Linking ice observations to laboratory studies of water ice structure

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Formation and evolution of water ice in star forming regions

Influence of mixing state on IR spectra of ices

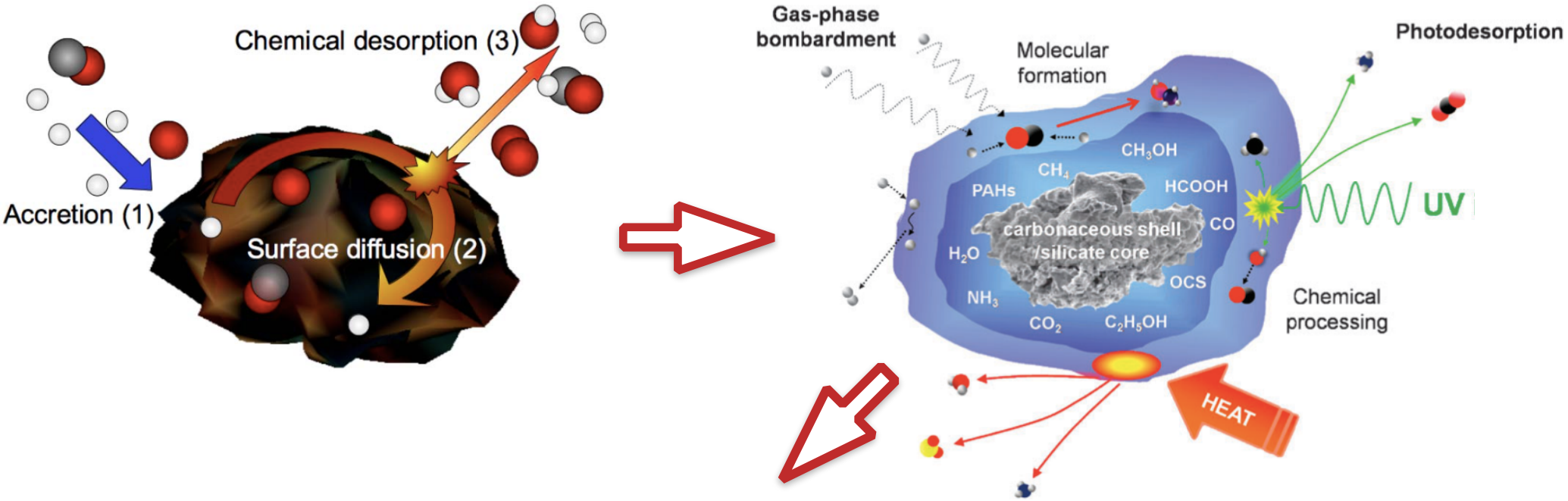
Influence of processing on IR spectra of ices

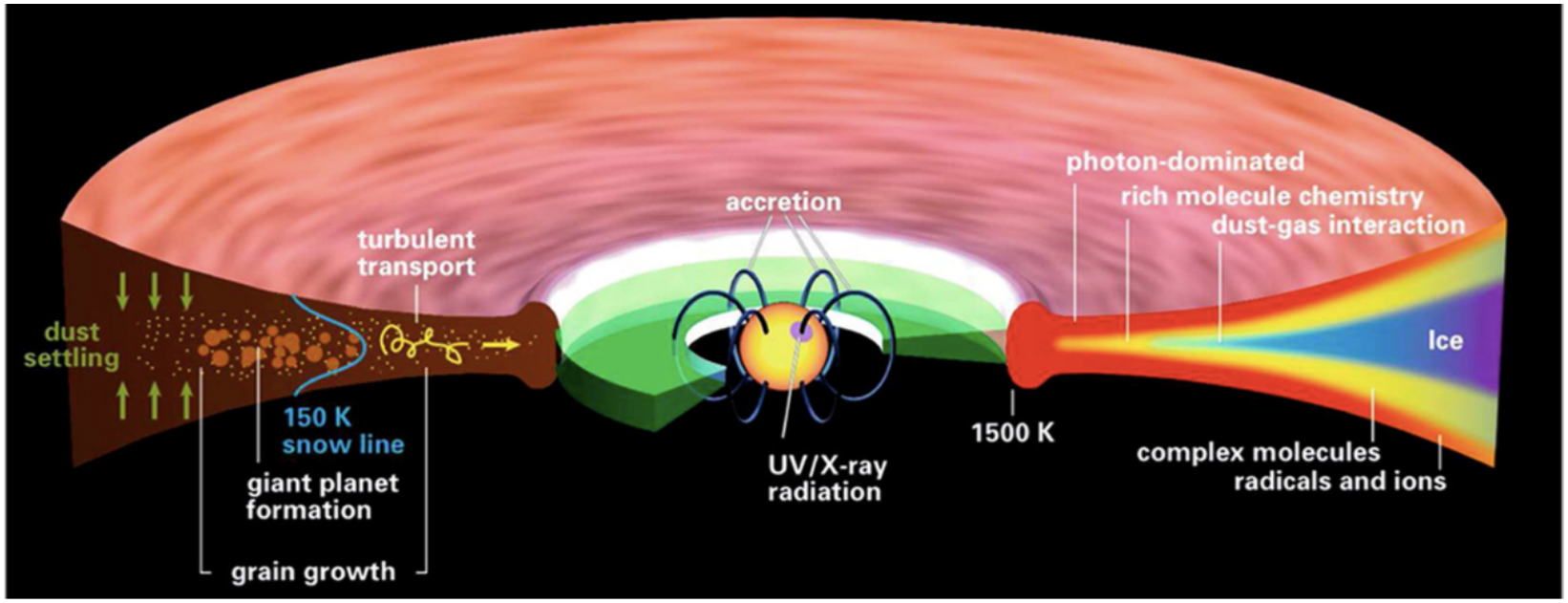
Formation and evolution of water ice in star forming regions

Influence of mixing state on IR spectra of ices

Influence of processing on IR spectra of ices

Ice formation and evolution during the star formation process





Dulieu+ *2013 Scientific Reports* , Brown & Burke *2010* PCCP, *Rab+ SpaceSciRev, 2016*

Observing ices in the ISM and solar system

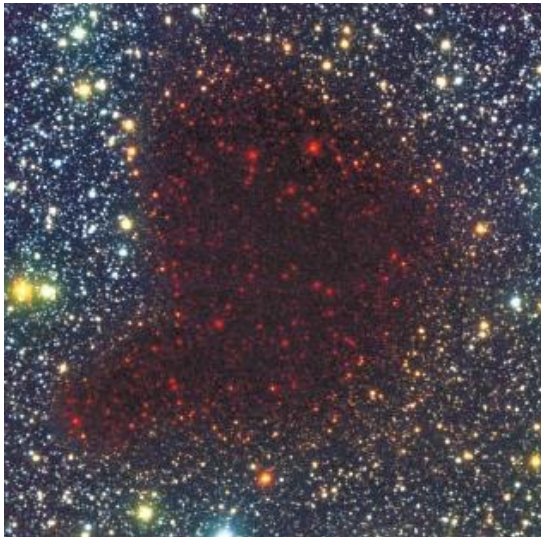
Direct methods

Indirect methods

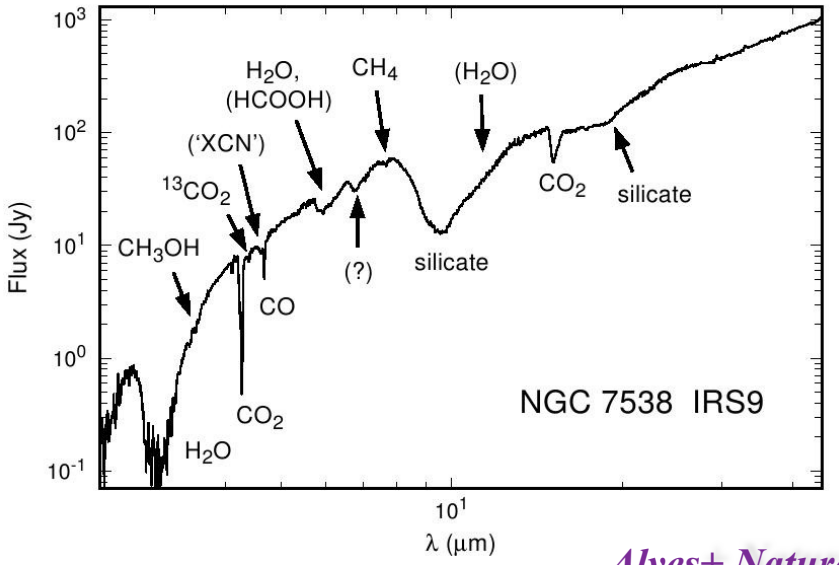
Alves+ Nature 2001, Whittet+ A&A 1996, Qi+ Science 2013, Altwegg+ ARAA 2019

Observing ices in the ISM and solar system

Direct methods



IR spectrum of embedded protostar NGC 7538 IRS9



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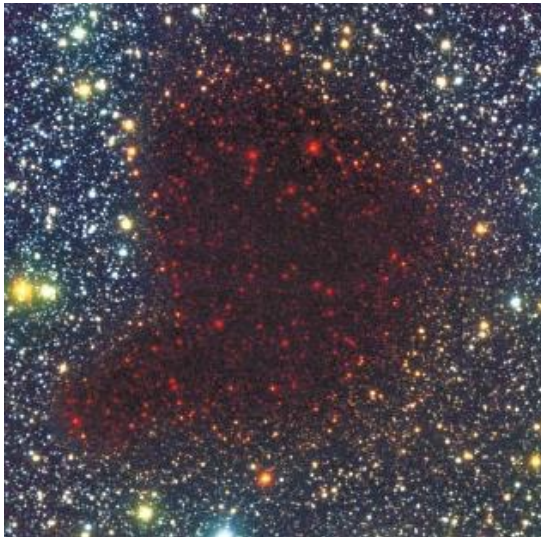
Observing ices in the ISM and solar system

Direct methods



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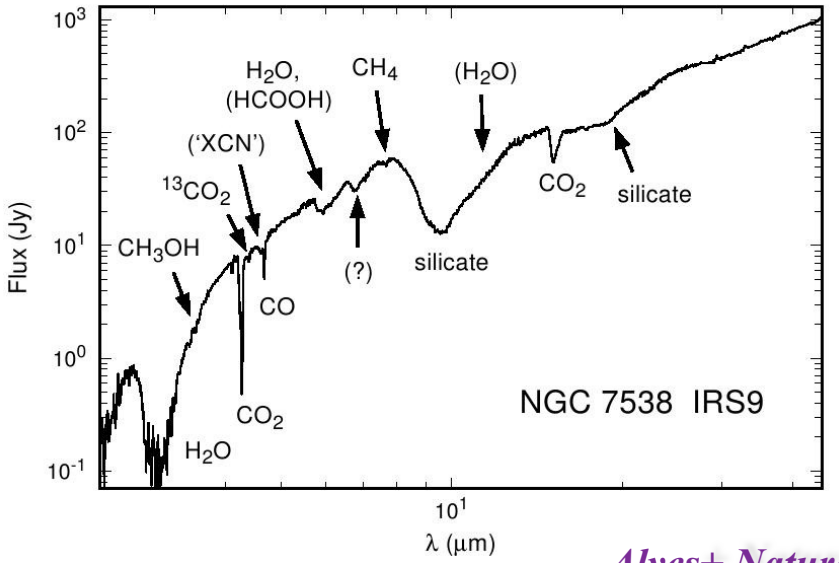
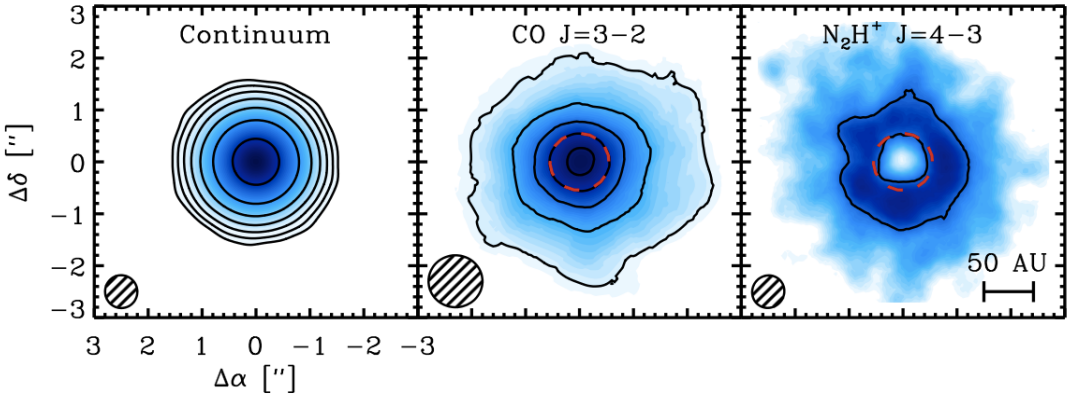
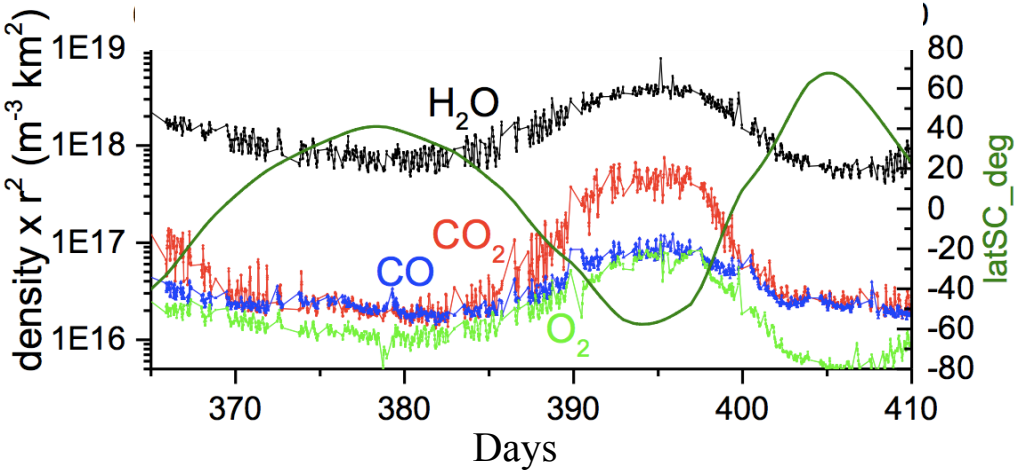


