The Molecular Universe
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(EXO)PLANETARY ATMOSPHERES CHEMICAL MODELS

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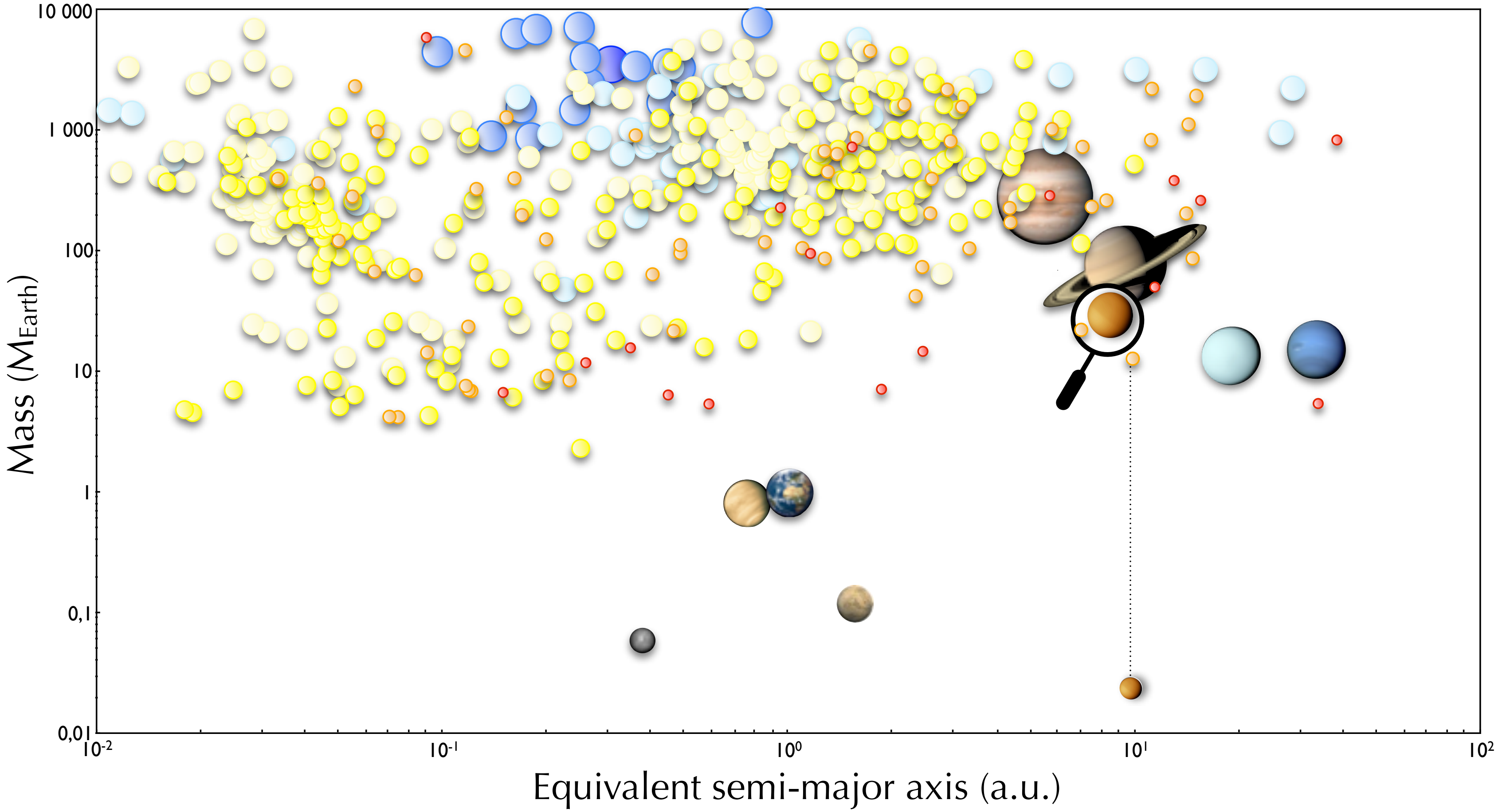
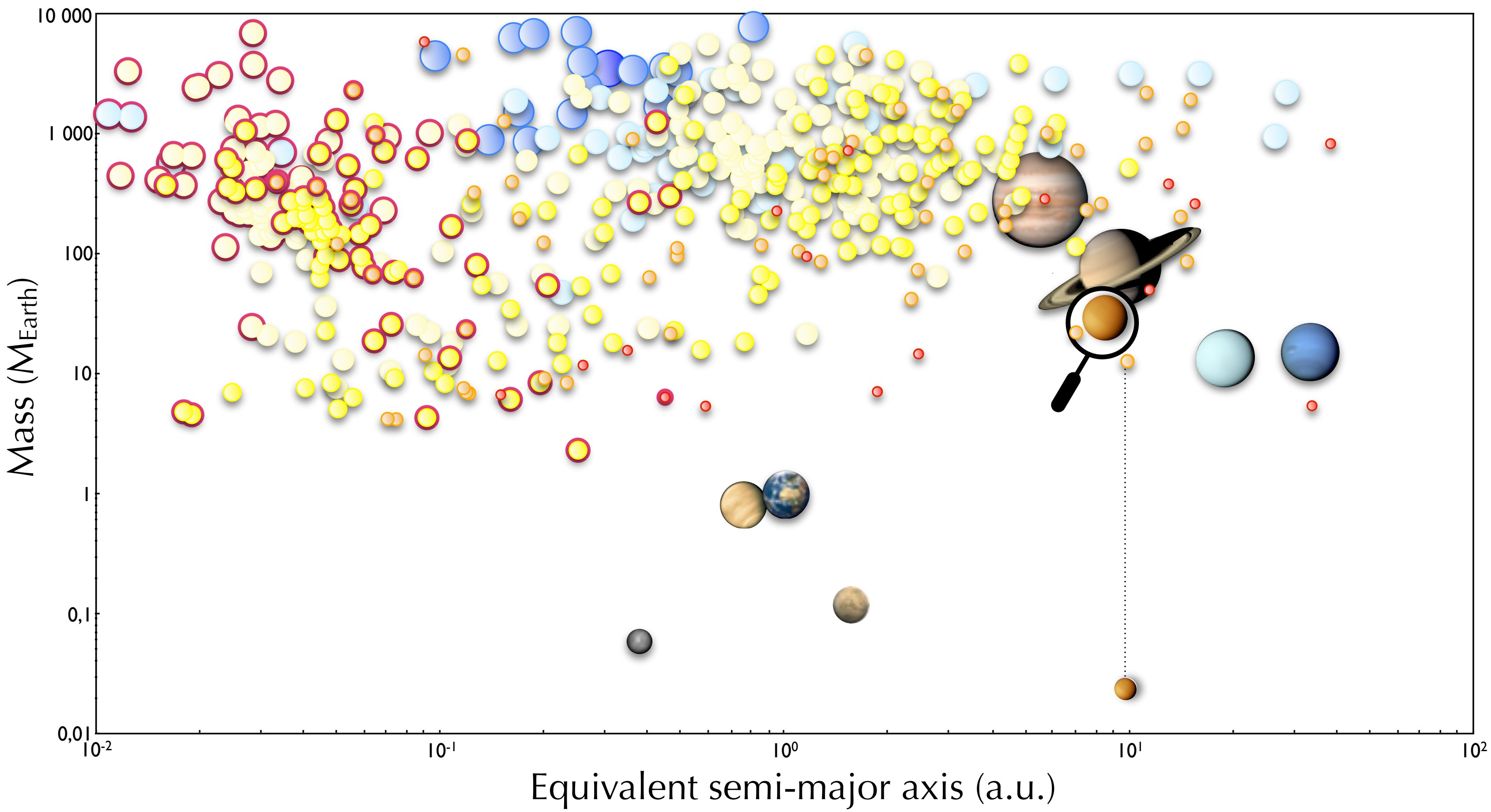
