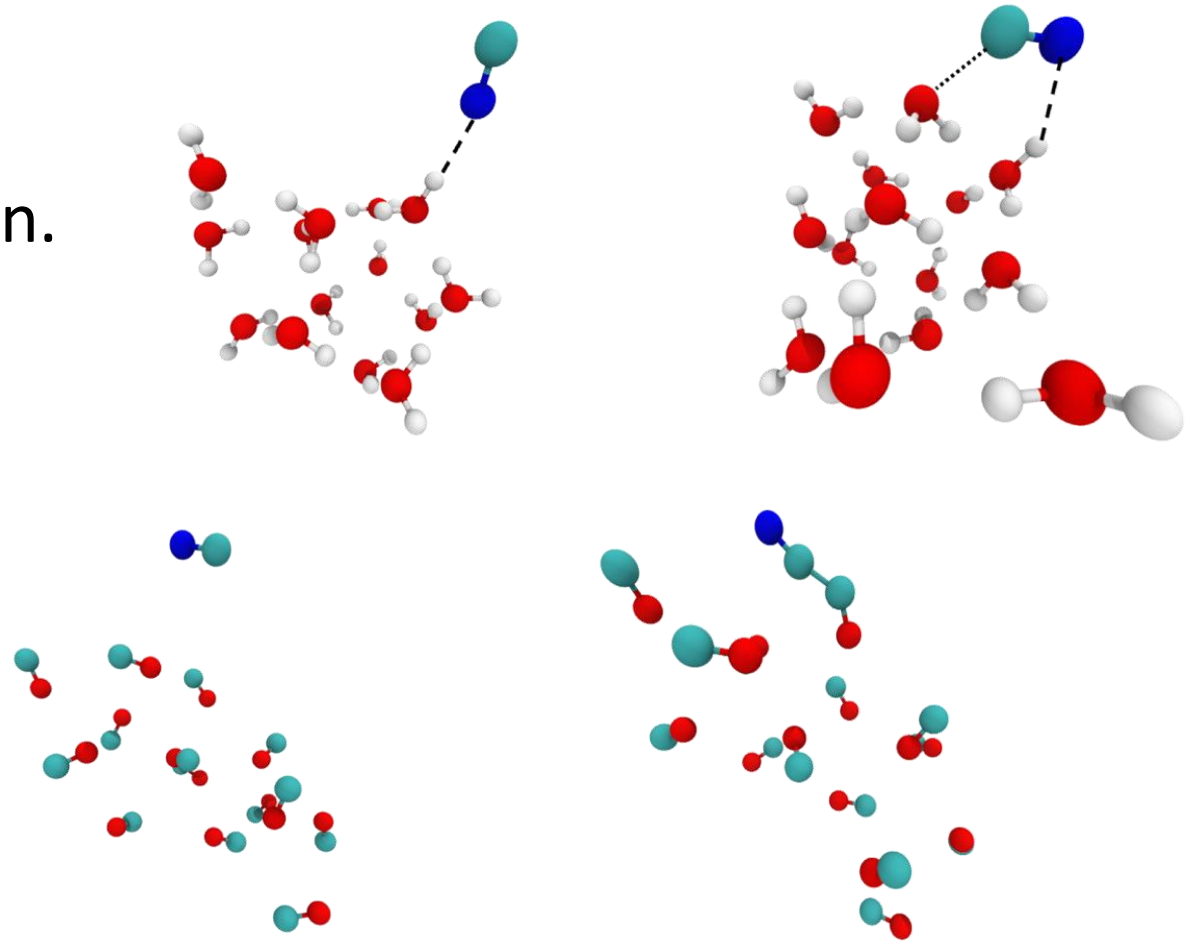


Figure courtesy: Joan Enrique-Romero

Example: Energetics of binding sites

Method of choice: DFT + NN or ONIOM

- Generation of the ice
  - Periodic Boundary Conditions vs. cluster
  - Pure ices vs. mixtures
- Reorganisation of the ice
- Dual-level approach
- Benchmark!
- Corrections:
  - BSSE
  - Zero Point Energy
  - Dispersion

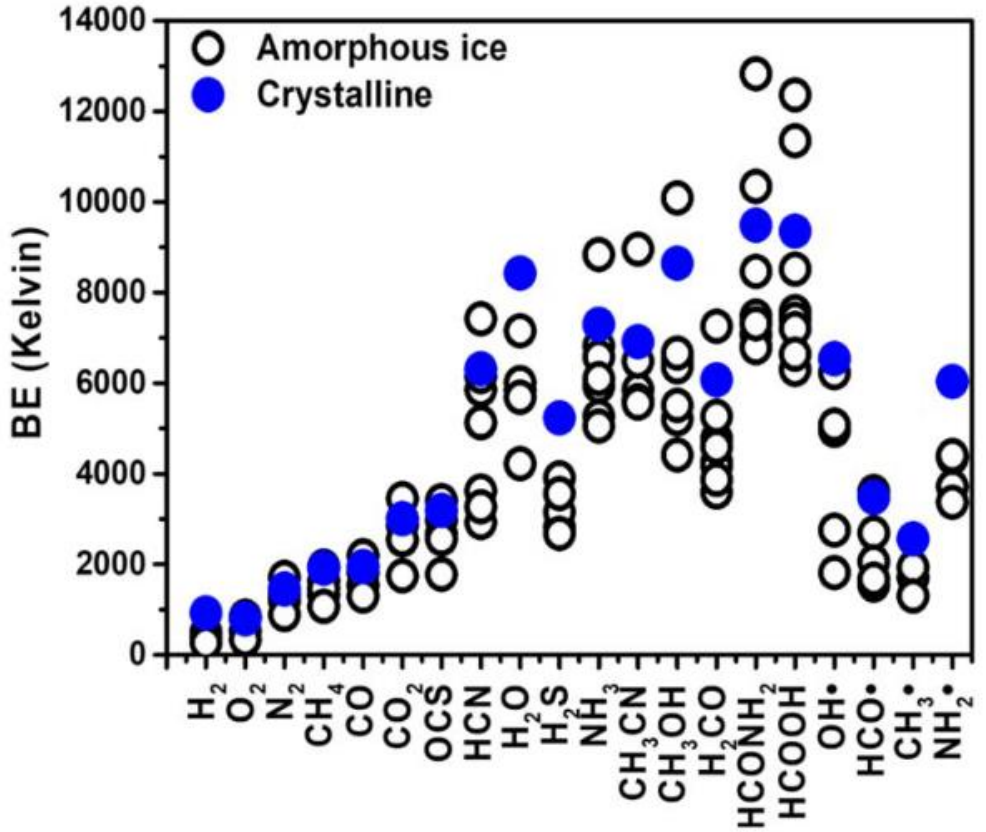
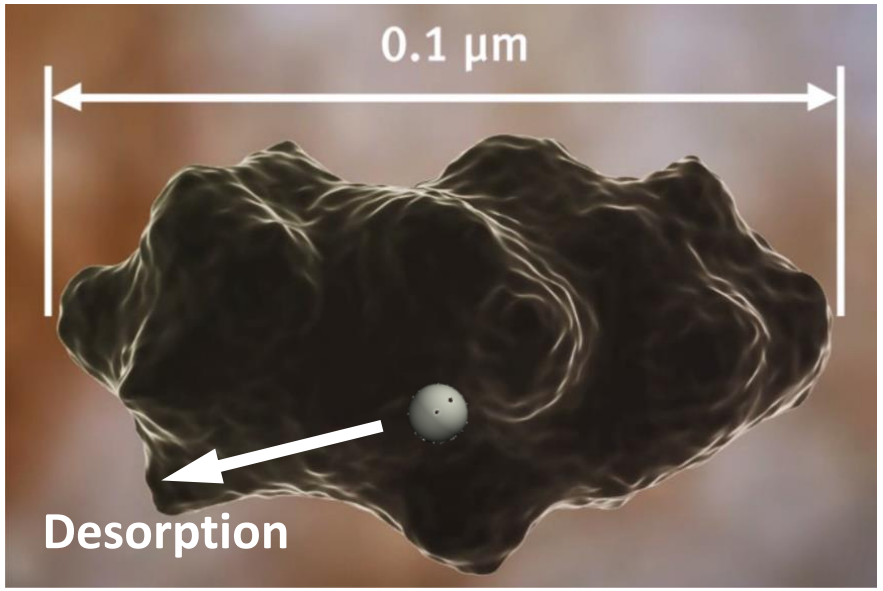


Figure 9. Comparison between the DFT//HF-3c BEs (in kelvin) computed on the crystalline ice (filled blue circles) and ASW (open circles), respectively, for 20 species studied here: HCl is missing as it dissociates on the ASW (see text).

Ferrero *et al.* ApJ 904 (2018) 11

Desorption

Opposite of adsorption: return of a species to the gas phase. Governed by interaction with the surface: Binding energy



$$f_{des,X} = k_{des,X}\, n_s(X) \quad \text{with:}$$

$$k_{des,X} = \nu_{trial} \exp\left(-\frac{E_{bind,X}}{T}\right) \quad \text{and} \quad \nu_{trial} = \sqrt{\frac{2N_s E_{bind,X}}{\pi^2 m_X}}$$

Assumptions underlying typical formula

Transition state theory ☺

$$k = \nu \exp\left(-\frac{E_a}{k_B T}\right) \qquad \nu_{TST} = \frac{k_B T}{h}\frac{q^{\ddagger}}{q_{ads}}$$

$$\nu_{TST} = \frac{k_B T}{h} q^{\ddagger}_{tr,2D} q^{\ddagger}_{rot,3D}$$

$$q^{\ddagger}_{tr,2D} = \frac{A}{\Lambda^2} \qquad q^{\ddagger}_{rot,3D} = \frac{\sqrt{\pi}}{\sigma h^3}(8\pi^2 k_B T_{peak})^{3/2}\sqrt{I_x I_y I_z}$$

Up to 7 or Exercises? magnitude difference!