Indirect methods

Observations of dust & gas emission towards TW Hya disk



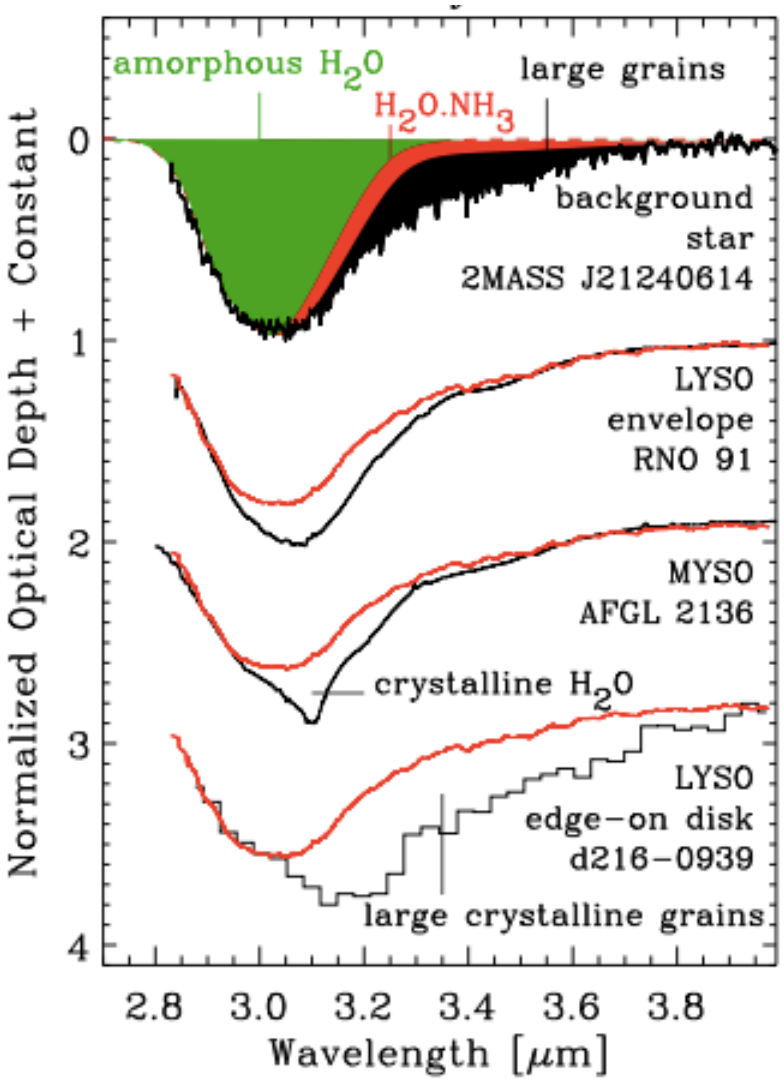
Remote sensing of comet 67P/Churyumov-Gerasimenko

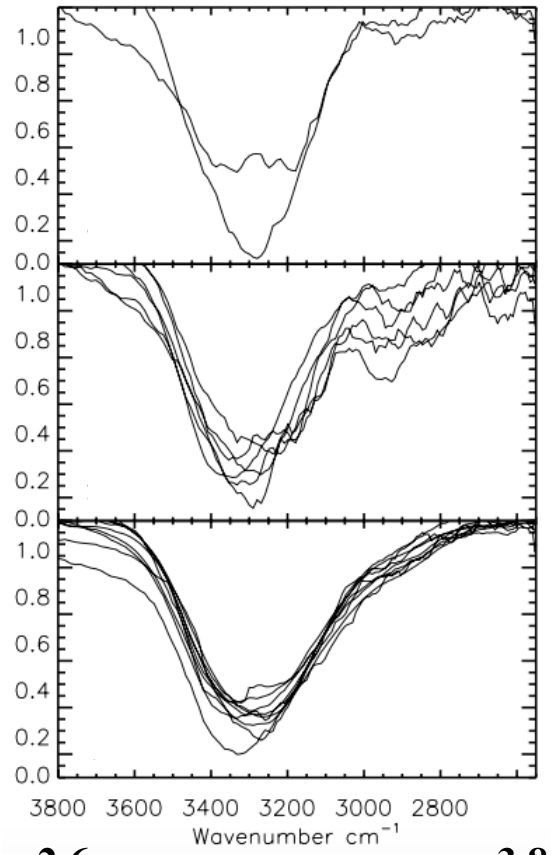


Alves+ Nature 2001, Whittet+ A&A 1996, Qi+ Science 2013, Altwegg+ ARAA 2019

Ice evolution traced through IR adsorption band profiles

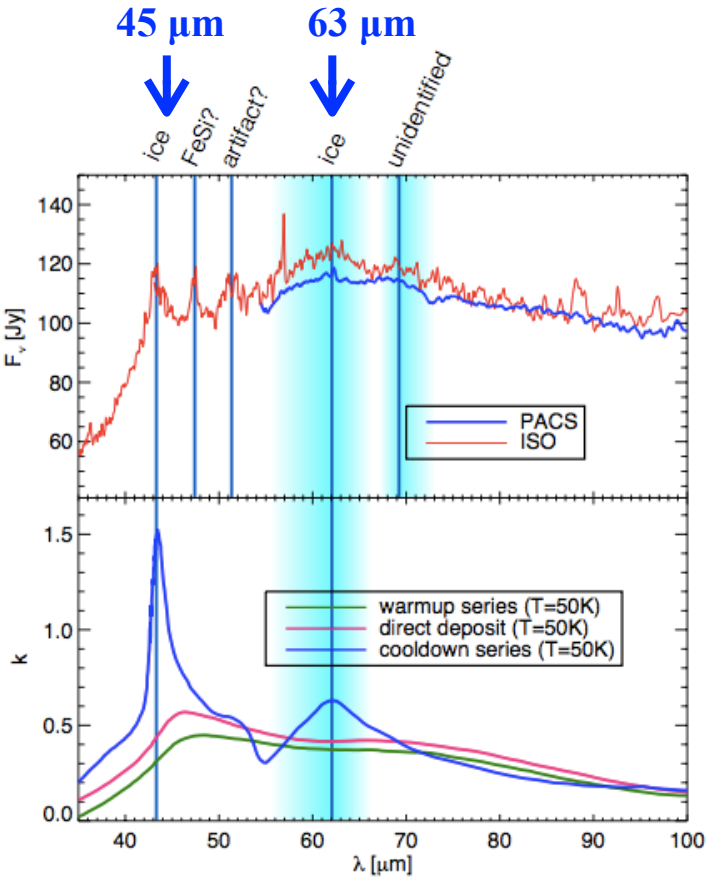
3 μm band (clouds, cores, envelopes)





2.6 μm 3.8

THz modes (disks)

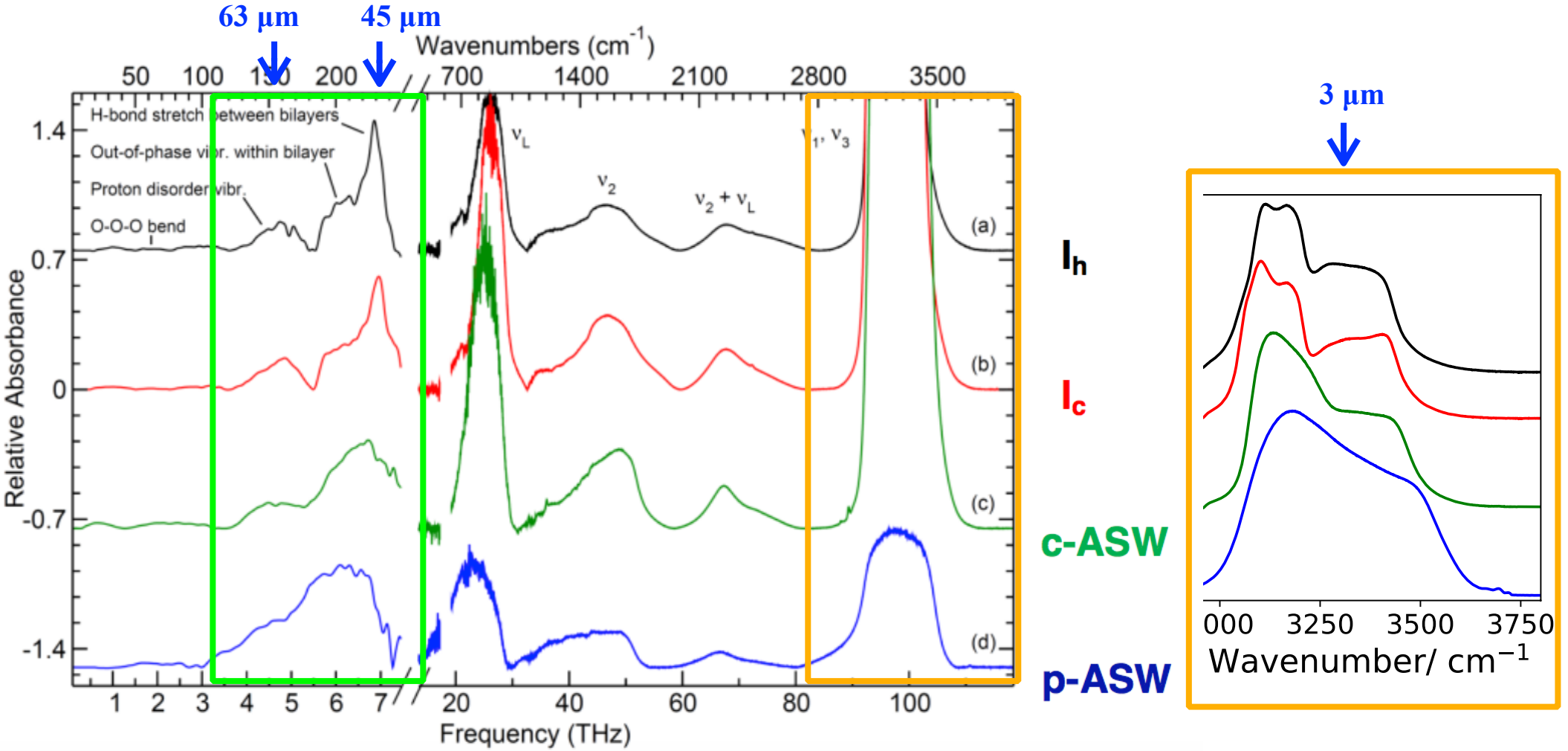


Boogert+ ARAA 2015; Noble+ ApJ 2013; Min+ A&A 2016

Evidence from laboratory IR spectroscopy

THz modes

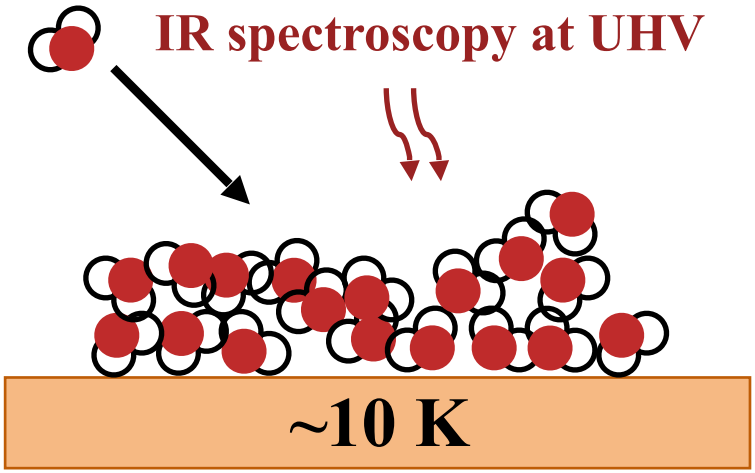
3 µm band



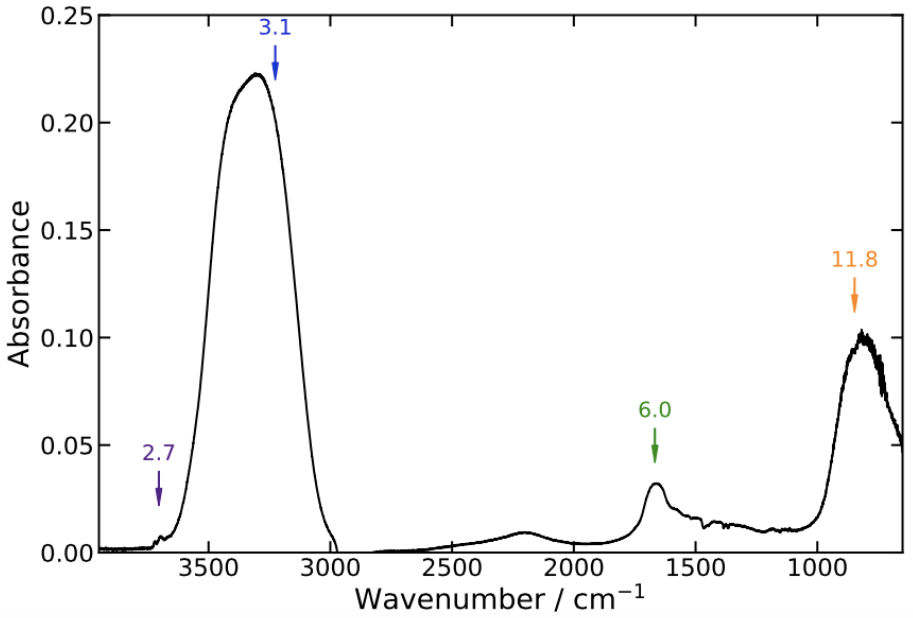
- 3 µm (stretch) and 50 µm (lattice) most sensitive to ice structure

Ioppolo+ Faraday Discuss. 2014

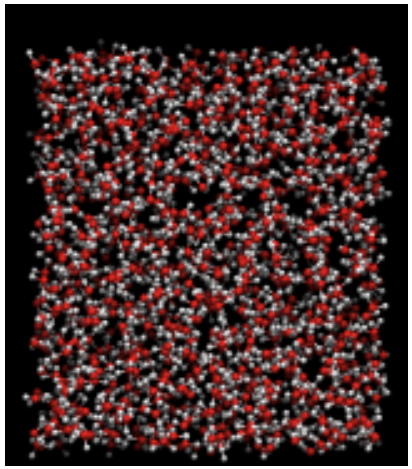
Evidence from laboratory IR spectroscopy