Observatoire Aquitain des Sciences de l'Univers

LAB

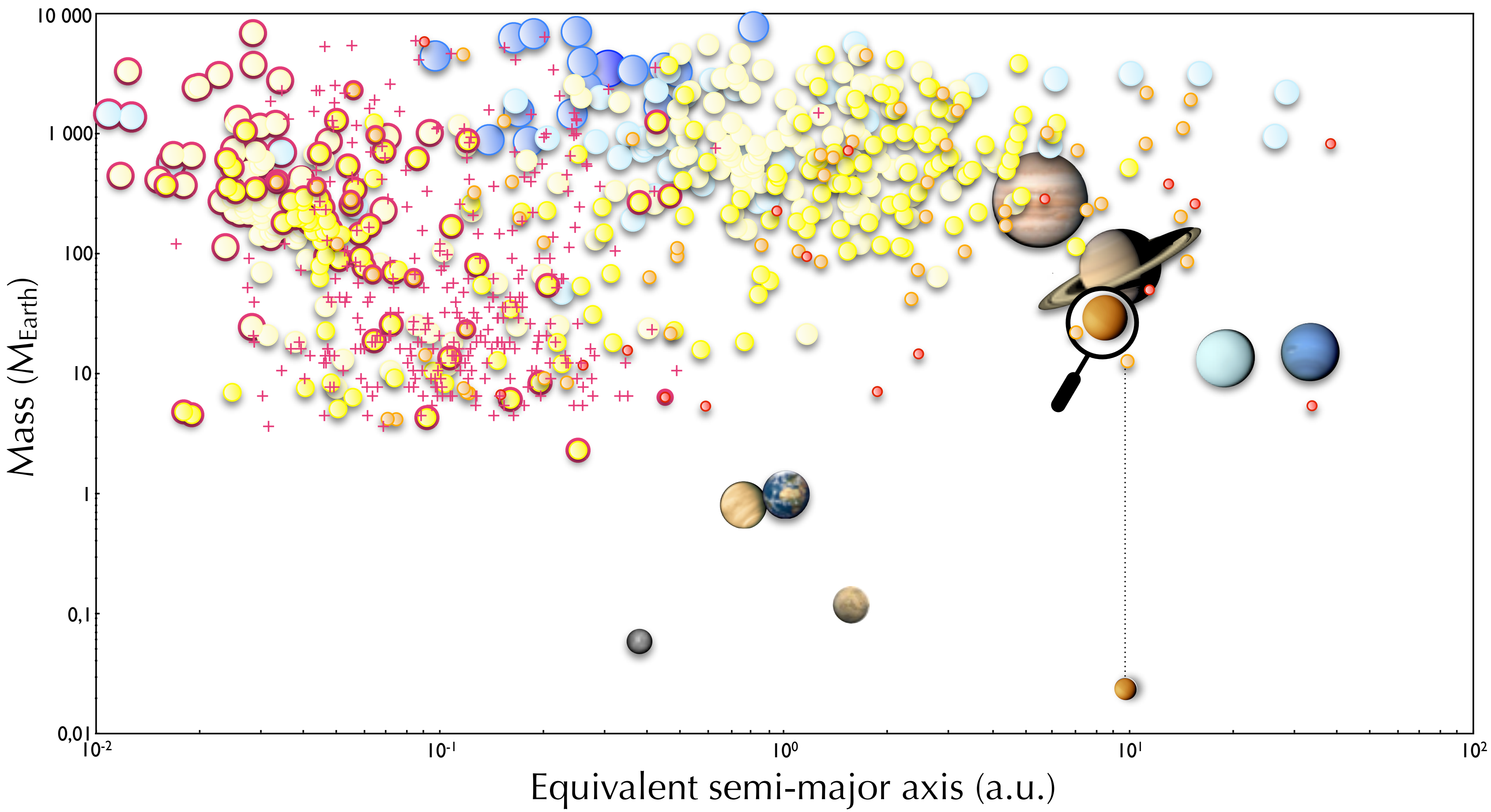