ACS EARTH AND SPACE CHEMISTRY

http://pubs.acs.org/journal/aesccq

Thermal Desorption of Interstellar Ices: A Review on the Controlling Parameters and Their Implications from Snowlines to Chemical Complexity

Marco Minissale,* Yuri Aikawa, Edwin Bergin, Mathieu Bertin, Wendy A. Brown, Stephanie Cazaux, Steven B. Charnley, Audrey Coutens, Herma M. Cuppen, Victoria Guzman, Harold Linnartz, Martin R. S. McCoustra, Albert Rimola, Johanna G.M. Schrauwen, Celine Toubin, Piero Ugliengo, Naoki Watanabe, Valentine Wakelam, and Francois Dulieu

Cite This: *ACS Earth Space Chem.* 2022, 6, 597–630

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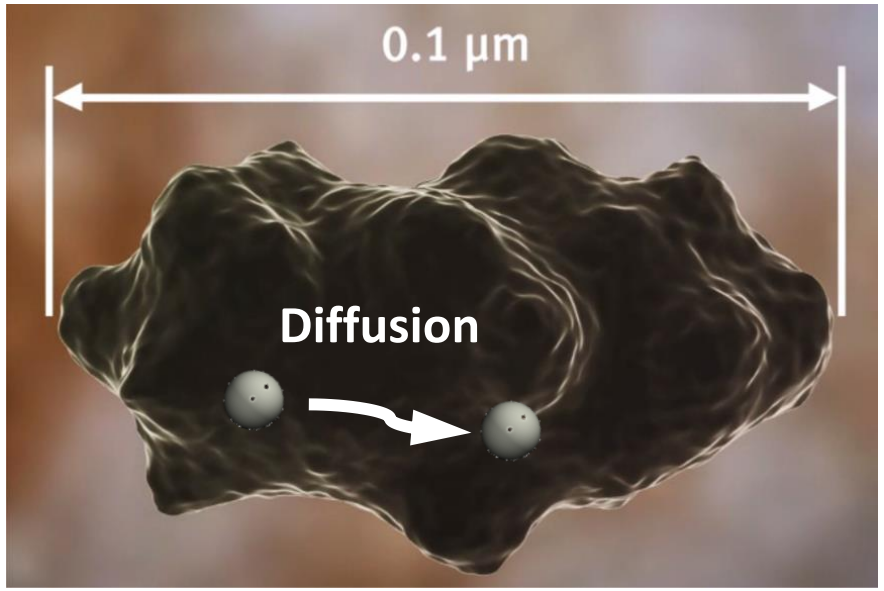
Diffusion

Movement across the surface allows reactants to meet. Governed by interaction with the surface: Diffusion Barrier



$$k_{diff,X} = \nu_{trial} \exp\left(-\frac{E_{diff,X}}{T}\right) \quad \text{and} \quad E_{diff,X} = \alpha \cdot E_{bind,X} \text{ with } \alpha < 1$$

Imagine: heavier species, typically bind stronger, and diffuse slower.

Validity of the α factor

Monthly Notices of the ROYAL ASTRONOMICAL SOCIETY

MNRAS 510, 3063–3070 (2022)
Advance Access publication 2021 December 13

https://doi.org/10.1093/mnras/stab3631

Neural-network assisted study of nitrogen atom dynamics on amorphous solid water – II. Diffusion

Viktor Zaverkin, Germán Molpeceres and Johannes Kästner ★

Computational studies need to include many degrees of freedom

- Nudged Elastic Band approach for locating TS
- Surface-coverage dependence of diffusion (α > 1)

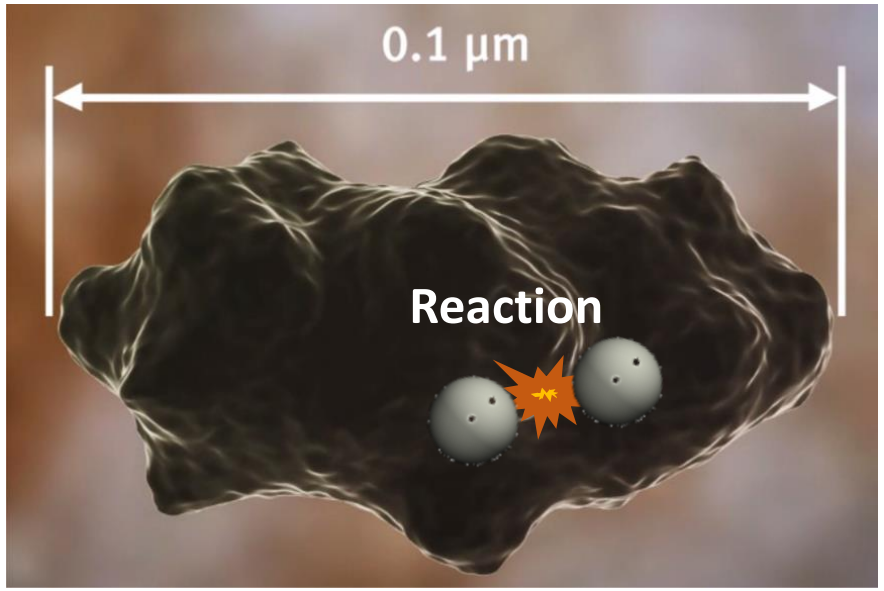
Sneak-peak at the molecular scales

- Introduction Astrochemistry

- Surface processes & Timescales
  - Dissipation (3rd body)
  - Adsorption
  - Desorption
  - Diffusion
  - **Reaction**
    - **Energetics of a chemical reaction**
    - Surface reaction mechanisms

- Energetic Processing & Non-thermal Desorption

Reaction



When two reactants meet: possibility for a reaction to occur

Simplest and most abundant molecule is formed on grain surfaces: H_2

$H\cdot_{ads} + H\cdot_{ads} \rightarrow H_{2\ ads}$

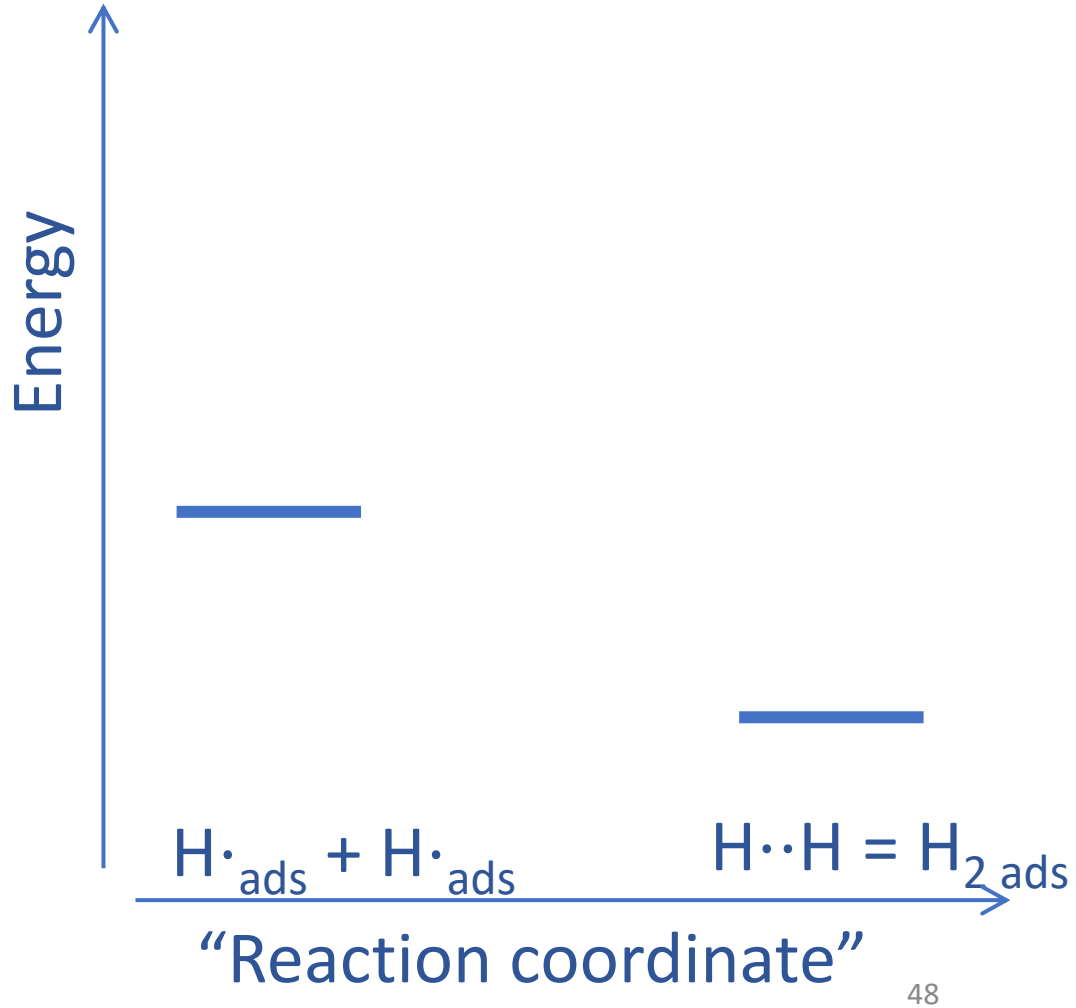
Barrierless and efficient! Detected despite UV radiation in PDR's.

Reaction energetics: Radical-radical

"Electrons like to be paired"

Radical-radical reactions are barrierless (*)