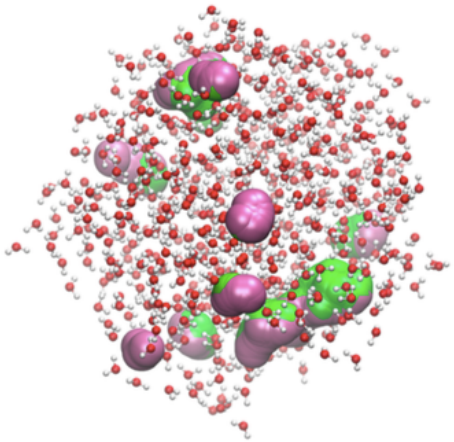


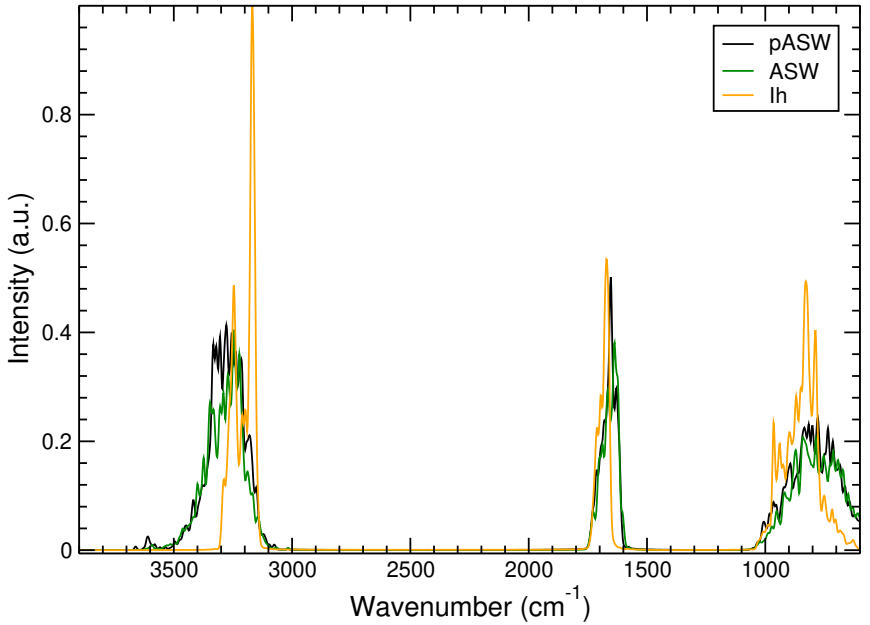
MIR spectrum of amorphous solid water



MD simulations



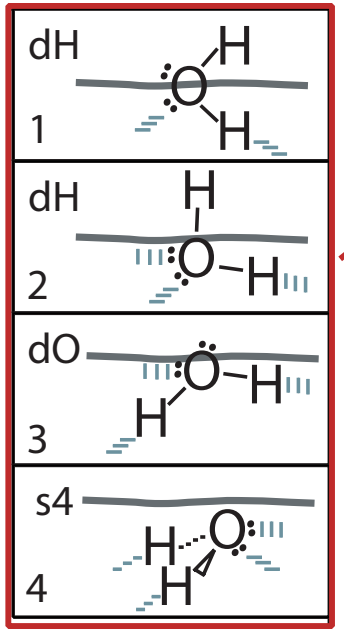


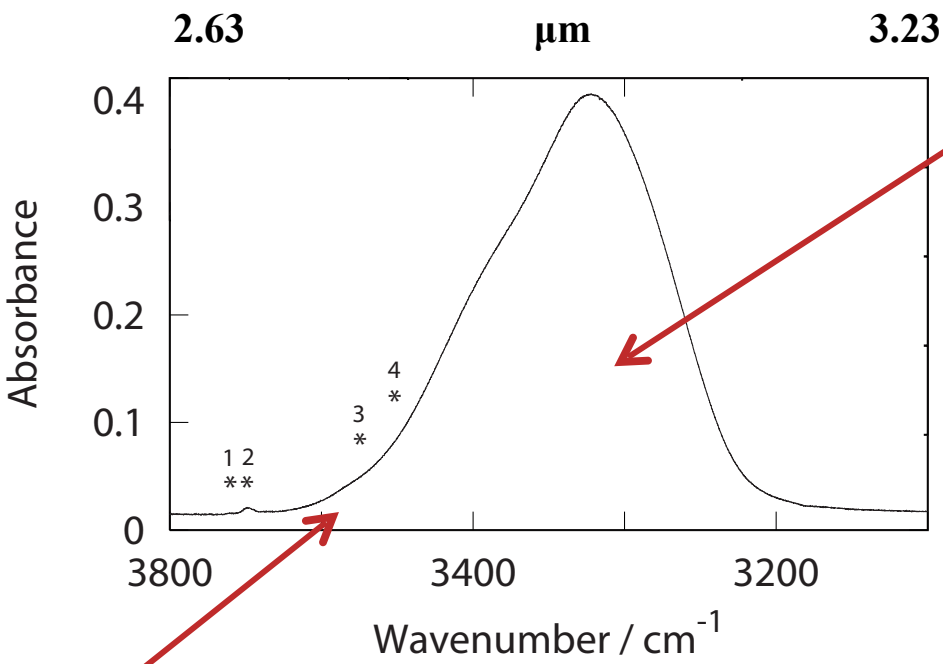


Noble+ to be submitted, Michoulier private comm, Cuppen private comm.

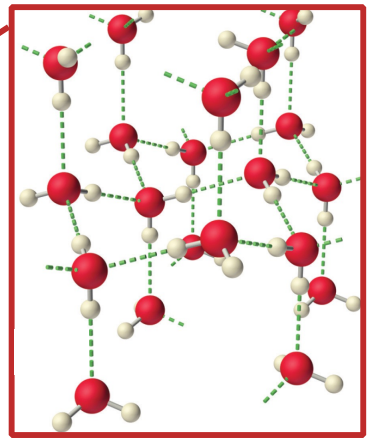
Structure of ASW determined in the laboratory

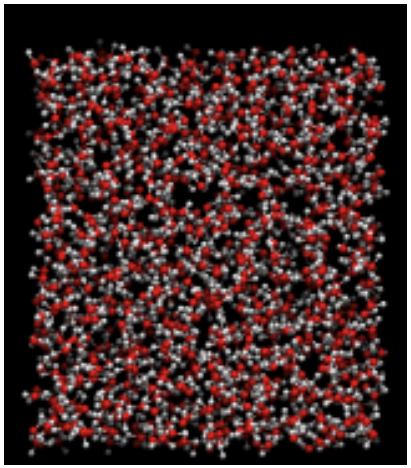
Surface :
Four distinct modes
"dangling bonds"

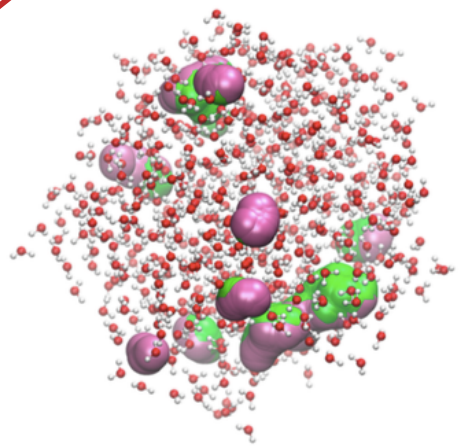




Bulk ice :
deformed tetrahedral

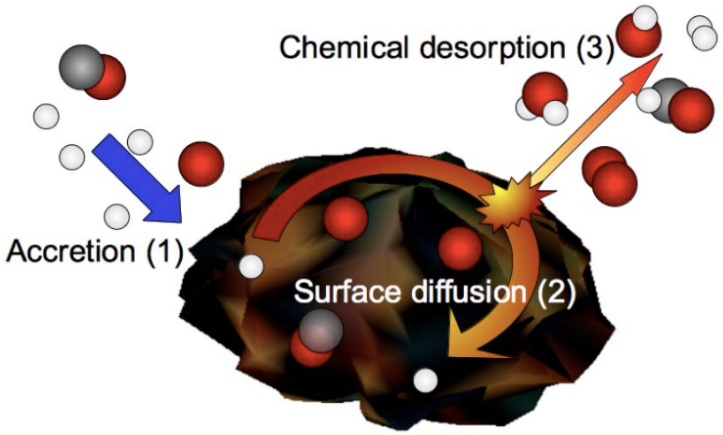






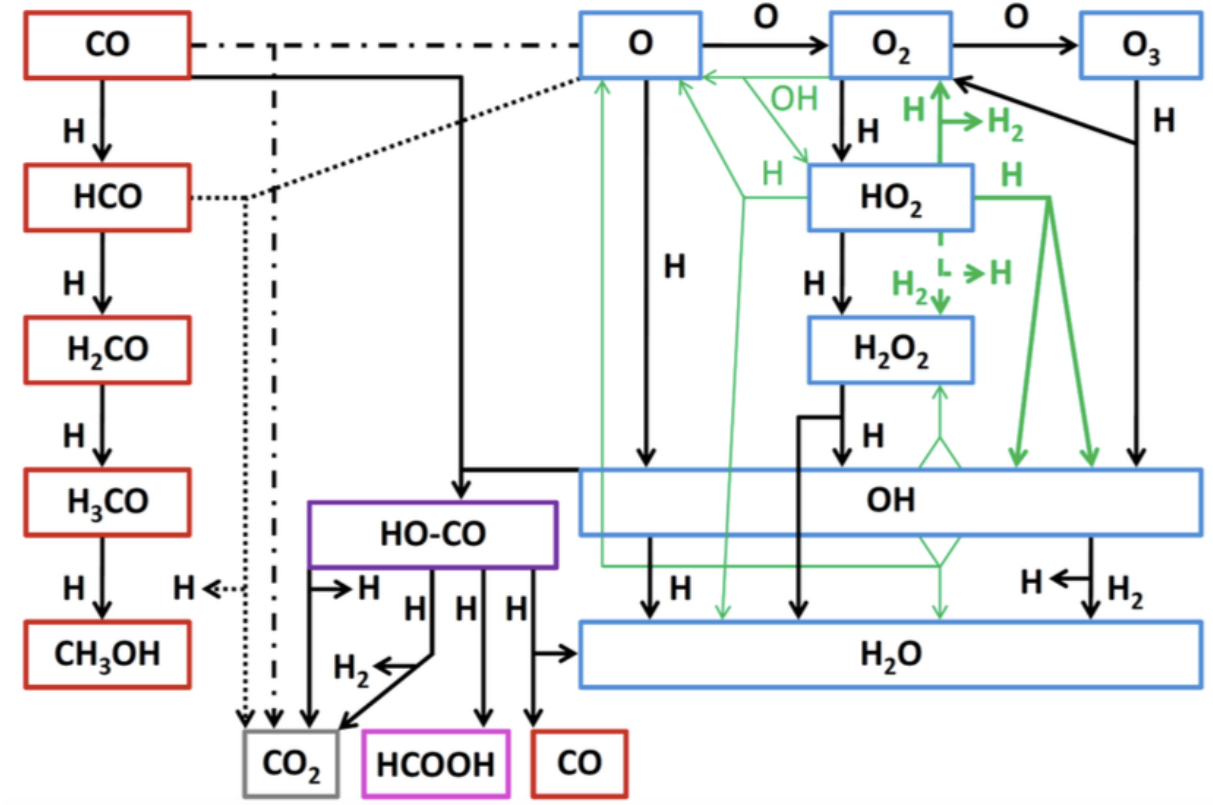
Devlin & Buch *J. Phys. Chem.* 1995; Bartels-Rausch + *Rev. Mod. Phys.* 2012

How porous is amorphous ice upon formation?



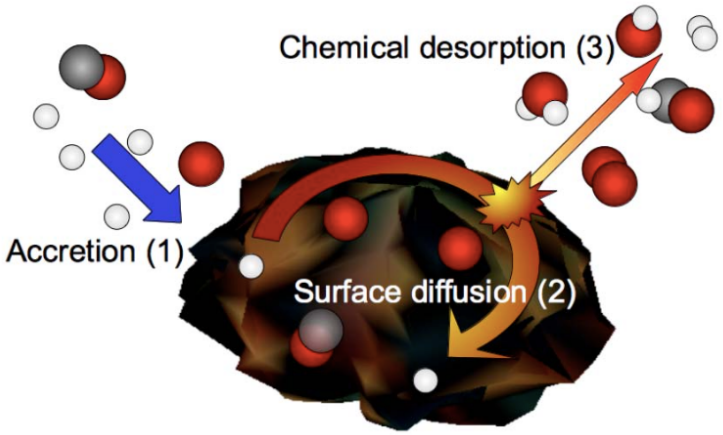
Cloud density $n_H \sim 10^3 - 10^4$ cm^{-3}

Temperature ~ 10 - 20 K



Dulieu+ *2013 Scientific Reports;* Linnartz+ 2015 *Int Rev Phys Chem*

How porous is amorphous ice upon formation?



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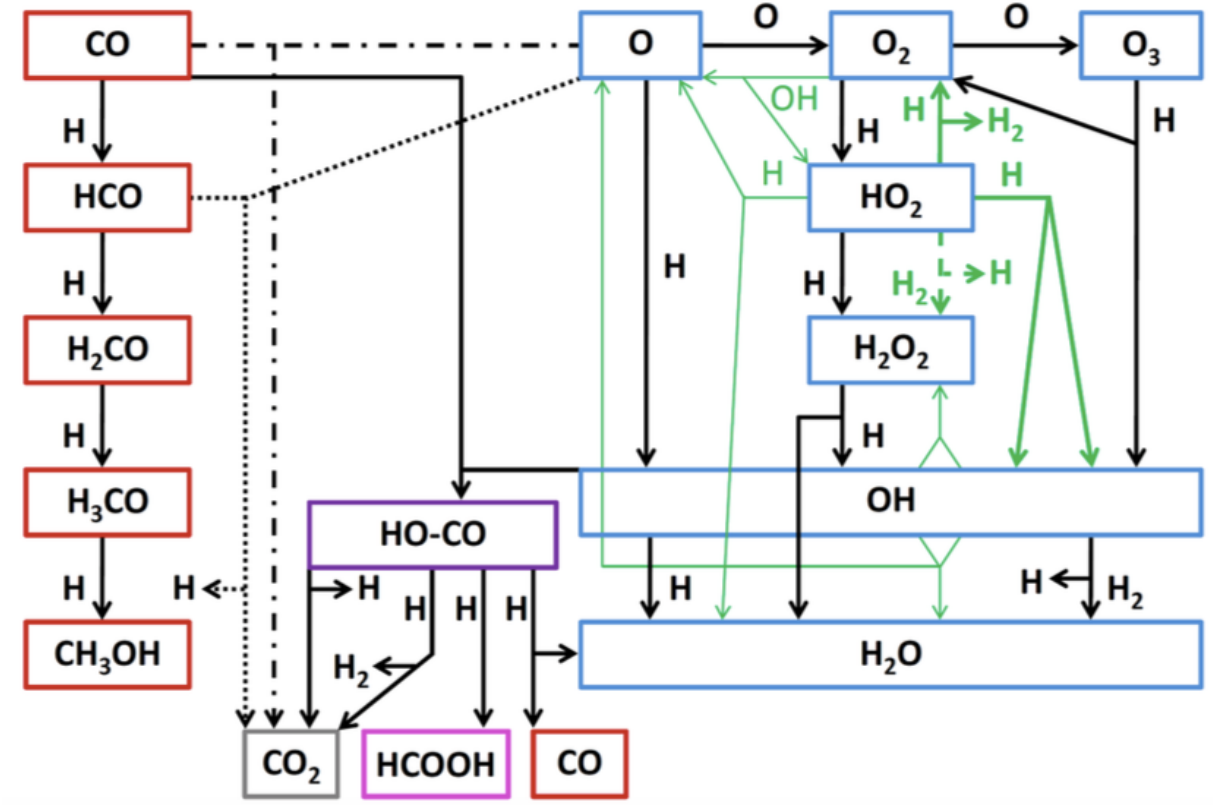
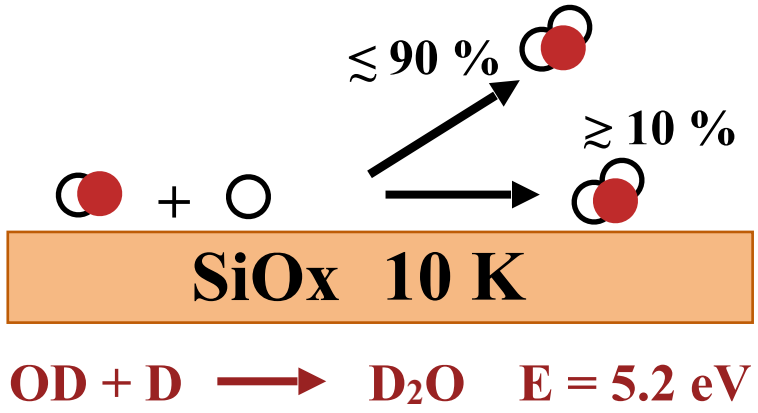