Physical/chemical diversity of (exo)planetary atmospheres



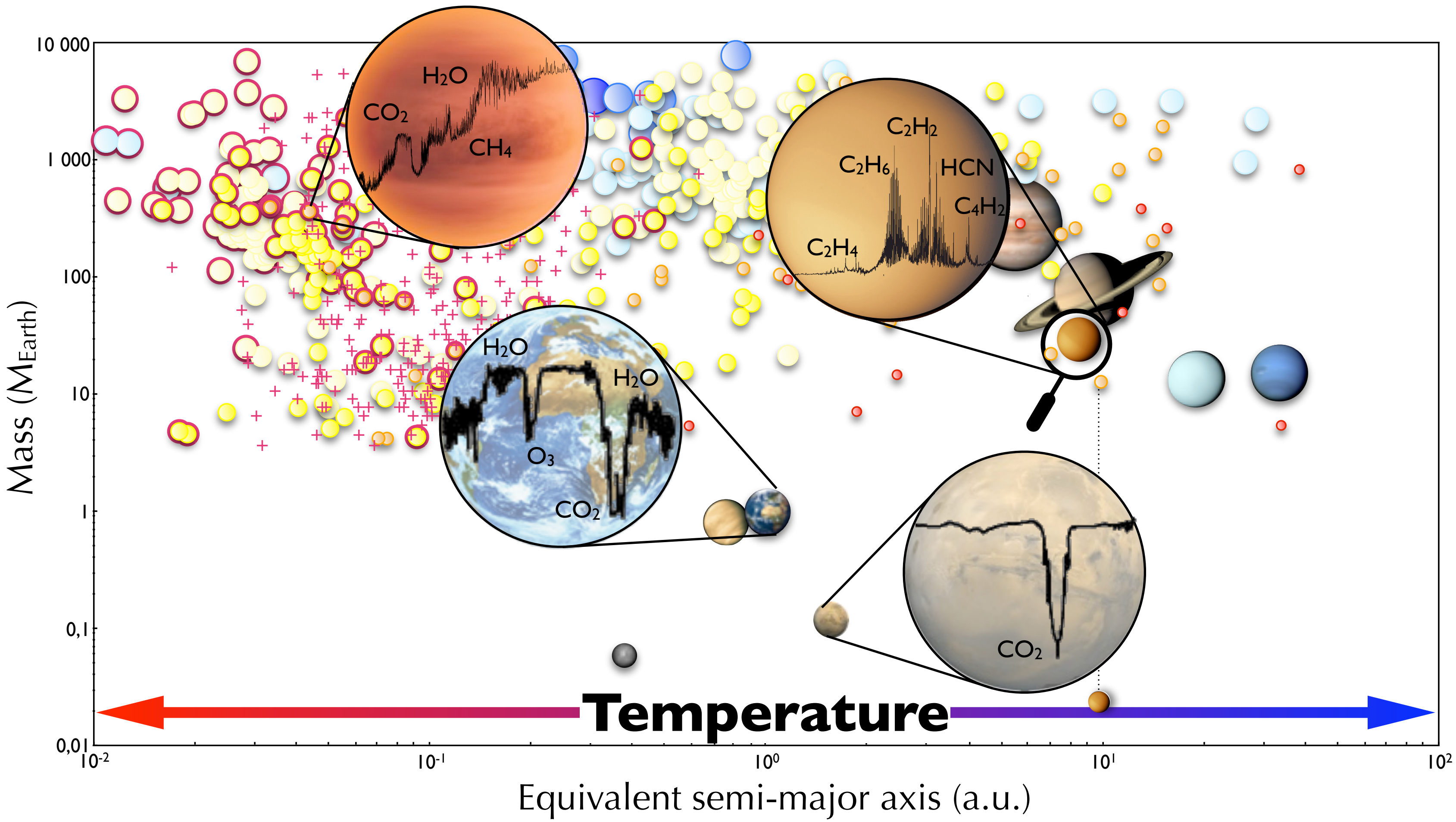
Physical/chemical diversity