(*) see exercises



Reaction energetics: Radical-neutral

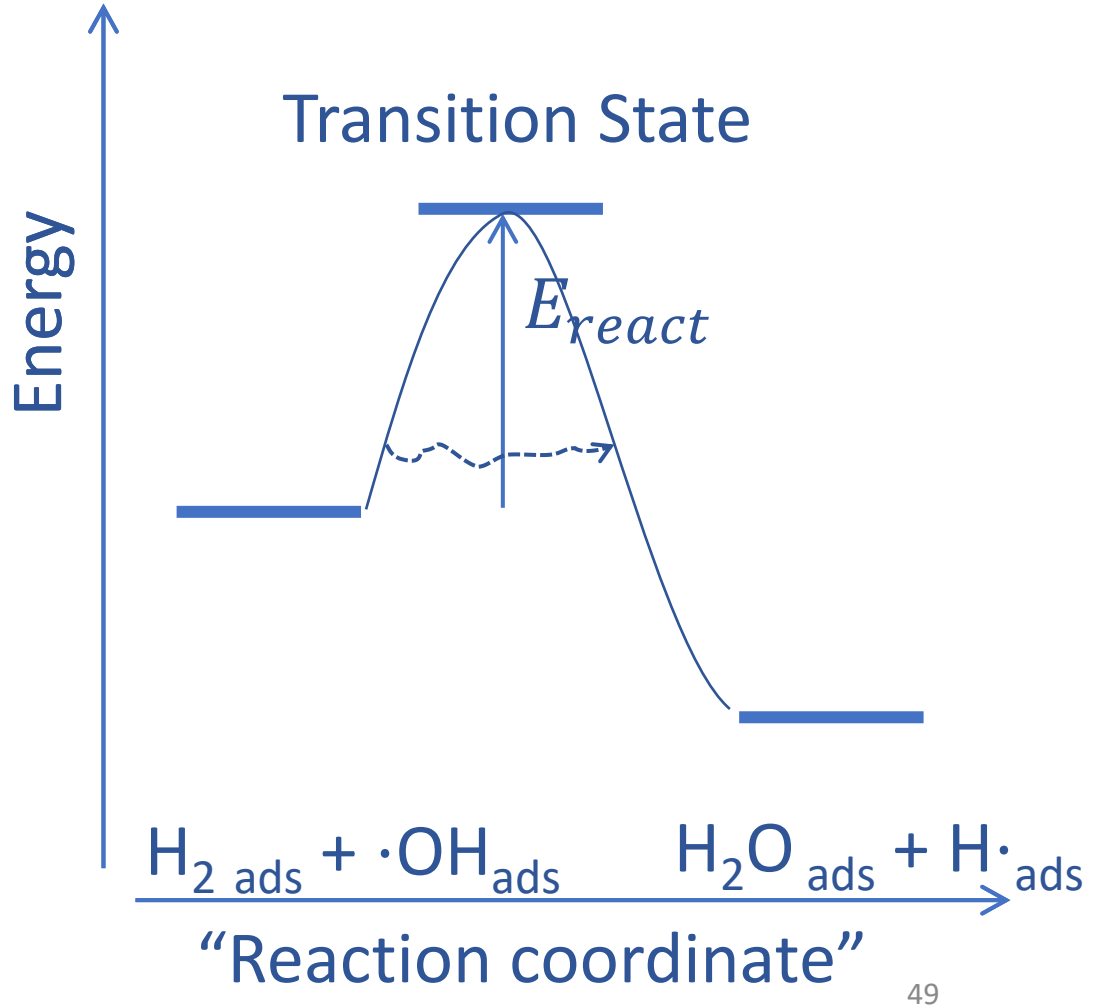
Usually a reaction with a barrier:

1. Thermally activated:

$$k_{LH} = \nu_{trial} \exp\left(-\frac{E_{react}}{T}\right)$$

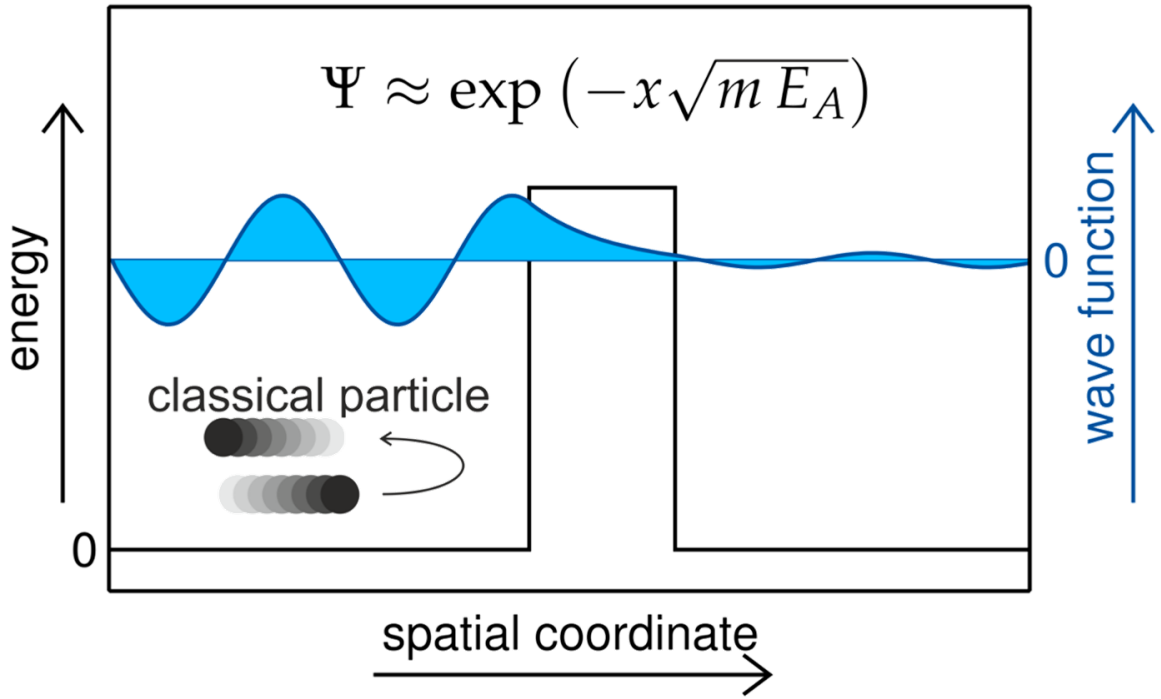
2. Tunneling mediated:

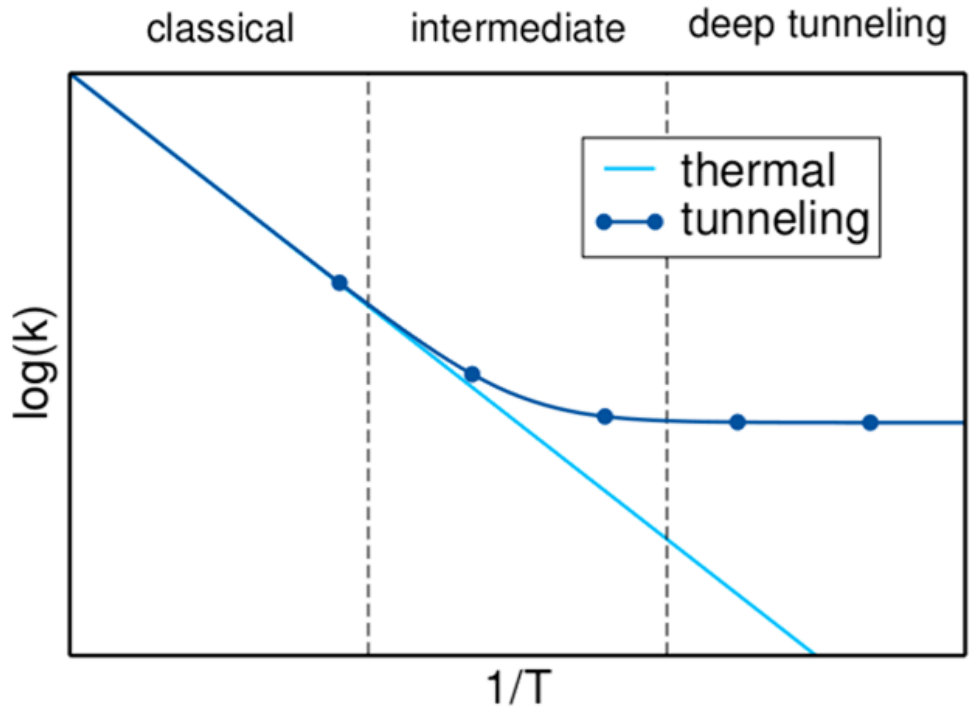
Depends on barrier height and width



Meisner et al. ACSESC 2017

Low-temperature effects: tunneling





Minimum energy path is not a good approximation to the tunneling path:
Rectangular barrier, Eckart, Instanton theory

Figure courtesy Meisner & Kästner ACIE 55, 5400 (2016)

Example: H + HC_3N 😉

Method of choice: usually DFT

- Including or excluding explicit treatment of ice
- Benchmark!
- Corrections:
  - BSSE
  - Zero Point Energy
  - Dispersion