- Water ice likely to be compact ASW upon formation
- Search for dOH feature at 2.8 µm / 3720 cm^{-1}

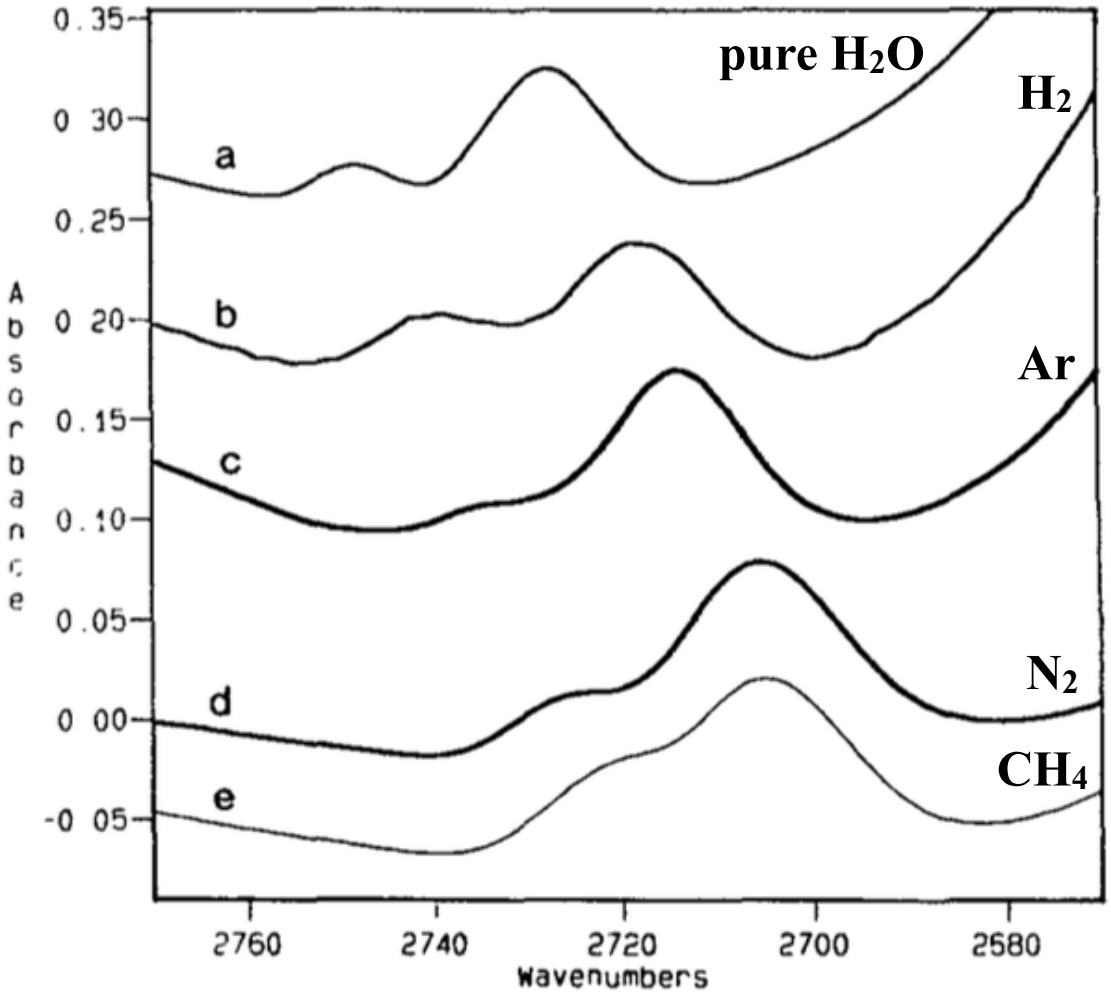
Dulieu+ *2013 Scientific Reports;* Linnartz+ 2015 *Int Rev Phys Chem*

Formation and evolution of water ice in star forming regions

Influence of mixing state on IR spectra of ices

Influence of processing on IR spectra of ices

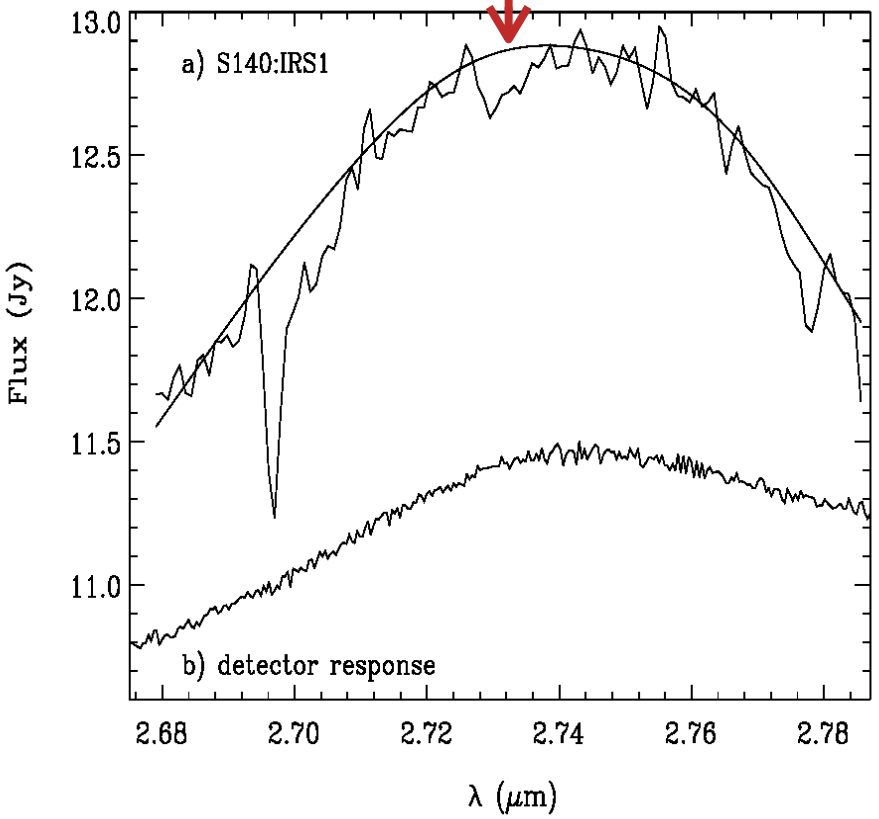
Influence of mixed ices on water ice surface



dOH redshift

$\Delta \sim 30\ cm^{-1}$

CO_2 on dOH?

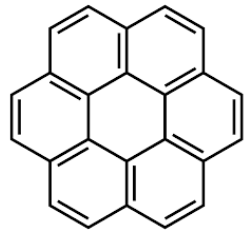


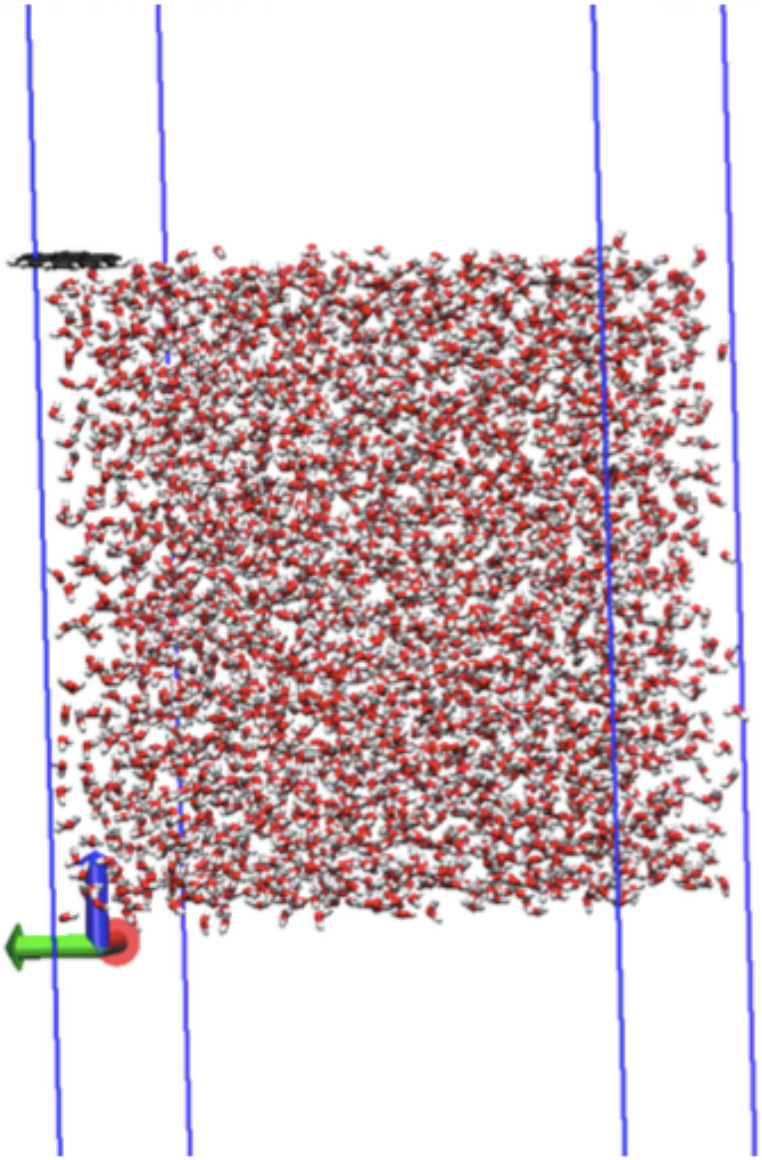
Luminous protostellar object S140:IRS1

Rowland+ J Chem Phys 1991; Keane+ A&A 2001

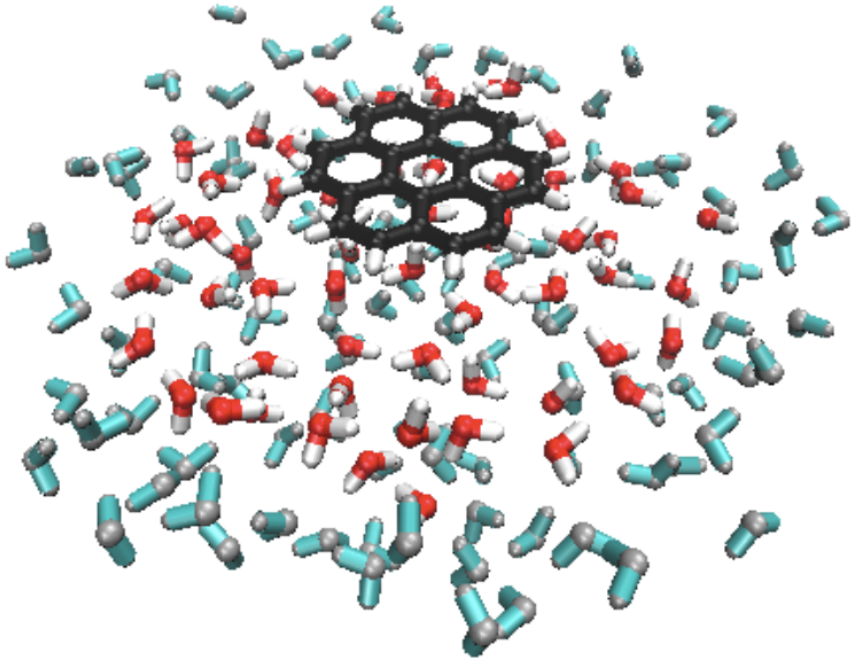
Simulations of the adsorption of PAHs on ice surfaces (multi-method)

Eric Michoulier, *PhD thesis* (C. Toubin & A. Simon)