of (exo)planetary atmospheres



Physical/chemical diversity of (exo)planetary atmospheres



Physical/chemical diversity of (exo)planetary atmospheres



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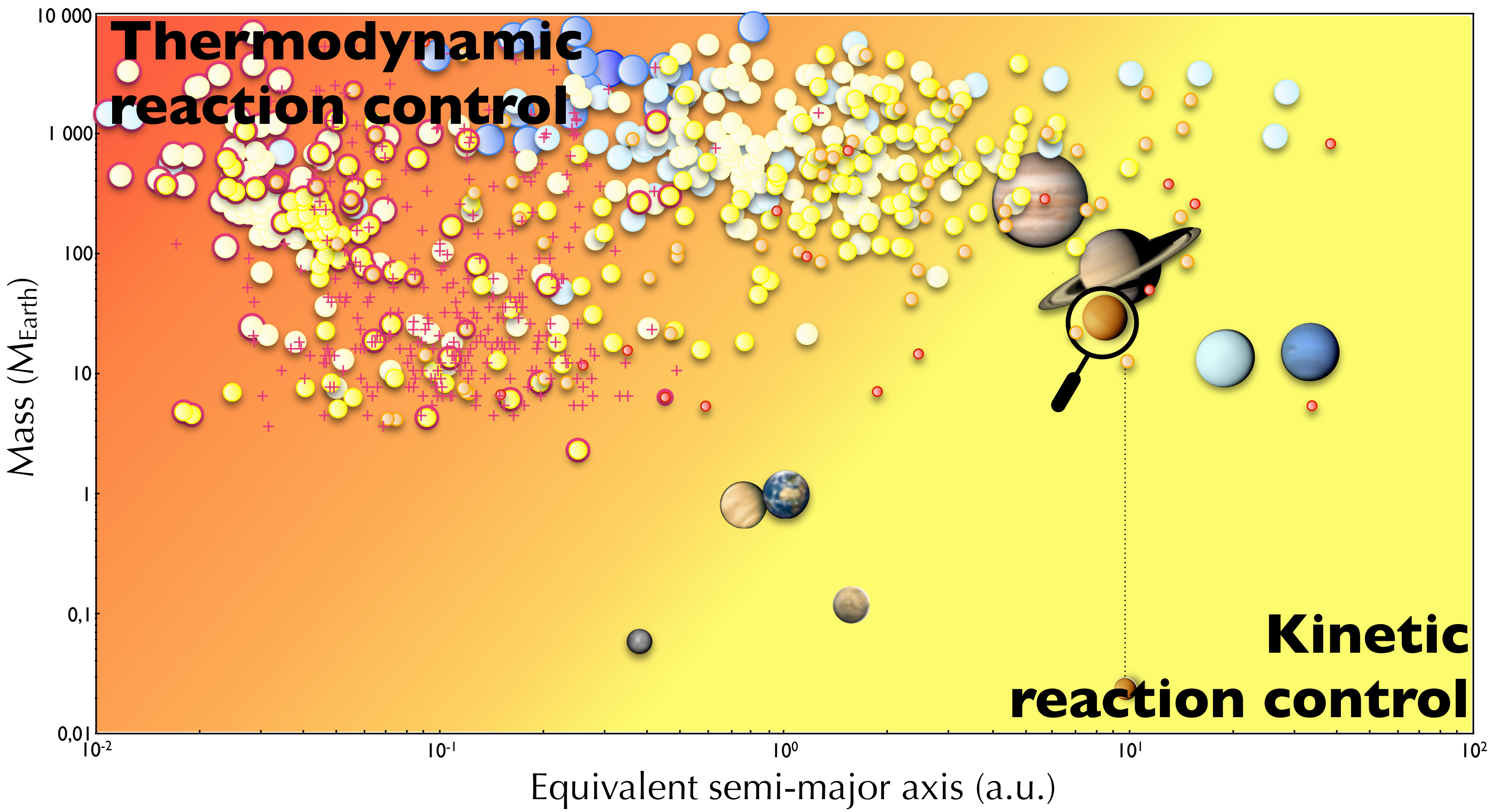