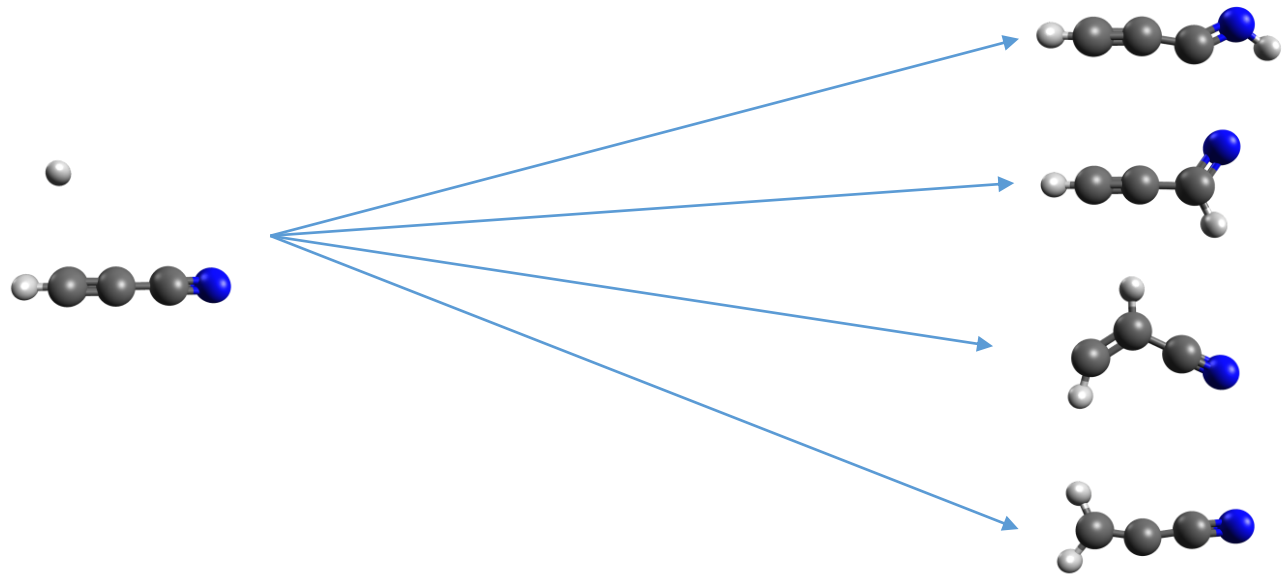


Figure courtesy: Marten Raaphorst

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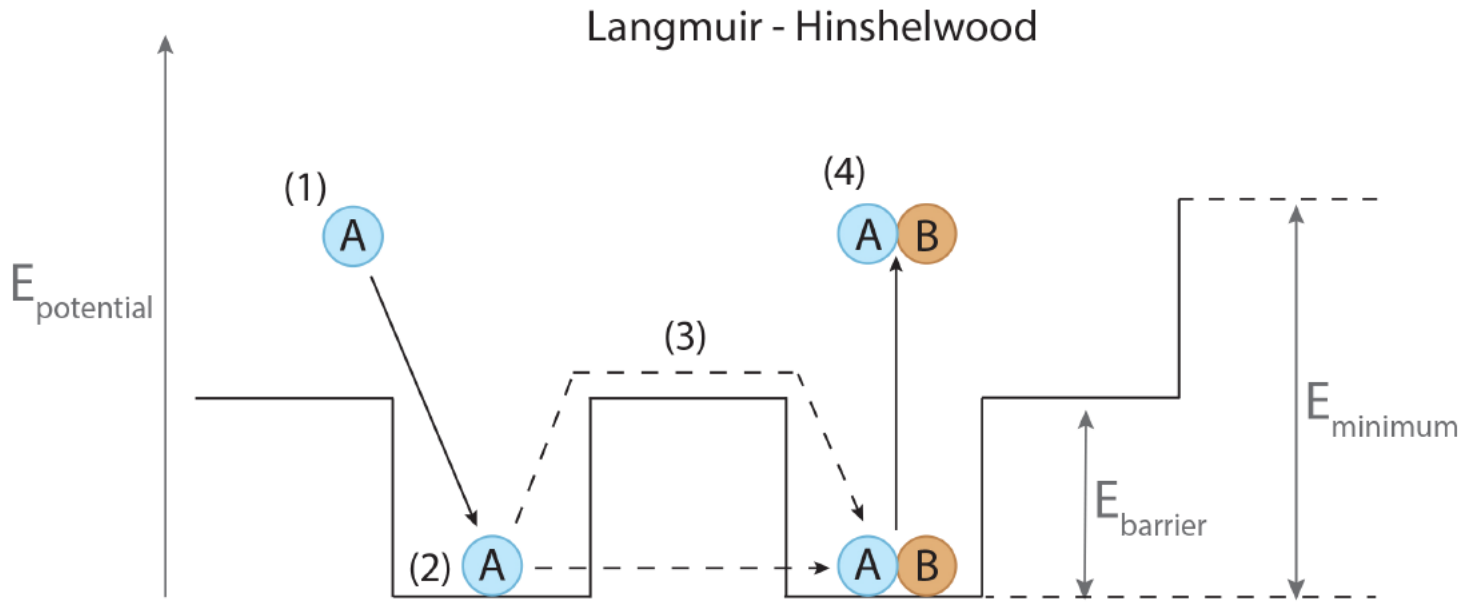
Reaction mechanism: Langmuir-Hinshelwood

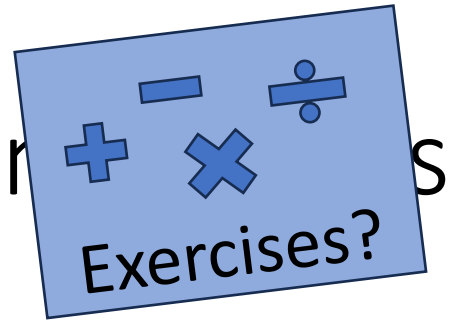
Thermalized and diffusive:



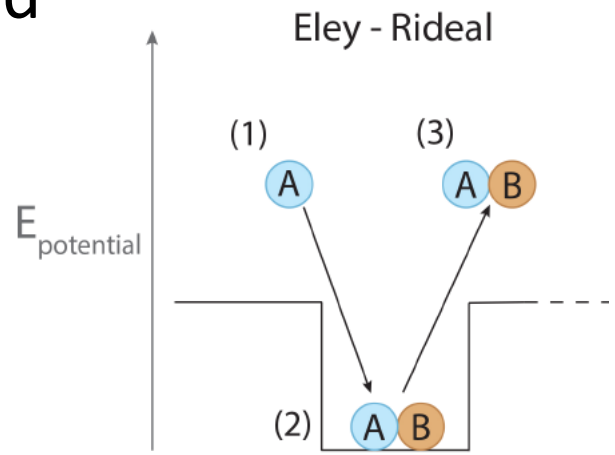
$A_{gas} + B_{ads} \rightarrow A_{ads} + B_{ads} \rightarrow (AB)_{ads} \rightarrow (AB)_{gas}$

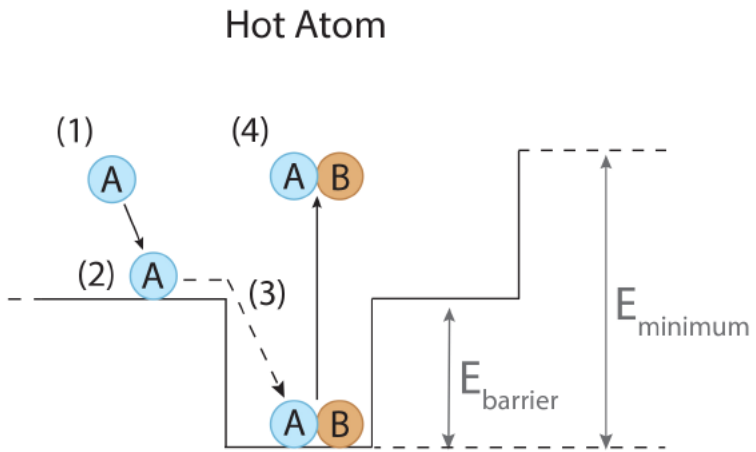
$$k_{LH} = \nu_{trial} \exp\left(-\frac{E_{react,A+B}}{T}\right)$$ with $E_{react,A+B}$ the reaction barrier

Reaction mechanism: Eley-Rideal or Hot Atom



Non-Thermalized





$A_{gas} + B_{ads} \rightarrow (AB)_{ads} \rightarrow (AB)_{gas}$

$A_{gas} + B_{ads} \rightarrow A_{not\text{-}ads} + B_{ads} \rightarrow (AB)_{ads} \rightarrow (AB)_{gas}$

Timescale comparisons (dark cloud @ 10 K)

Process	Timescale
Dissipation	Picoseconds – microseconds
Reaction	Microseconds – seconds
Diffusion	Microseconds – days
Adsorption	Days – months
Desorption	Seconds – months
Experiment	Days – weeks
Telescope lifetime	Years – decades
Molecular cloud	Million years

Surface processes in rate equation models

$$\frac{d}{dt}$$

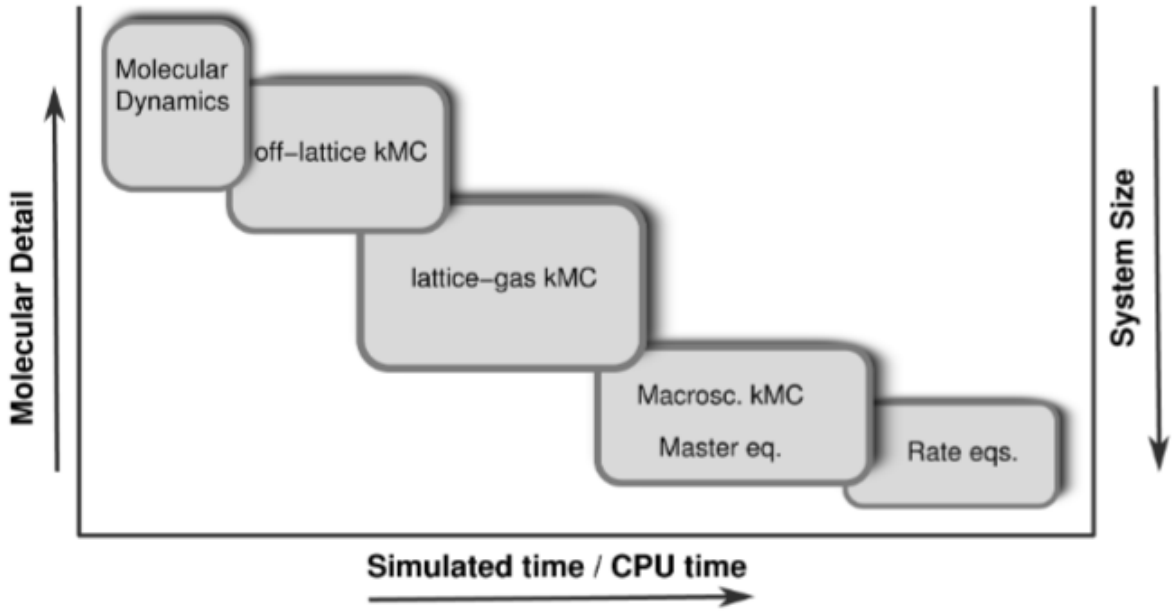
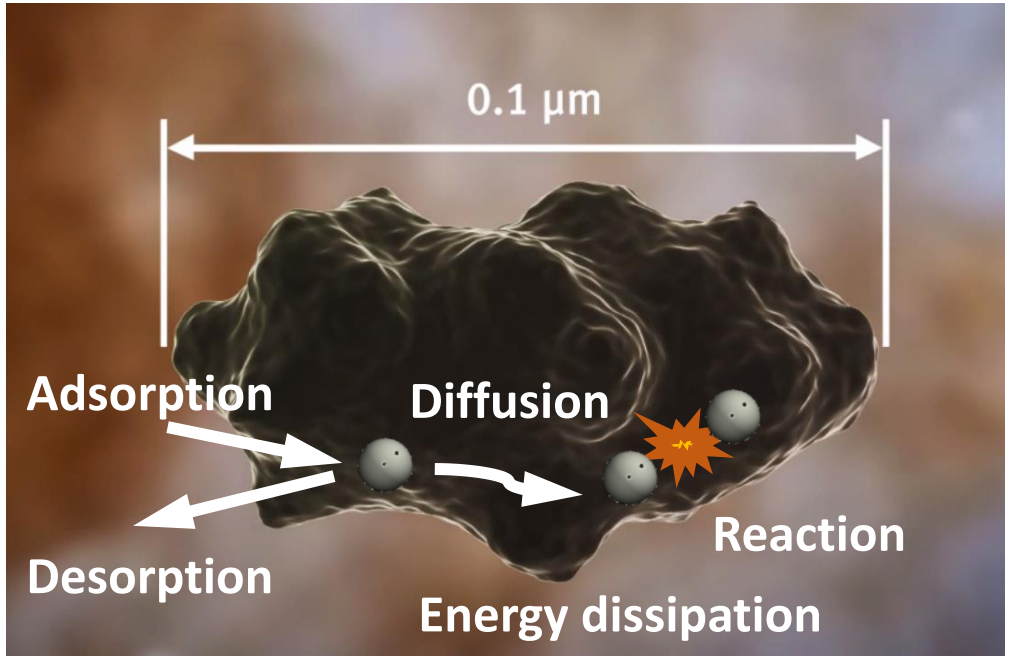
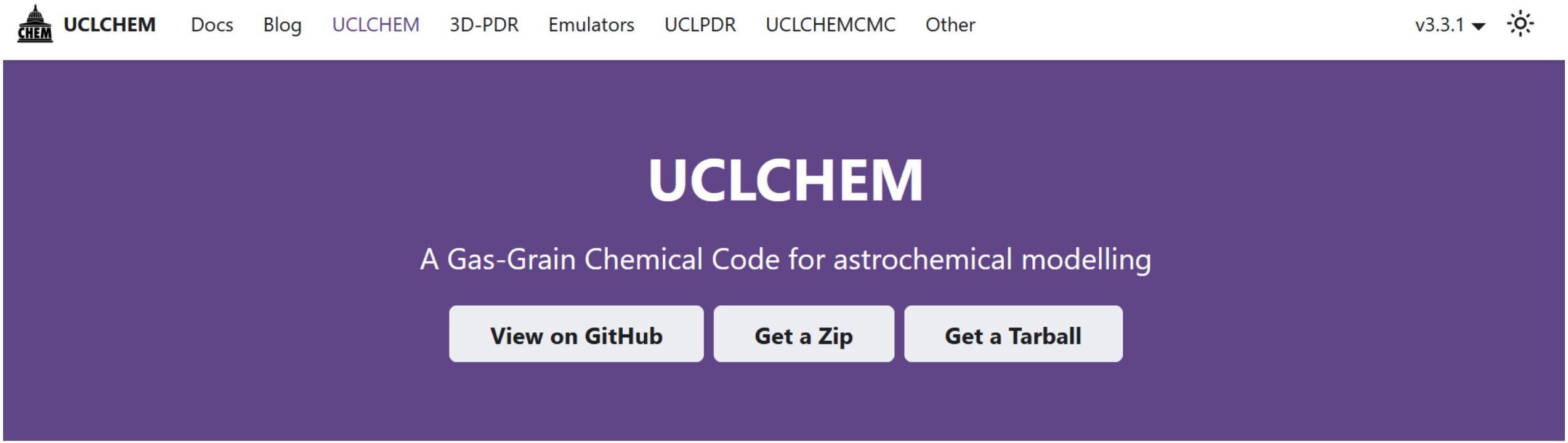