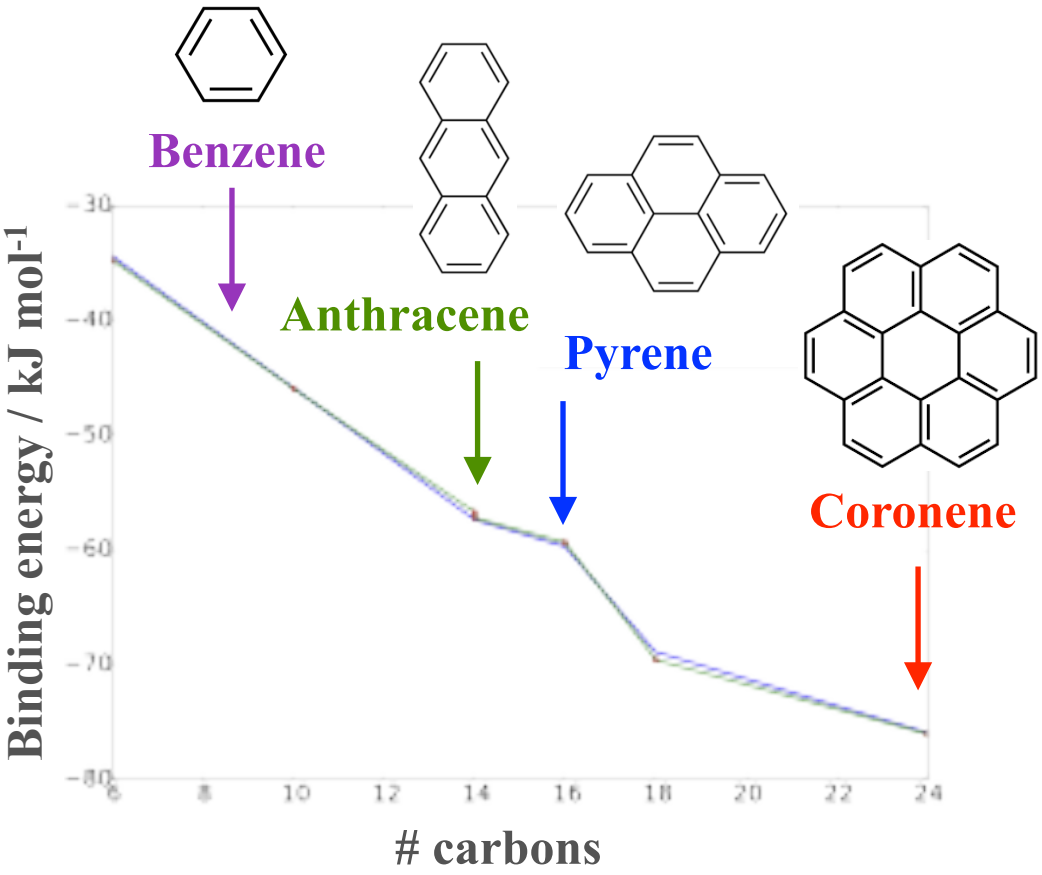
Classical MD simulation (ice + PAH)
(TIP4P/2005 Force Field + GOCPAC charges)



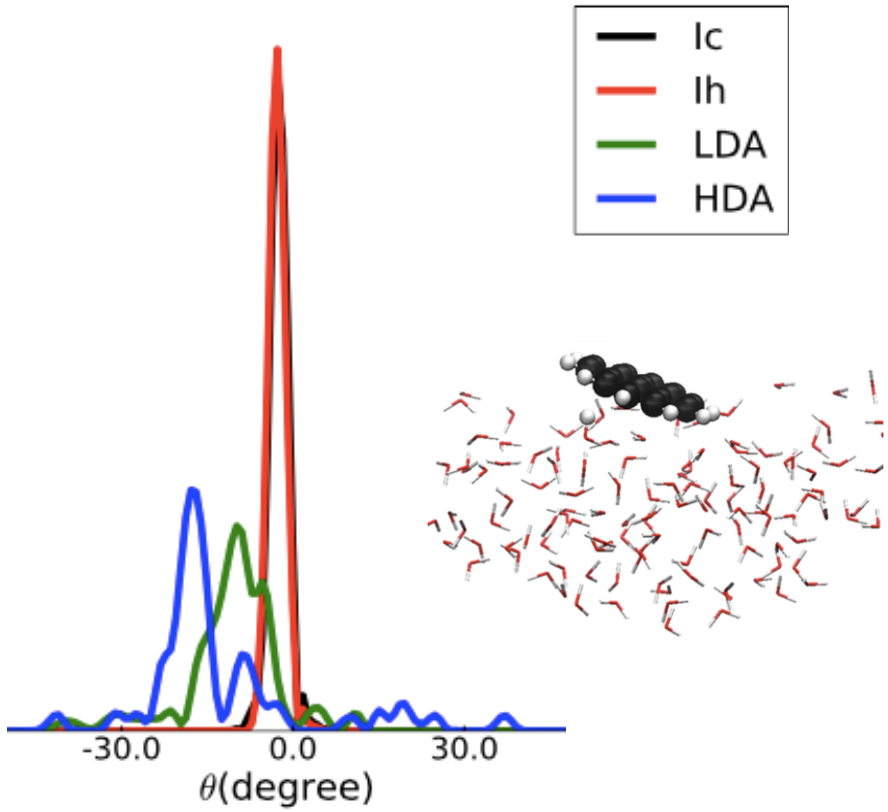
Electronic structure calculation
(DFTB 160 H_2O + 1 Coronene)

Sampling of 50 geometries

Binding energy and adsorption angle distribution



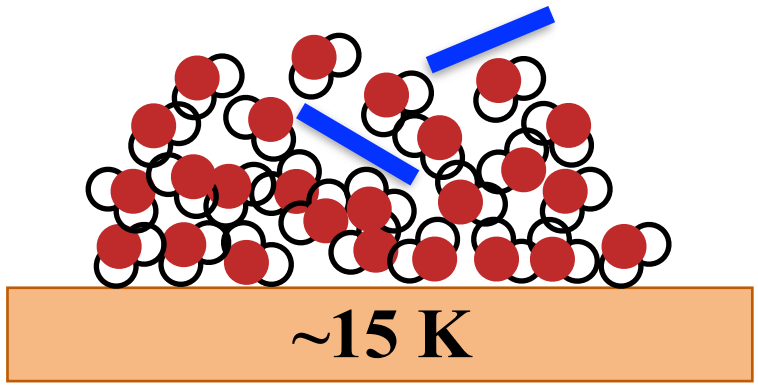
Binding energy increases with PAH size

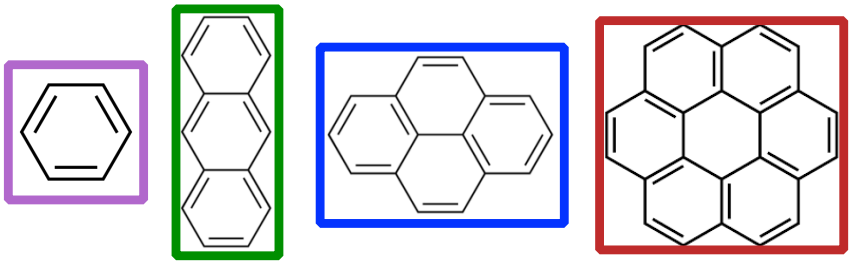


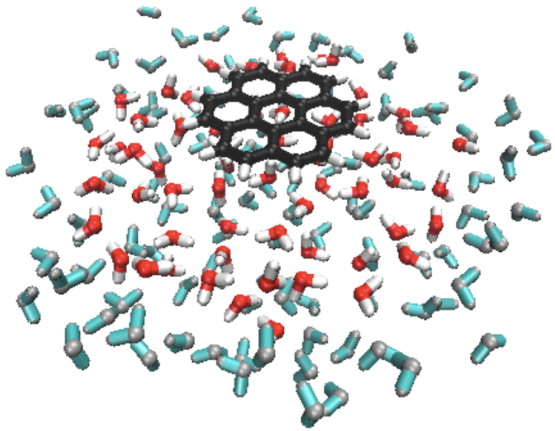
Adsorption geometry depends on ice structure

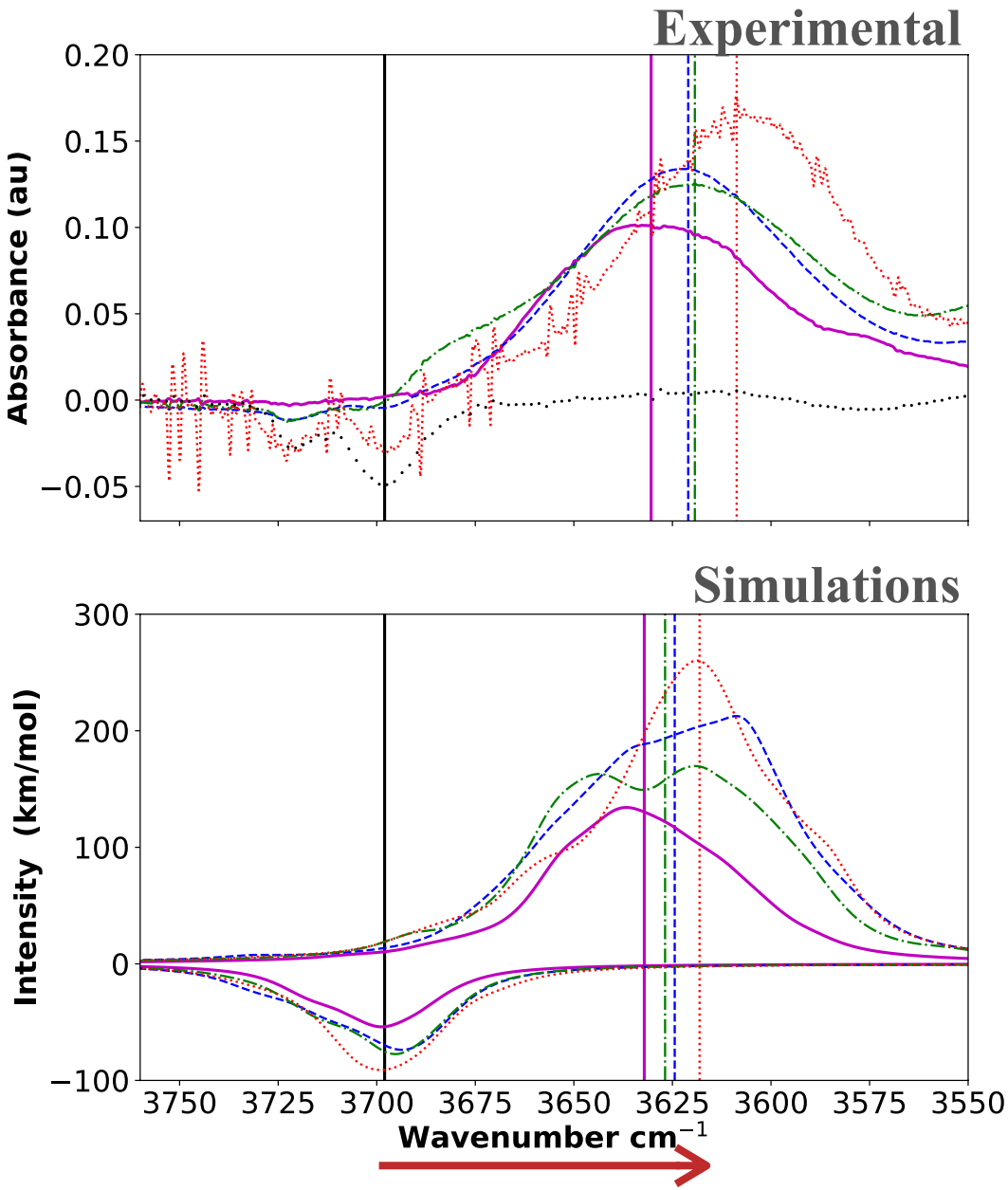
Michoulier+ 2018a PCCP, Michoulier+ 2018b PCCP