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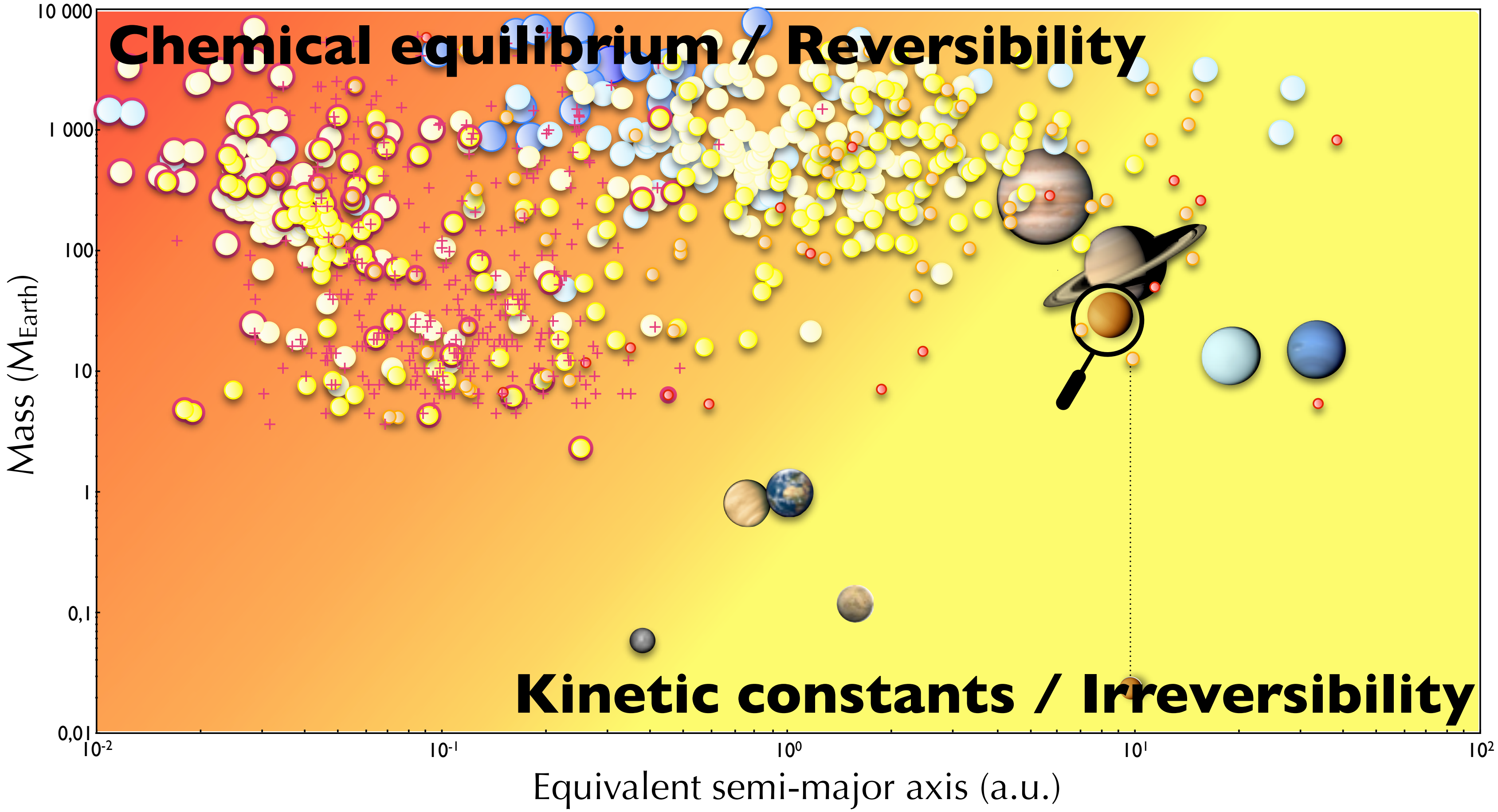