Figure 1. Overview of the different simulation methods mentioned in the present review.



Cuppen *et al.* 113 (2013) 8840

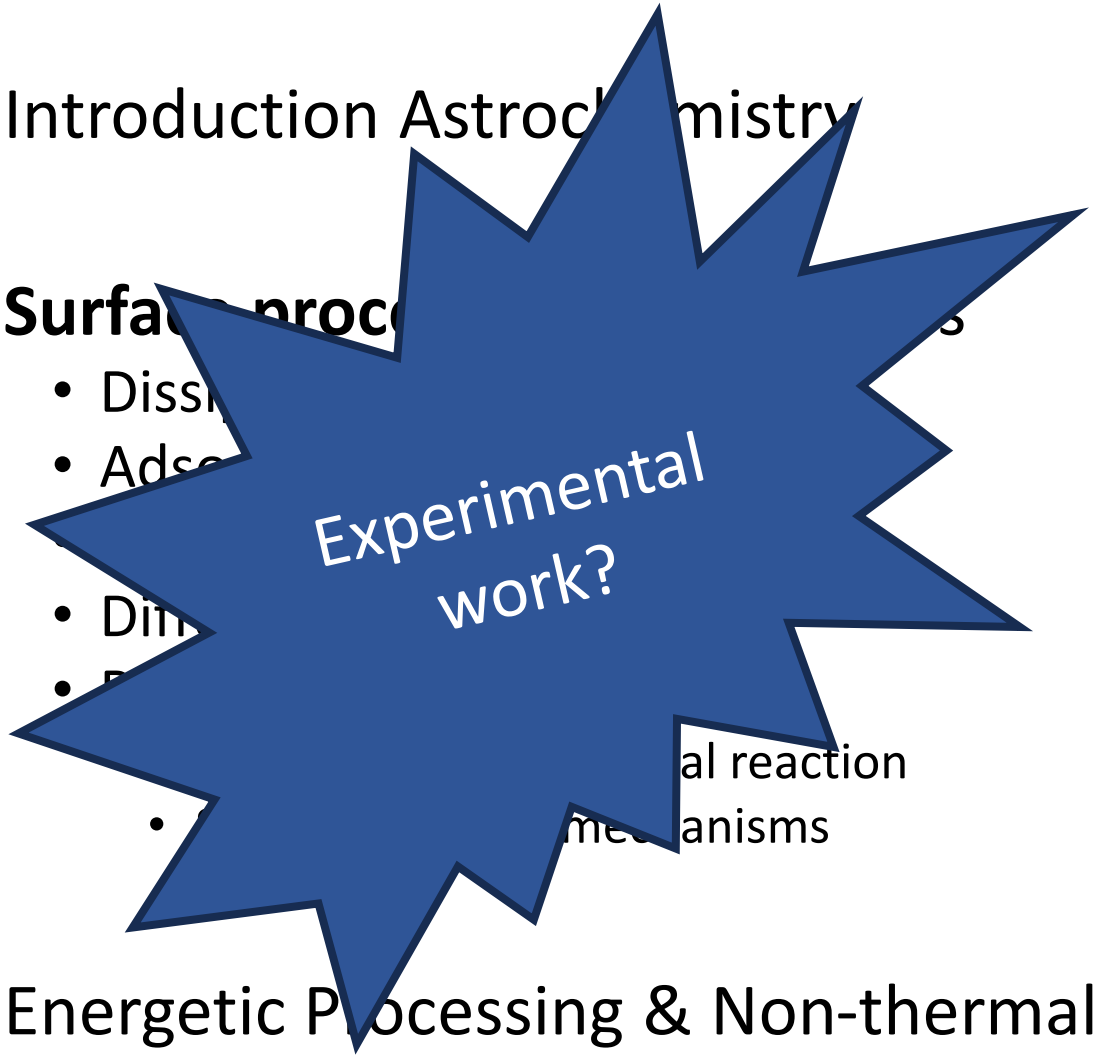
Surface processes in rate equation models