Adsorption impacts ice surface mode spectroscopy









dOH redshift ~ 70-80 cm^{-1}
& increases with PAH size

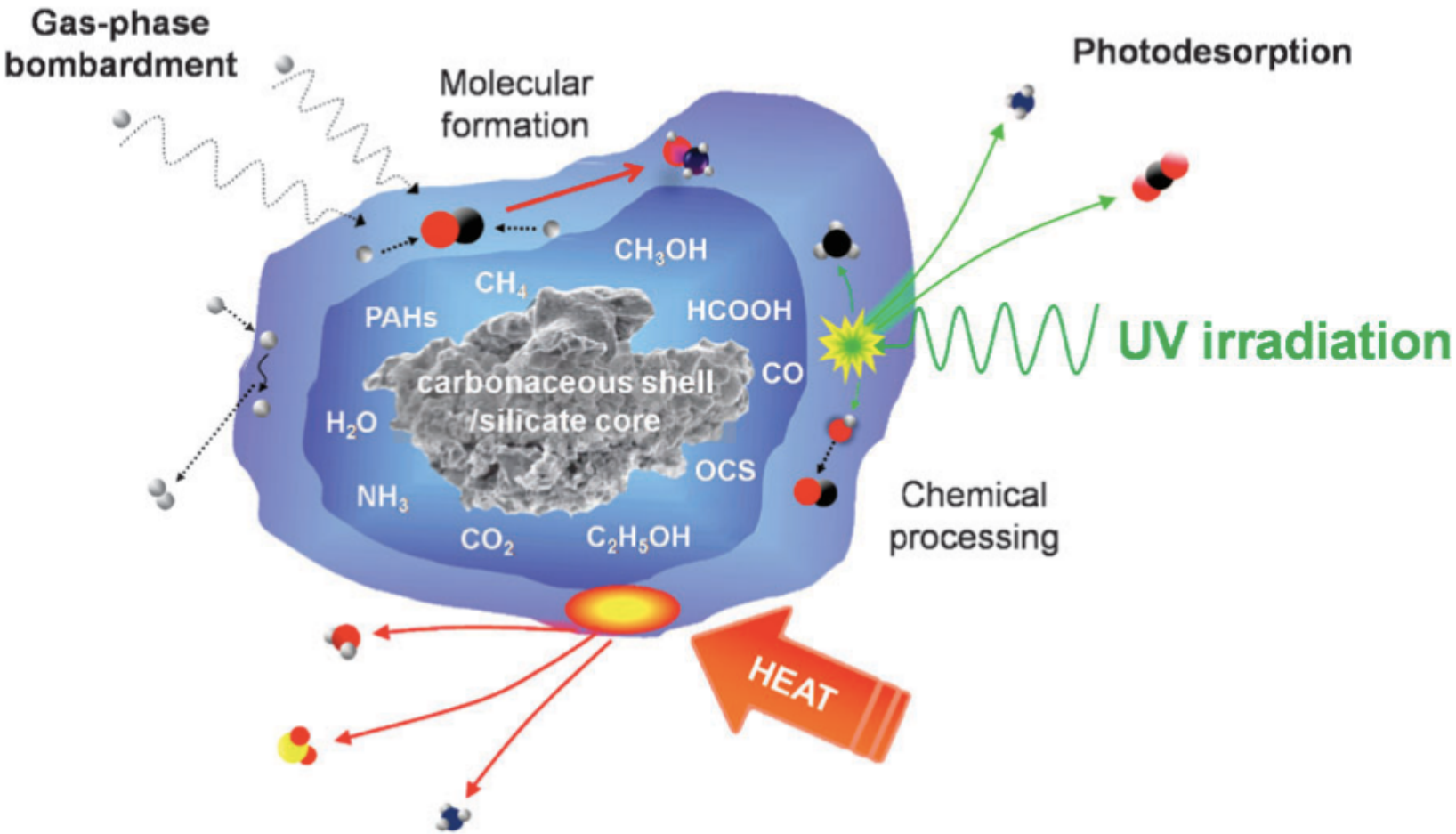
Michoulier+ *submitted*

Formation and evolution of water ice in star forming regions

Influence of mixing state on IR spectra of ices

Influence of processing on IR spectra of ices

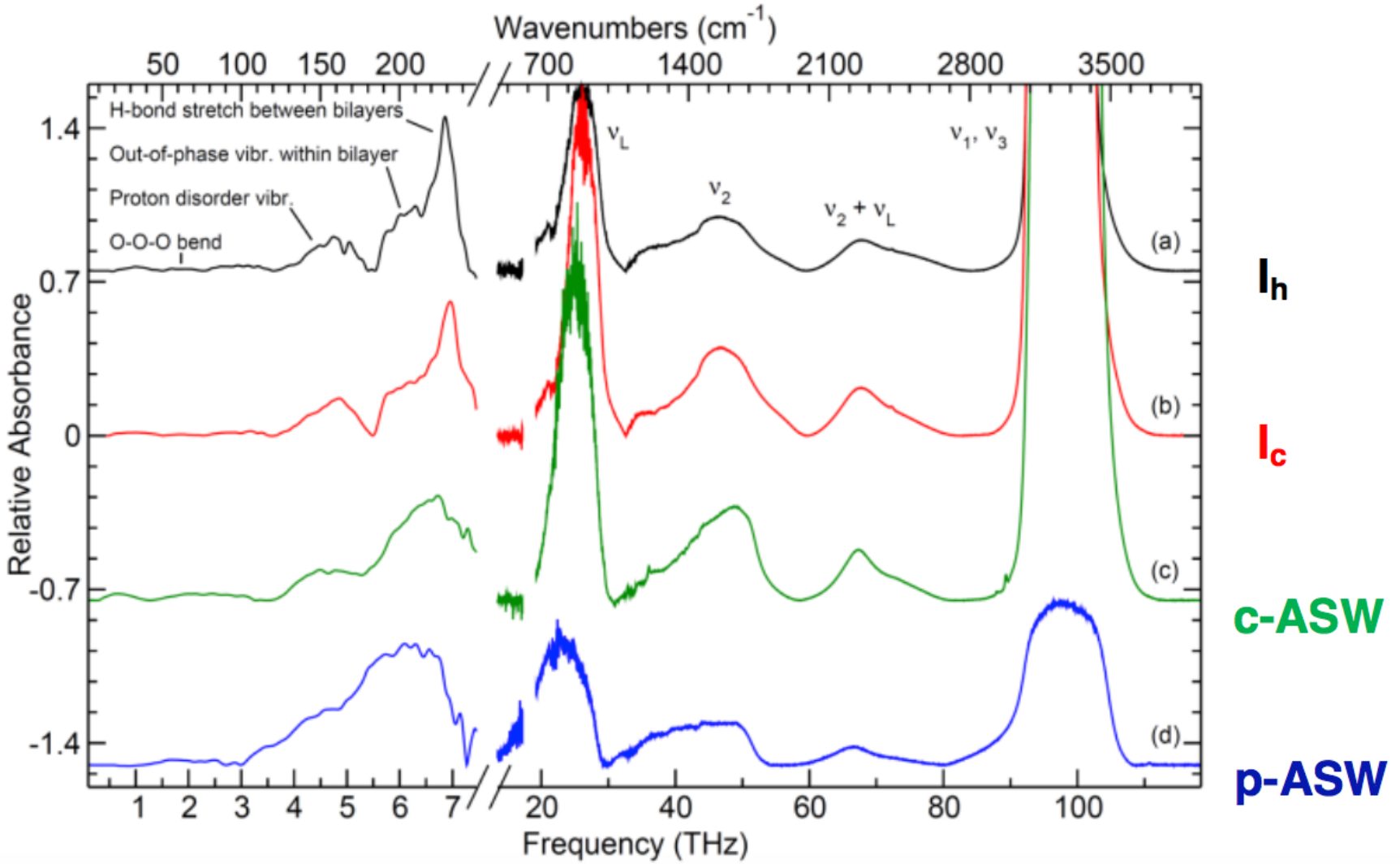
Energetic processing of ices in star formation cycle



How does amorphous ice relax injected energy?

Brown & Burke *2010* PCCP

MIR-THz irradiation of water ices with tuneable IR lasers

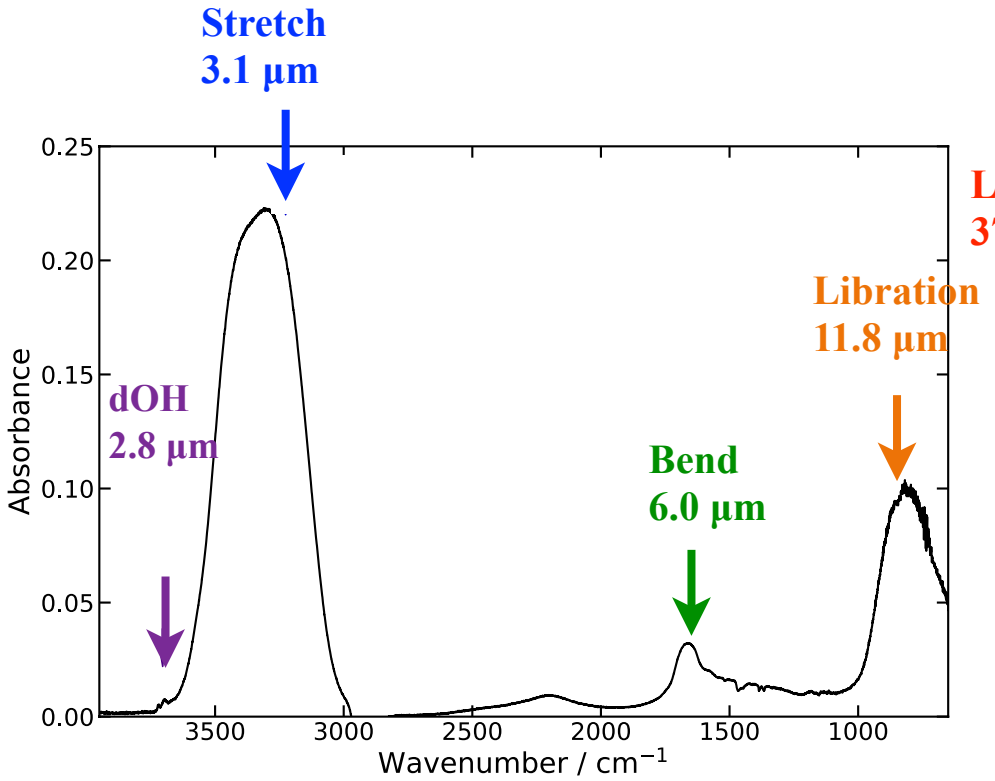


OPO tuneable range

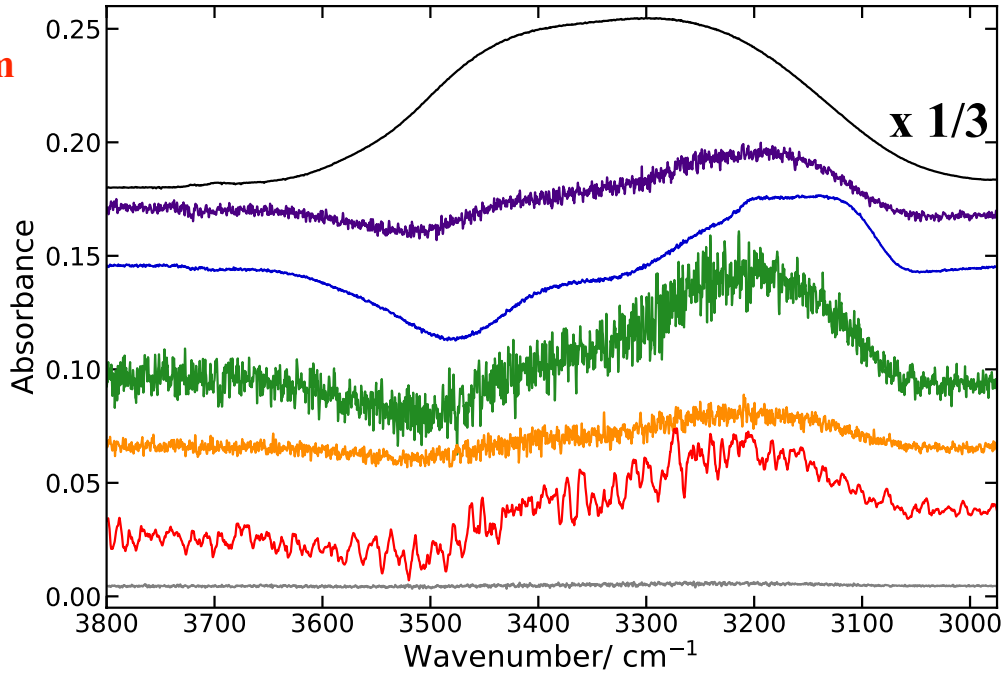
FELIX tuneable range

Ioppolo+ Faraday Discuss. 2014

Selective irradiation of pASW vibrational modes



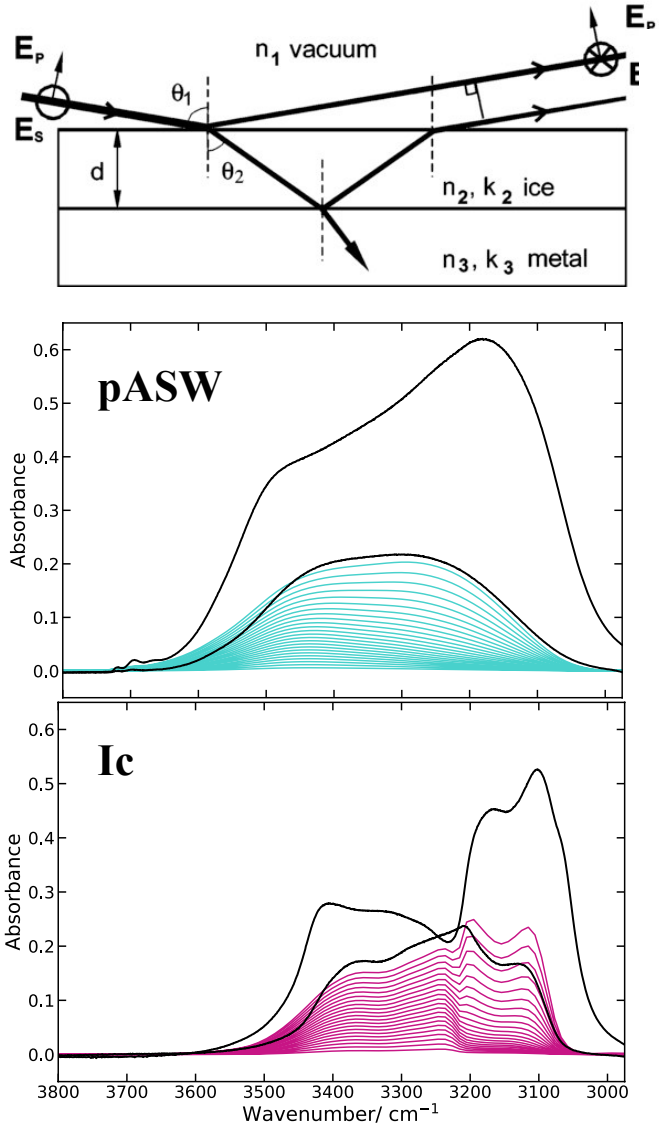
3 µm band - difference spectra after irradiation

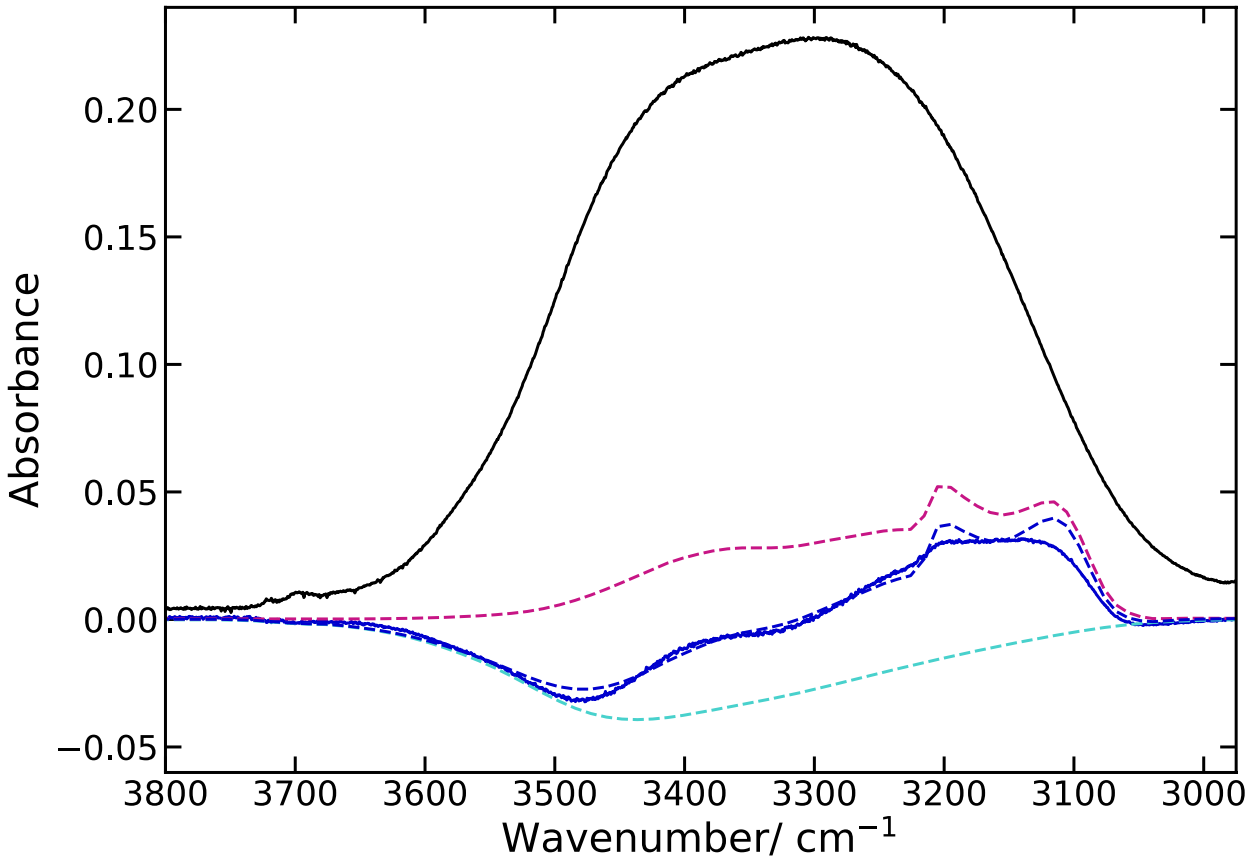


- Loss and gain of oscillators similar for energy injection into different modes
- Amorphous ice exhibits restructuring

Noble, Cuppen, Redlich, Coussan & Ioppolo *to be submitted.*

Synthetic ice spectra from optical constants

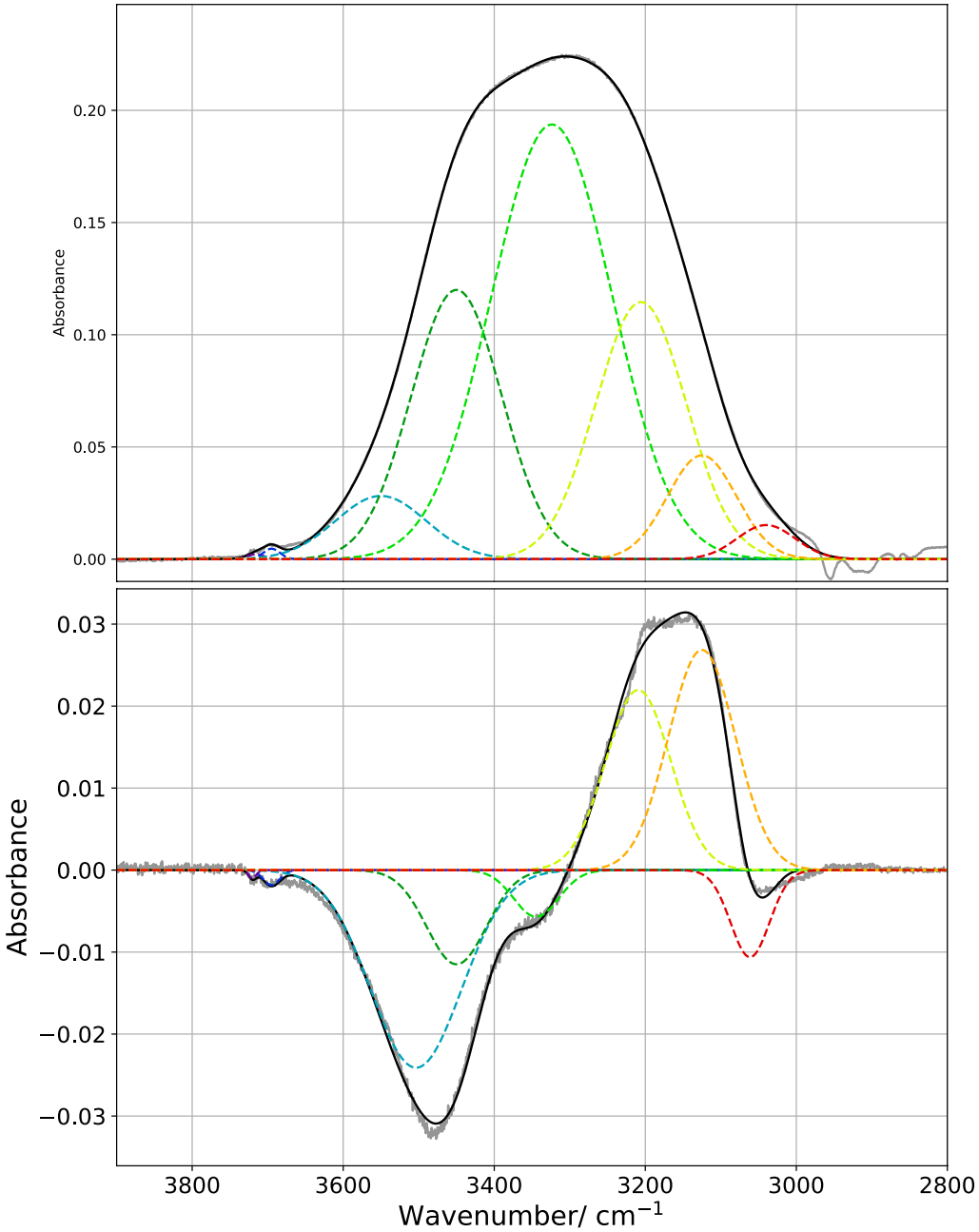


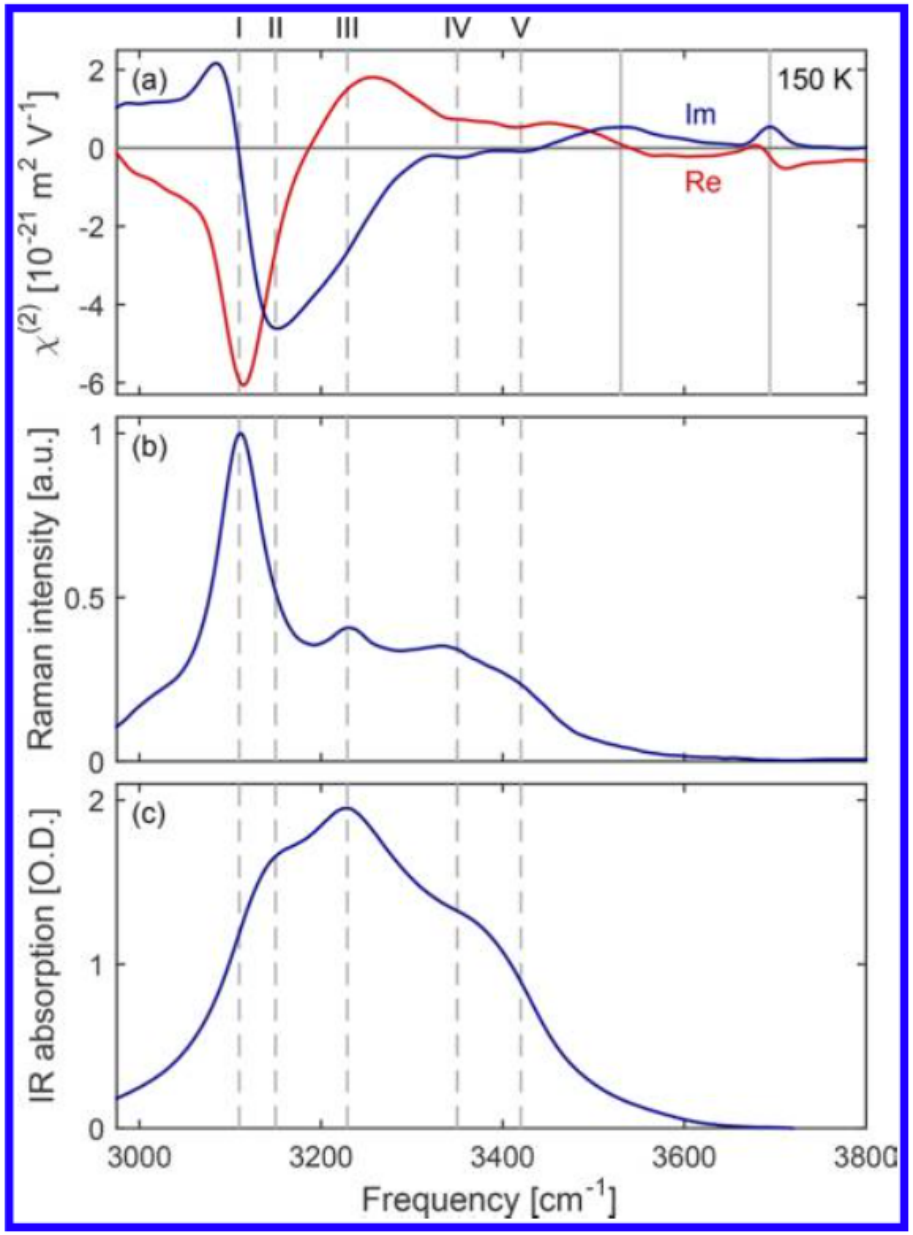


~ 33 % of pASW restructures ("crystallises")