Sneak-peak at the molecular scales

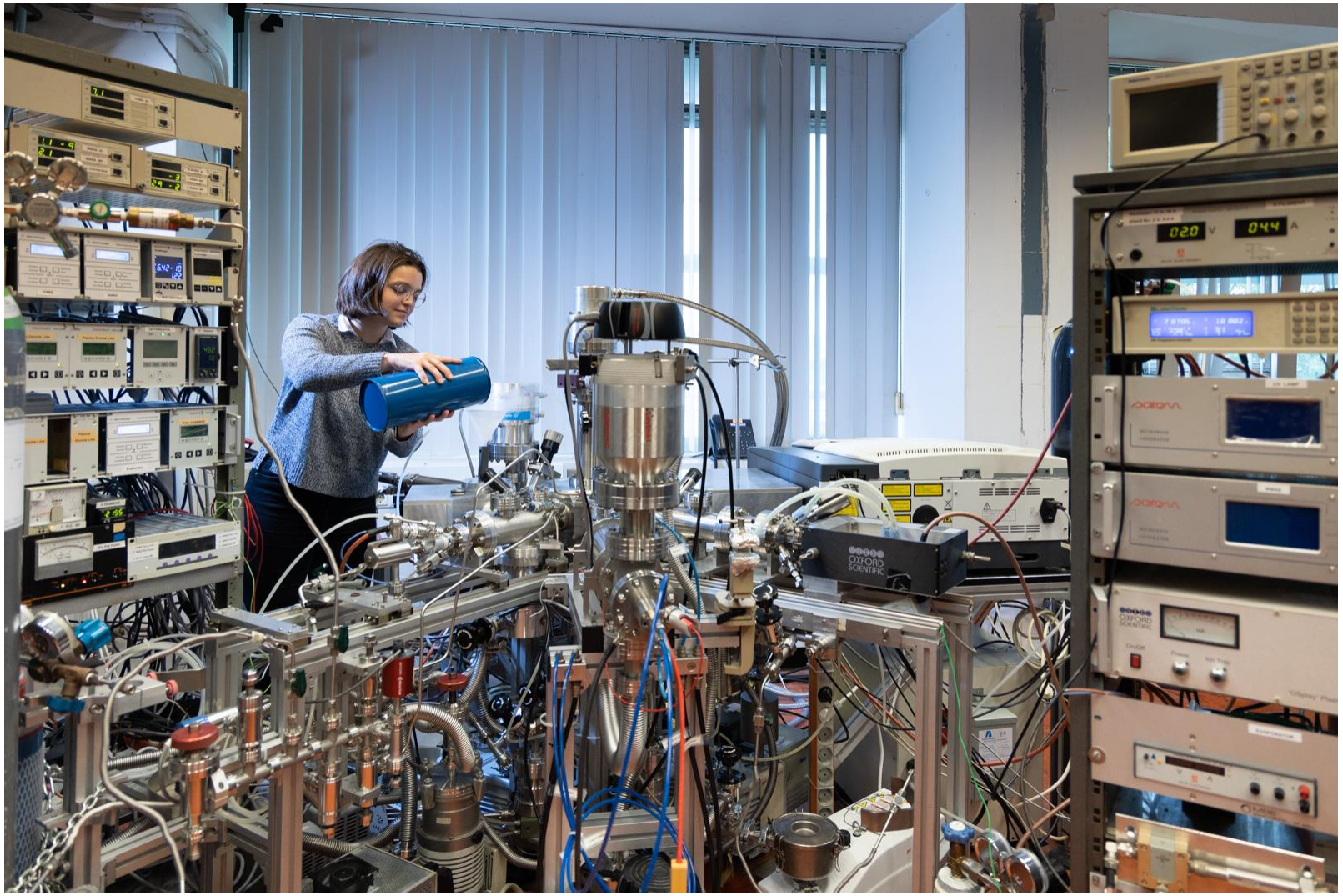
- Introduction Astroch mistry

- **Surfa proc**
  - Diss
  - Ads
  - Di
  - al reaction
  - anisms

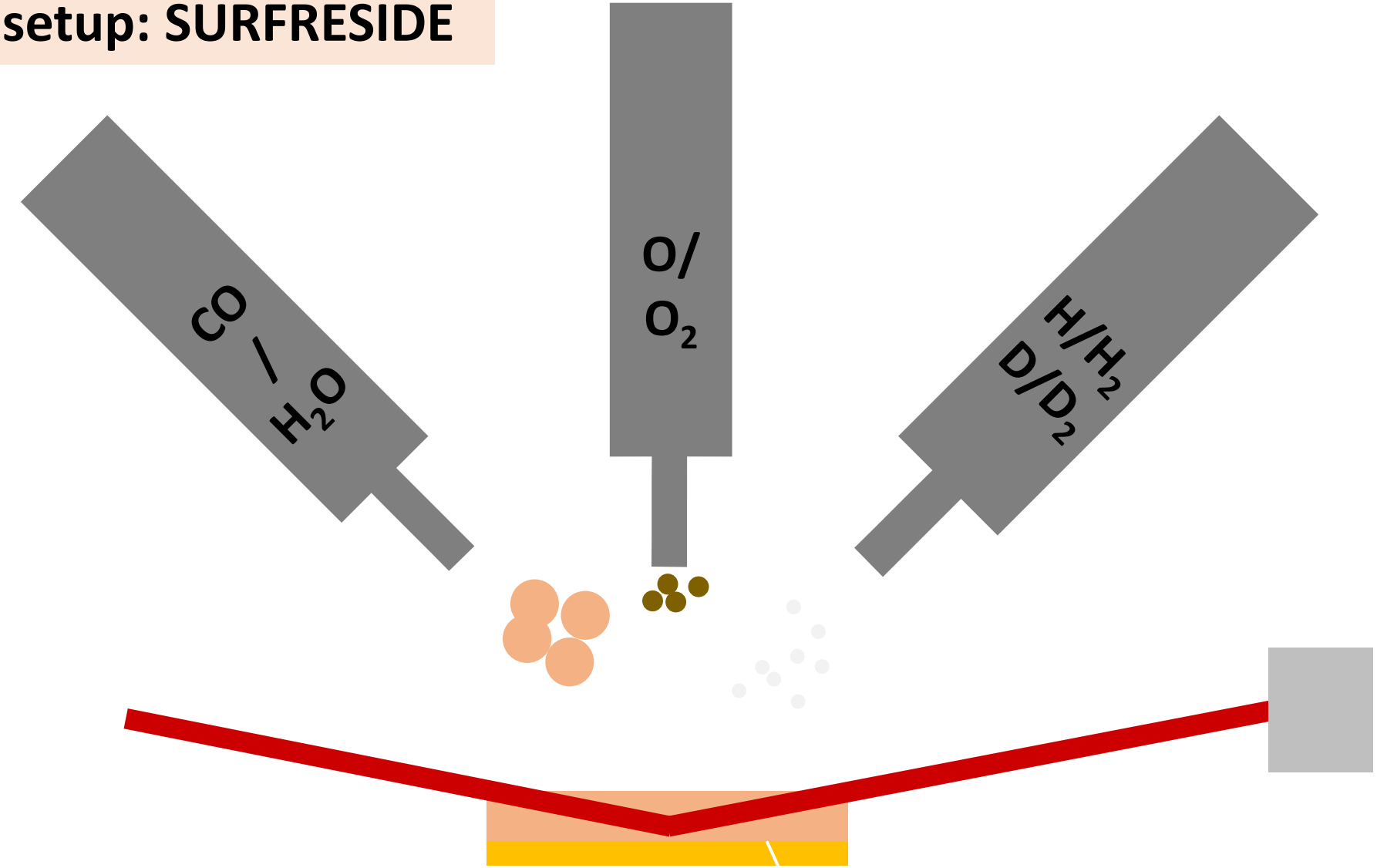


- Energetic P ocessing & Non-thermal Desorption

Laboratory for Astrophysics @ Leiden



Experimental setup: SURFRESIDE



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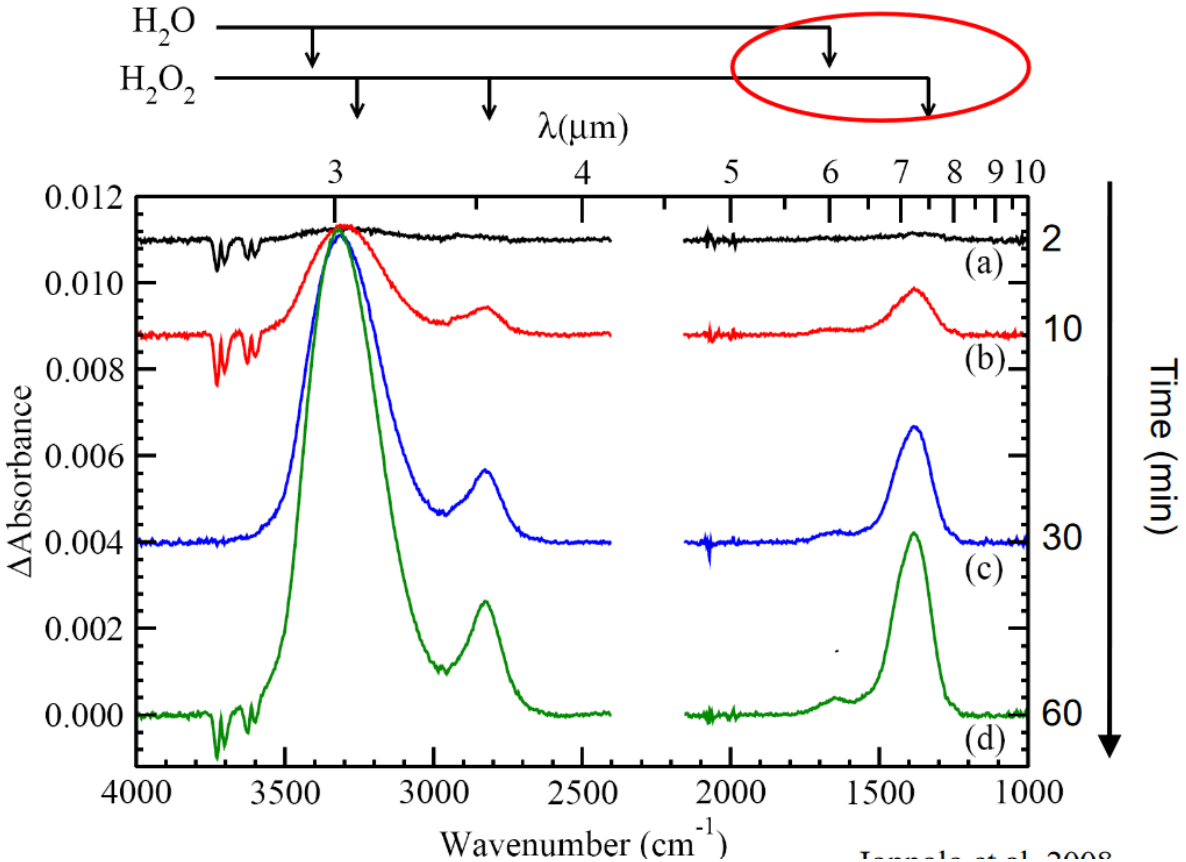
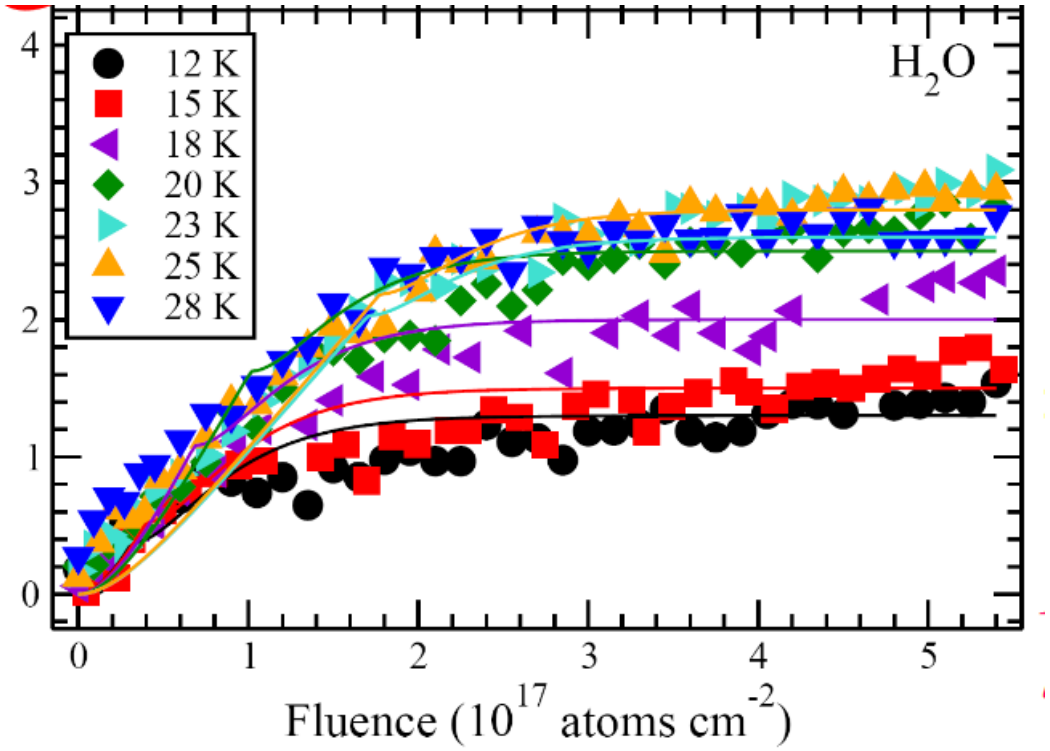




Ioppolo et al. ApJ 2008

Water reaction network

References:

Van de Hulst 1949

Tielens & Hagen 1982

Hiraoka et al. 1998

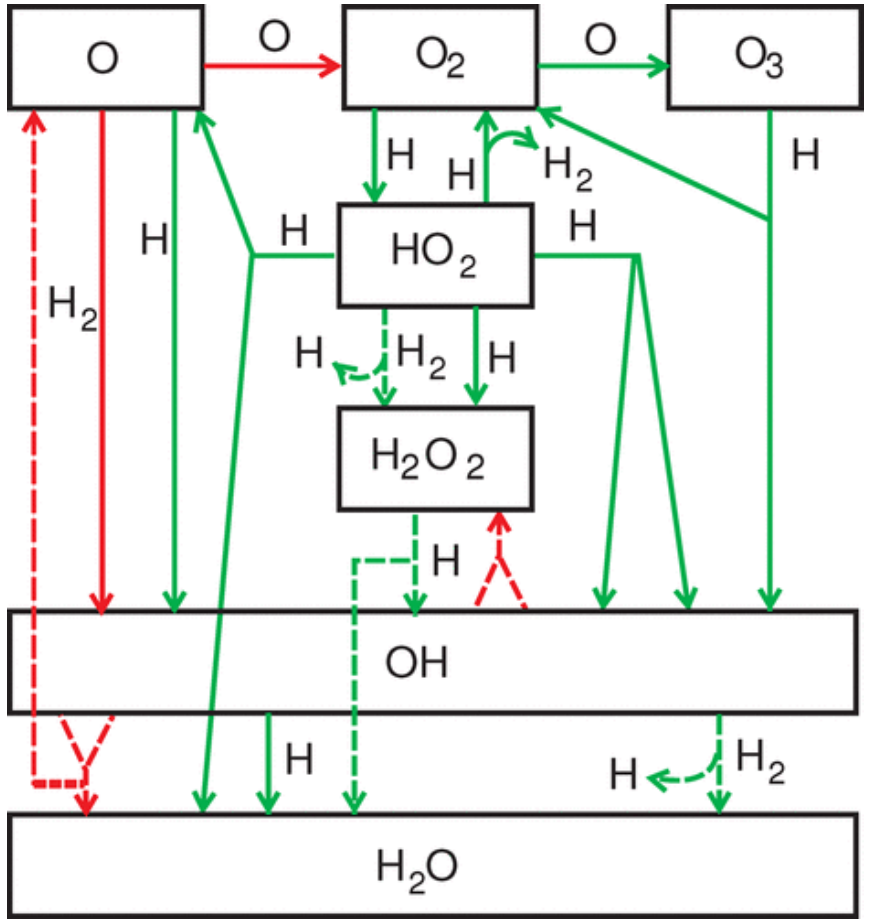
Ioppolo et al. 2008

Dulieu et al. 2010

Cuppen et al. 2010

Oba et al. 2012

Lamberts et al. 2017



Van Dishoeck et al. 2013

Theoretical work on water formation I

Kinetic Monte Carlo lattice-gas model

PCCP

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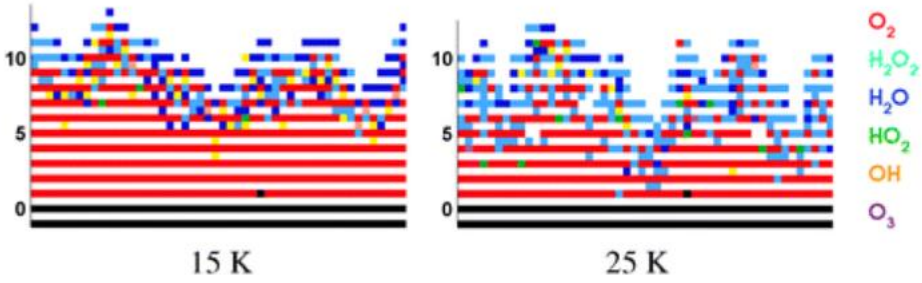
View Journal | View Issue

Water formation at low temperatures by surface O_2 hydrogenation III: Monte Carlo simulation

Cite this: *Phys. Chem. Chem. Phys.*, 2013, **15**, 8287

Thanja Lamberts,*[ab] Herma M. Cuppen,[b] Sergio Ioppolo†[a] and Harold Linnartz[a]



Faraday Discussions

Cite this: *Faraday Discuss.*, 2014, **168**, 327

PAPER

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The formation of ice mantles on interstellar grains revisited – the effect of exothermicity

T. Lamberts,[ab] X. de Vries[a] and H. M. Cuppen*[a]

$H + HO_2 \rightarrow 2\ OH$

Theoretical work on water formation II

Reaction rate constants

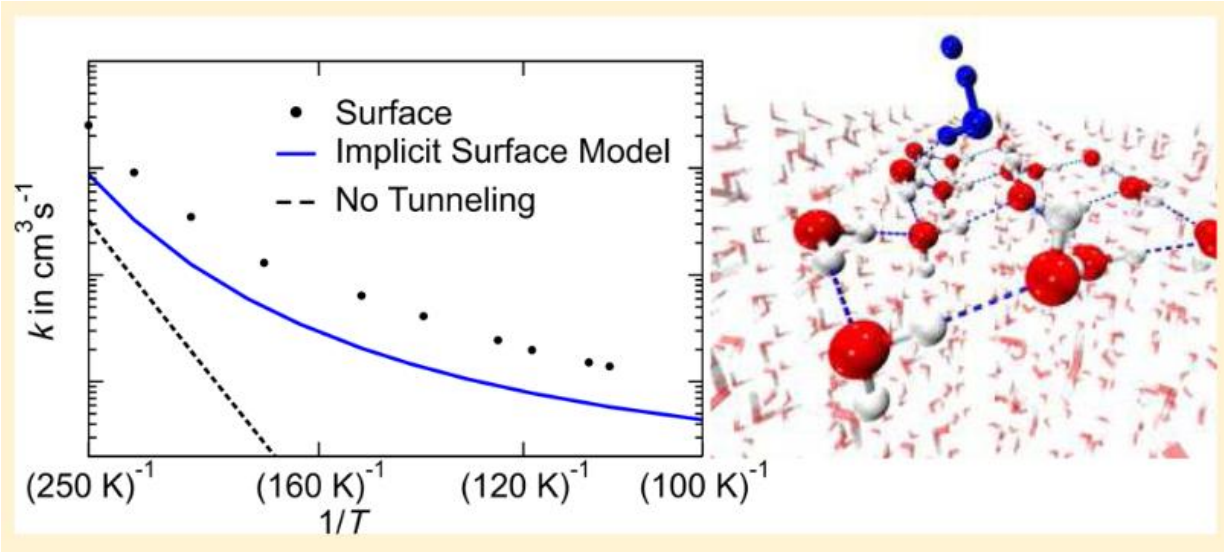
ACS EARTH AND SPACE CHEMISTRY

Article

http://pubs.acs.org/journal/aesccq

Atom Tunneling in the Water Formation Reaction $H_2 + OH \rightarrow H_2O + H$ on an Ice Surface

Jan Meisner, Thanja Lamberts, and Johannes Kästner*



Theoretical work on water formation II

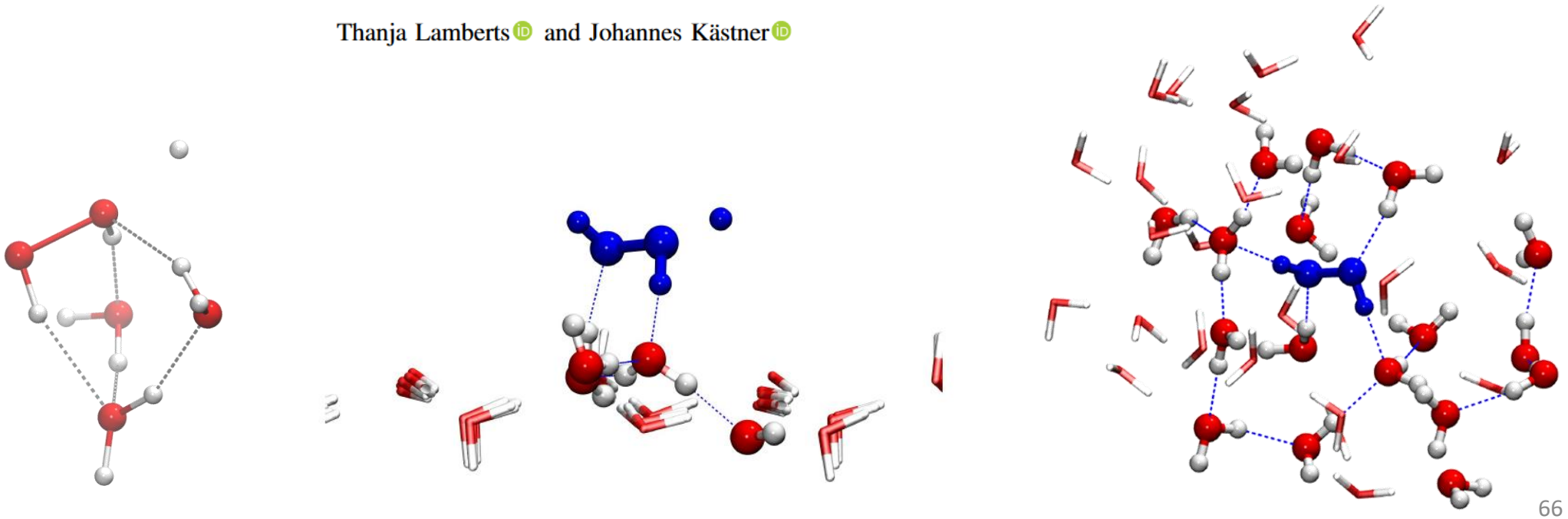
Reaction rate constants

THE ASTROPHYSICAL JOURNAL, 846:43 (7pp), 2017 September 1 https://doi.org/10.3847/1538-4357/aa8311

CrossMark

Influence of Surface and Bulk Water Ice on the Reactivity of a Water-forming Reaction