Noble, Cuppen, Redlich, Coussan & Ioppolo *to be submitted.*

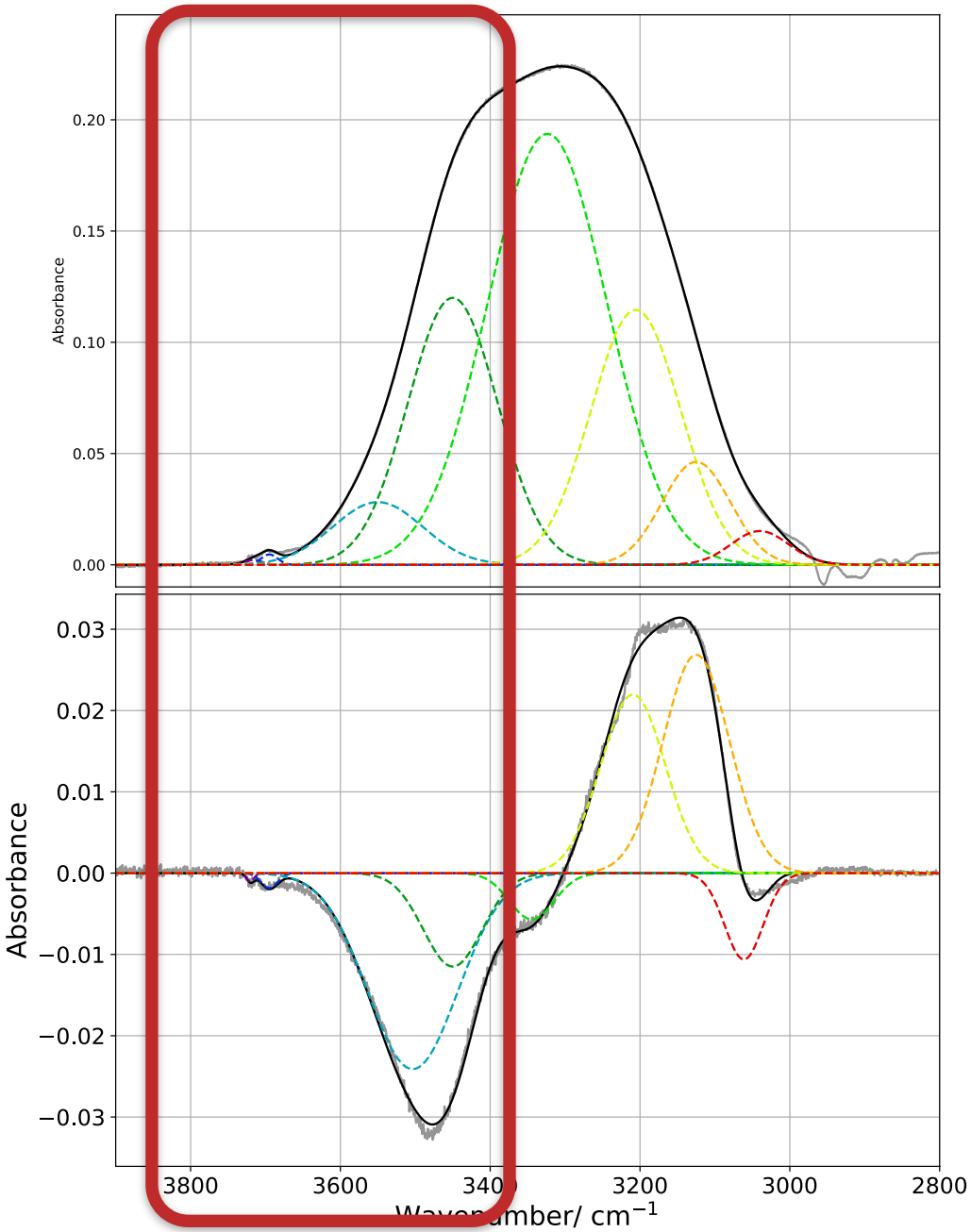
Oscillator fitting method

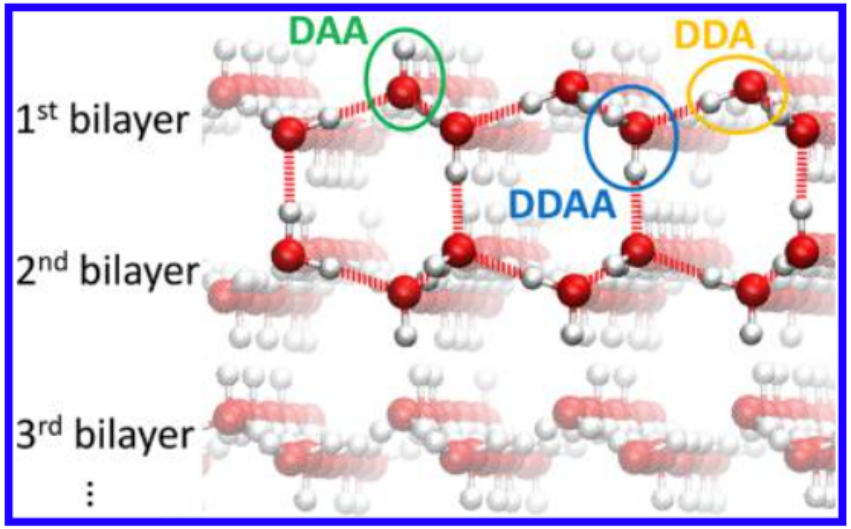


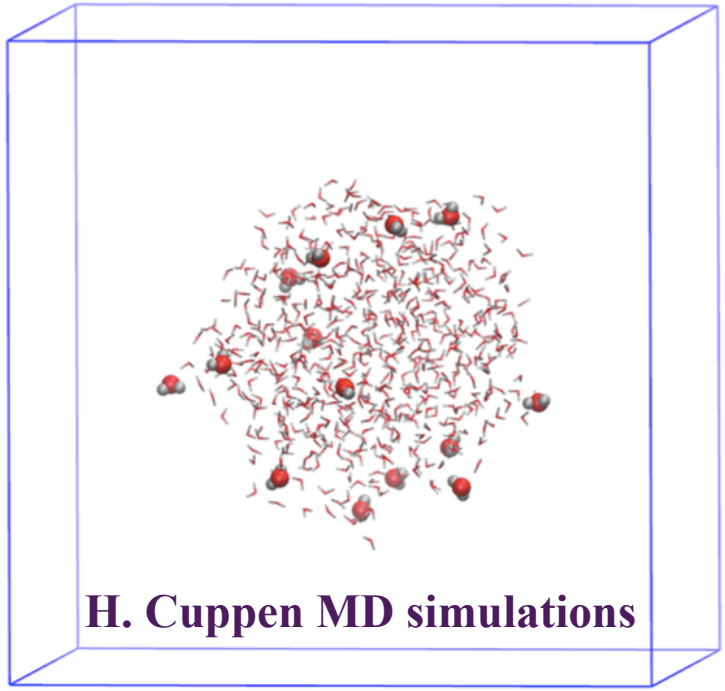


Smit et al. *J. Phys. Chem. Lett.* 2017

Oscillator fitting method

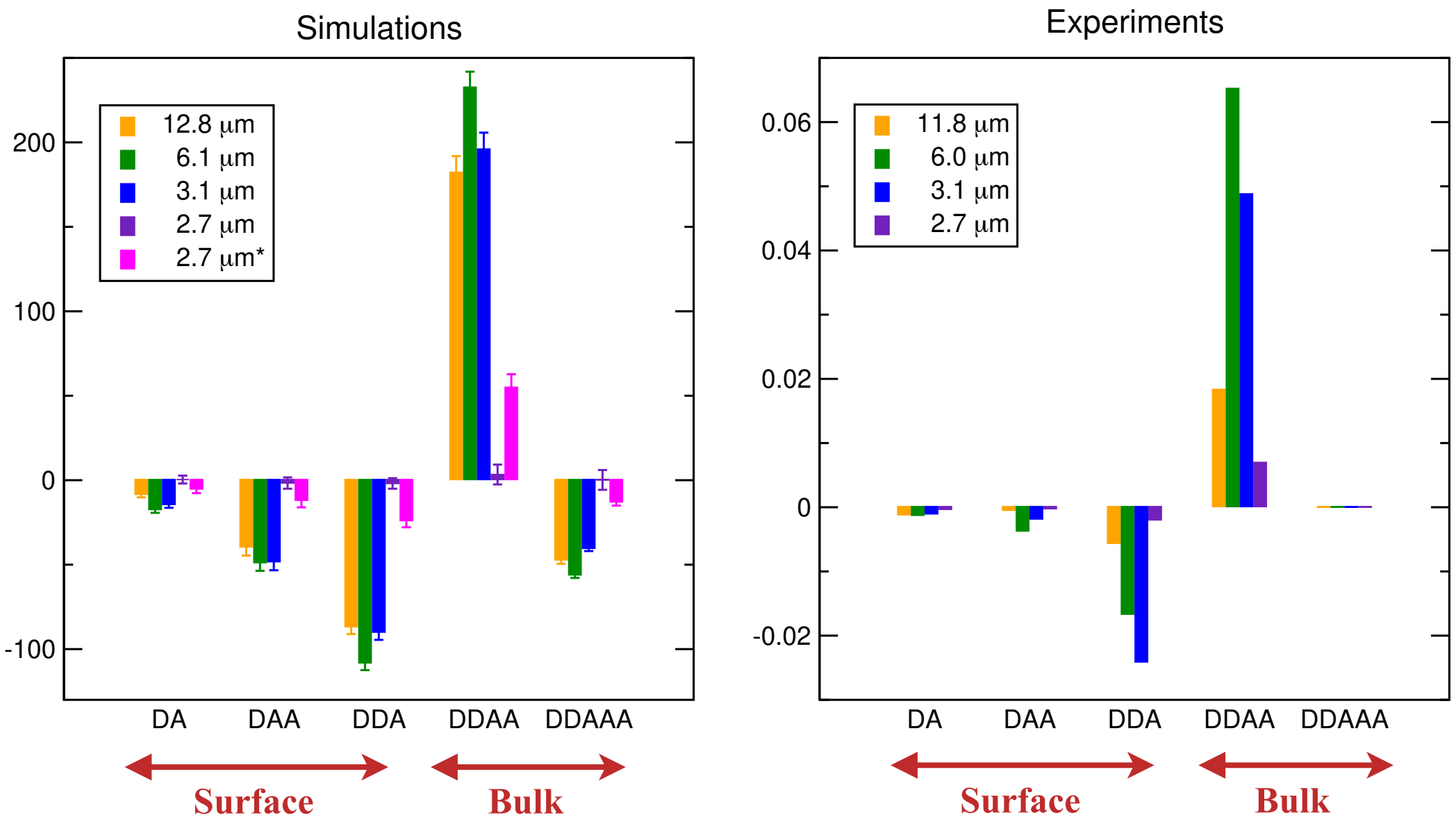






Noble, Cuppen, Redlich, Coussan & Ioppolo *to be submitted.*

Modelling energy relaxation in ASW



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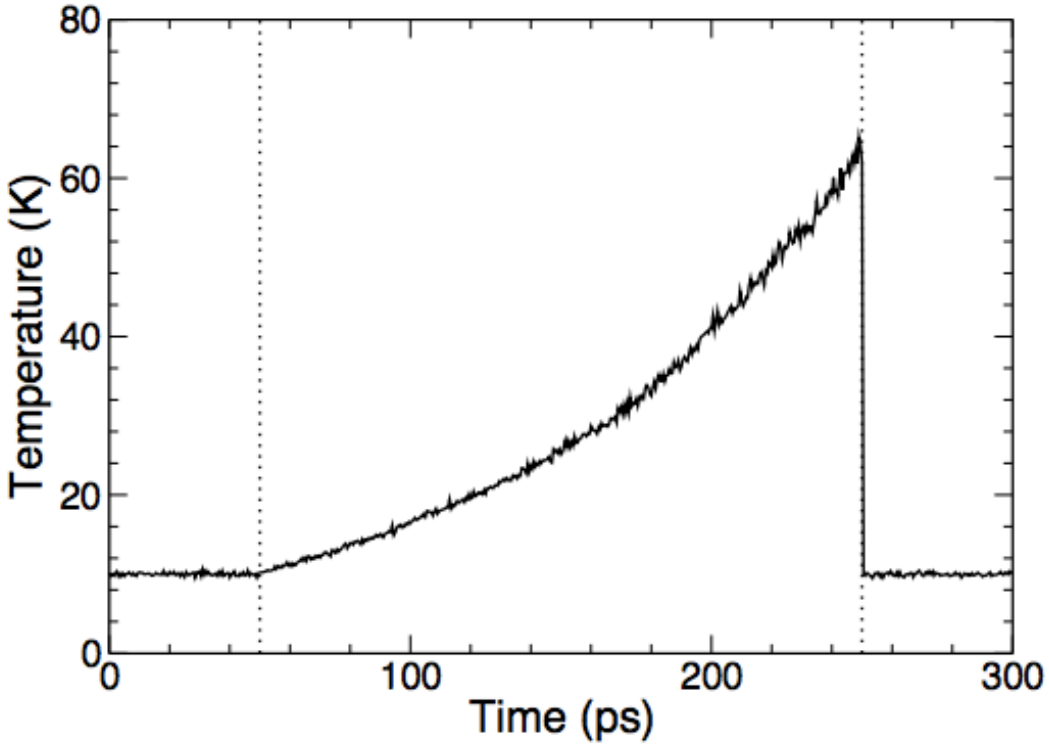
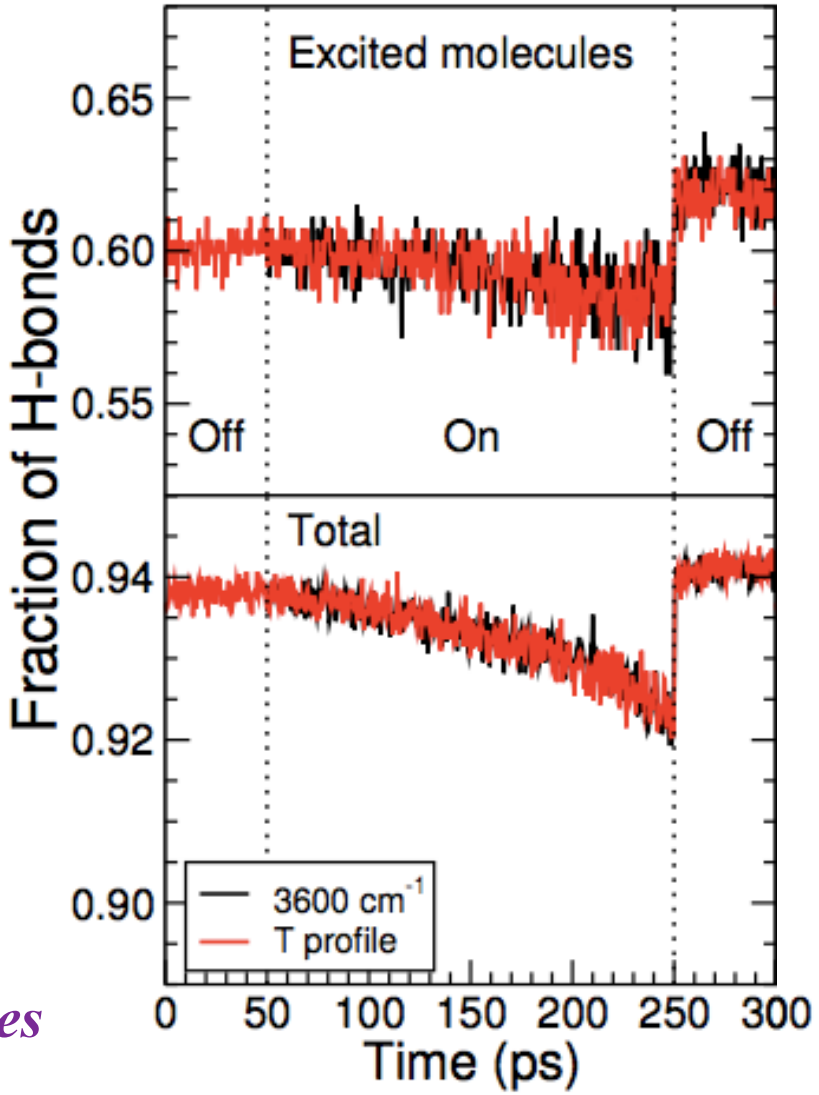
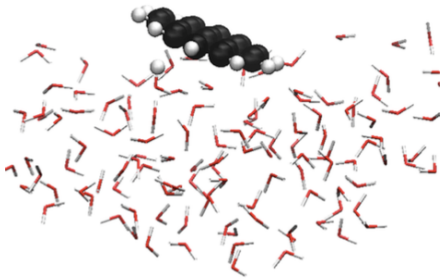




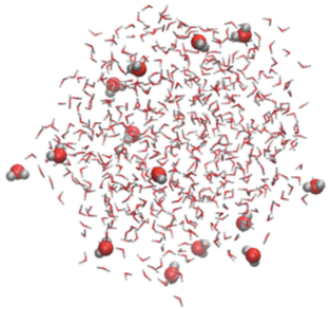
- **Irradiation heats ice locally**
- **Increases number of H-bonds *i.e. ice restructures***

Noble, Cuppen, Redlich, Coussan & Ioppolo *to be submitted.*

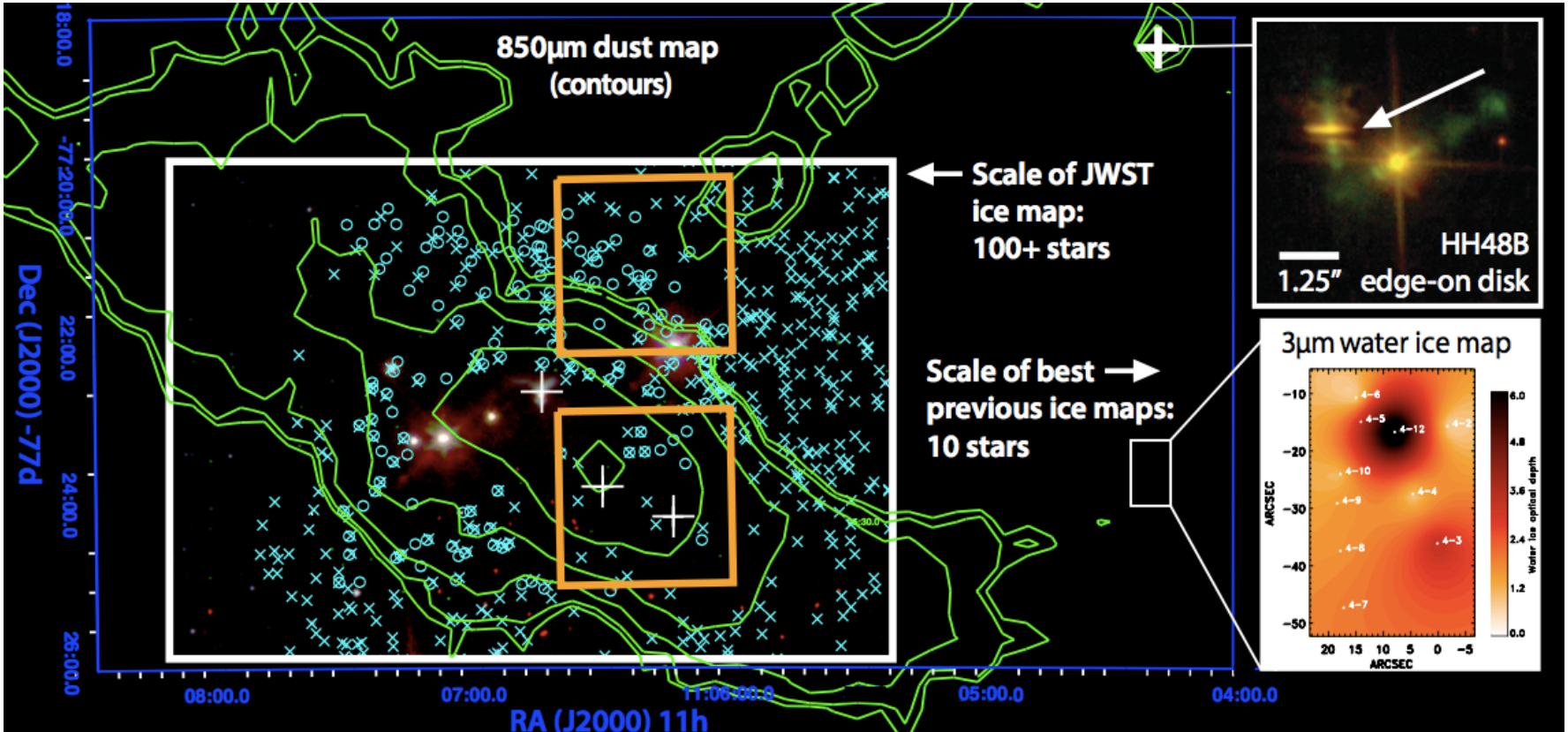
Future needs for astrochemistry of ices



- **Simulations** of molecular **orientation** and energy **dissipation** dynamics necessary to fully integrate ad-/desorption and reactivity into **astrochemical models**



- **JWST "IceAge" ERS program** will study objects at all stages of **evolution** from molecular cloud to protoplanetary disk



Cha 1 field
McClure+

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