Thanja Lamberts and Johannes Kästner



Theoretical work on water formation III

Diffusion parameters

THE JOURNAL OF PHYSICAL CHEMISTRY Letters

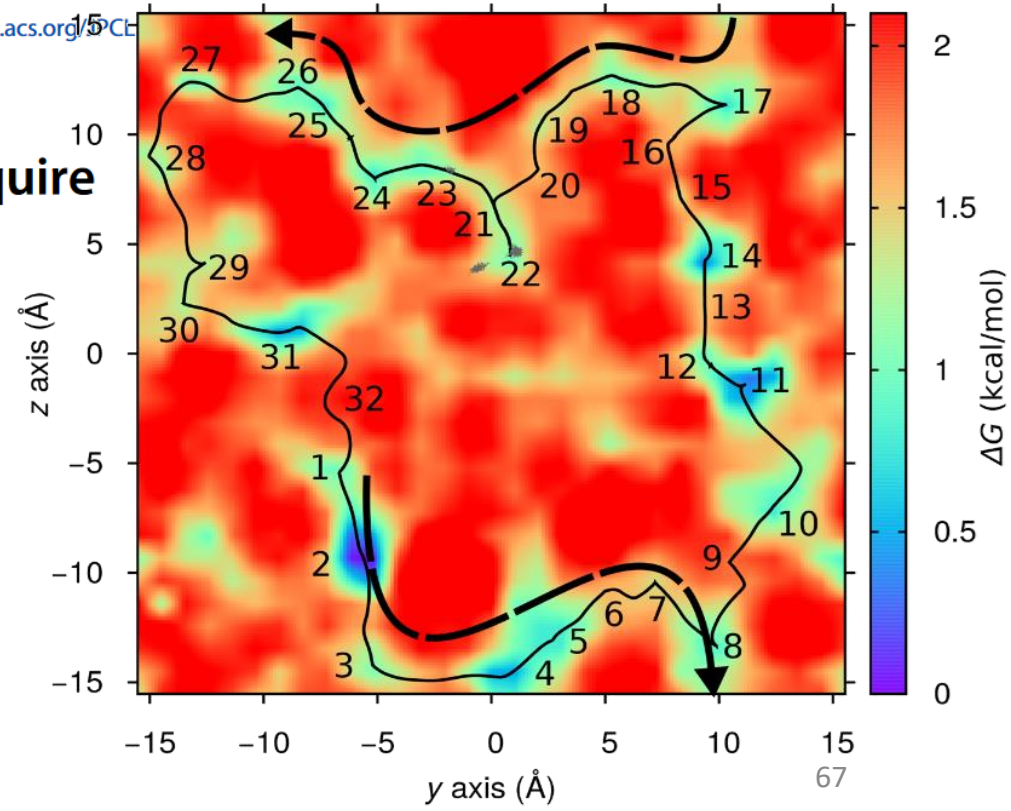
Letter

Cite This: J. Phys. Chem. Lett. 2018, 9, 1822−1826

pubs.acs.org/JPCL

Molecular Oxygen Formation in Interstellar Ices Does Not Require Tunneling

Marco Pezzella, Oliver T. Unke, and Markus Meuwly*



Theoretical work on water formation IV

Diffusion parameters

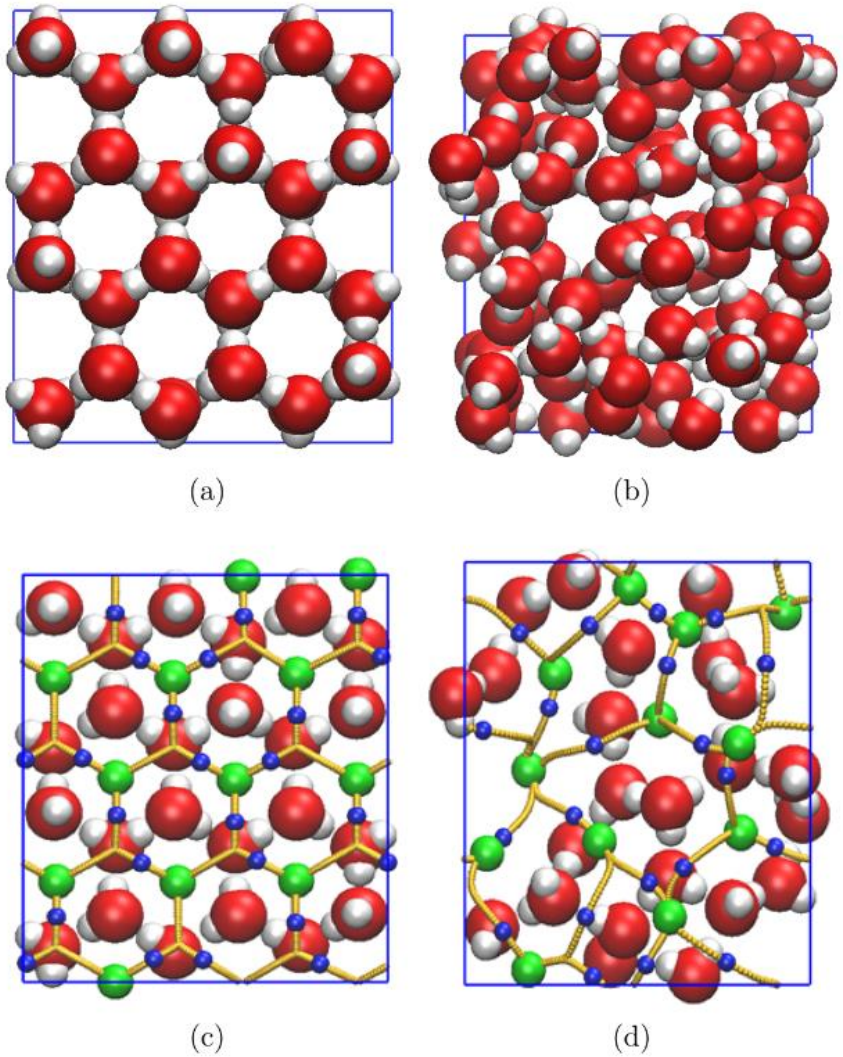
THE JOURNAL OF PHYSICAL CHEMISTRY C

Article

pubs.acs.org/JPCC

Long-Time Scale Simulations of Tunneling-Assisted Diffusion of Hydrogen on Ice Surfaces at Low Temperature

V. Ásgeirsson,[†,‡] H. Jónsson,[§] and K. T. Wikfeldt*[,†]



In summary:

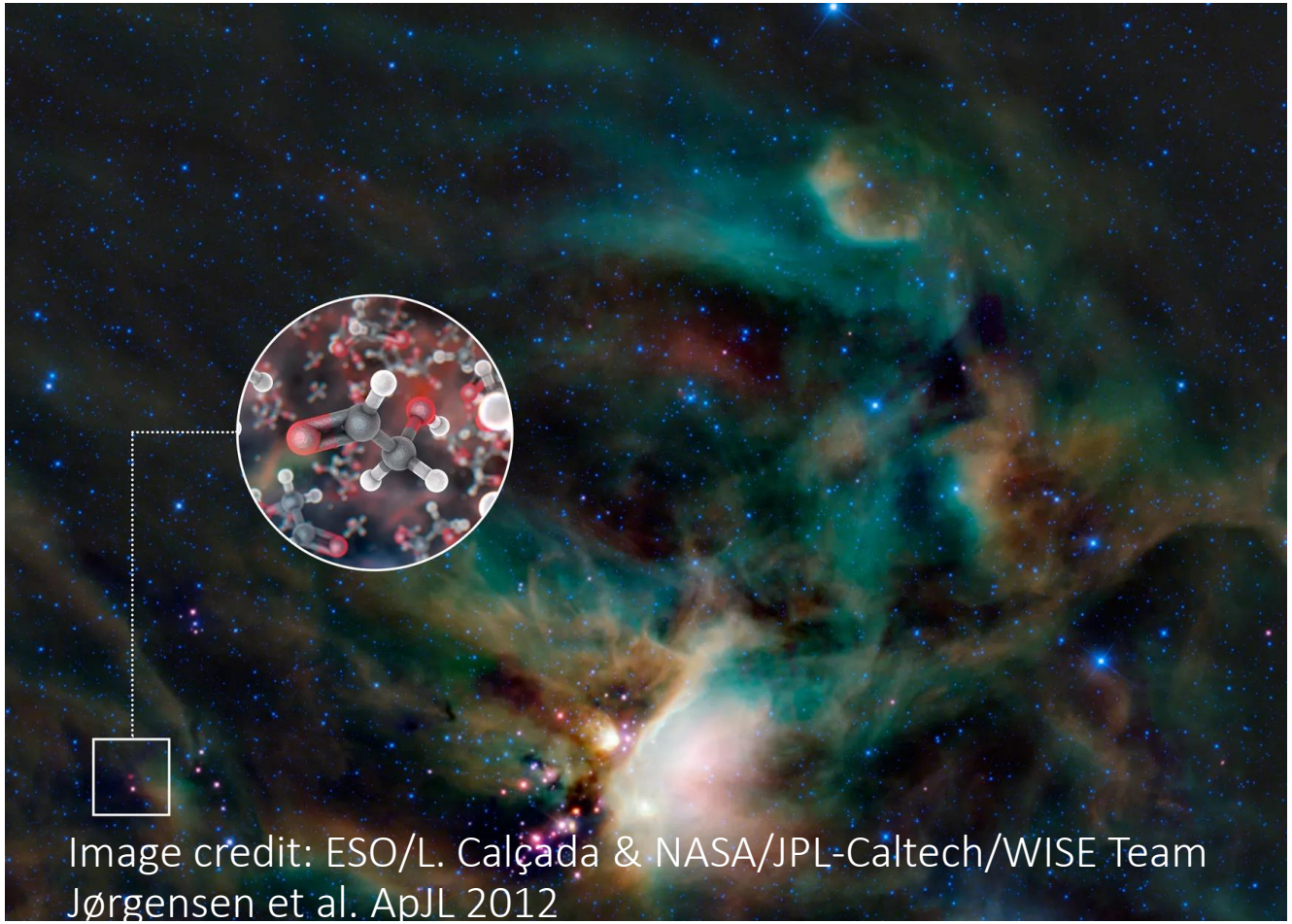
Courtesy: Lamberts & Van Dishoeck

Great, H_2O! But… what about biomolecules?

Simplest sugar: $CHOCH_2OH$

Ingredients: CO and H

We will look at molecules that can be formed with CO and H in the exercise



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- **Energetic Processing & Non-thermal Desorption**

Energetic Processing

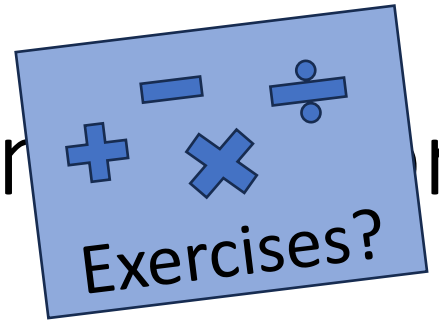
Different sources of radiation:

- UV
- X-Rays
- Cosmic Rays

Leads to:

- Excitation of molecules
- Dissociation of molecules
- Secondary electron generation
- UV generated radiation

Non-therr rption



At 10 K it is unlikely that molecules can desorb “thermally”

Alternative mechanisms that are proposed are:

- Desorption induced by energetic radiation
  - Problem: what about dissociation?
- Desorption induced by the excess energy of a chemical reaction
  - Problem: what about dissipation?

Take Home Messages

- Ice surface chemistry leads to formation of (saturated) molecules
- Dust grains are pivotal in taking up excess energy of reactions
- There are various elementary surface processes at play
- Surface reactions can be barrierless or with a barrier
- There are thermal and non-thermal desorption mechanisms

A plethora of computational chemical techniques is available to tackle the research questions above ☺

Further Reading Material

- Chapter from the book Surface Science written by Marco Griebling and Sharon Diamant, students of the MSc course Surface Science, as used to be taught by Ludo Juurlink

- Paper by Herma Cuppen et al.: Grain Surface Models and Data for Astrochemistry