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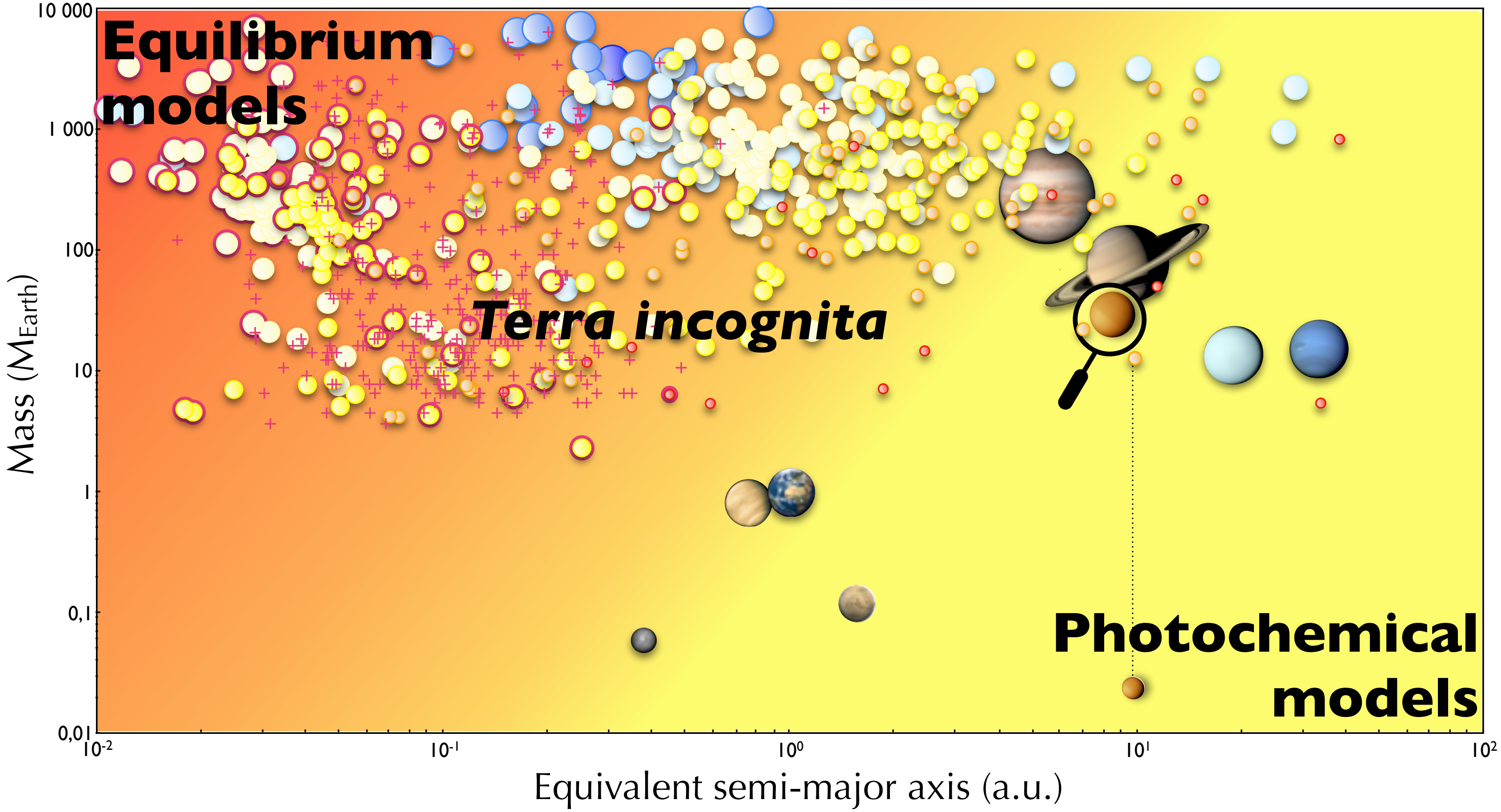
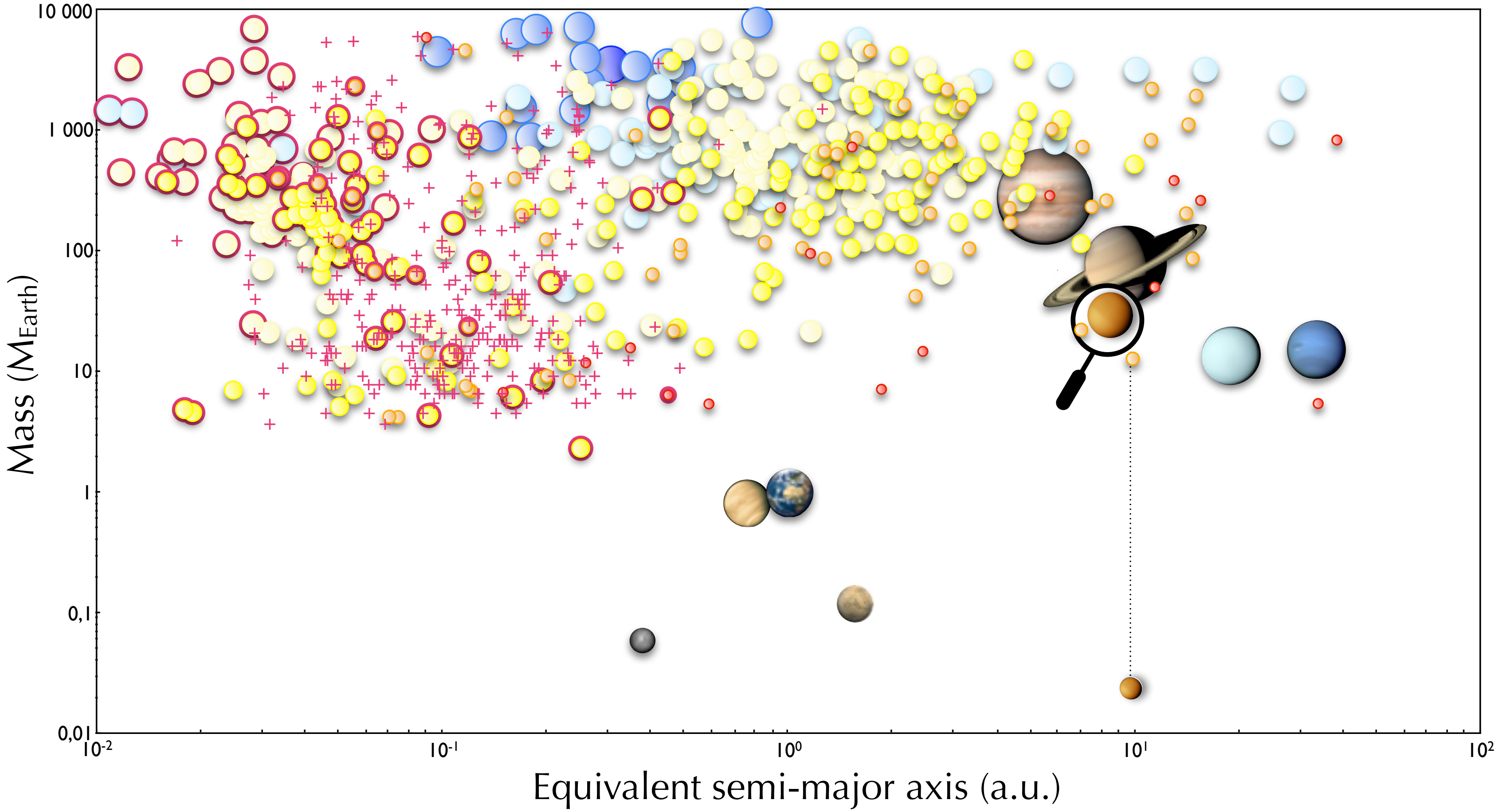
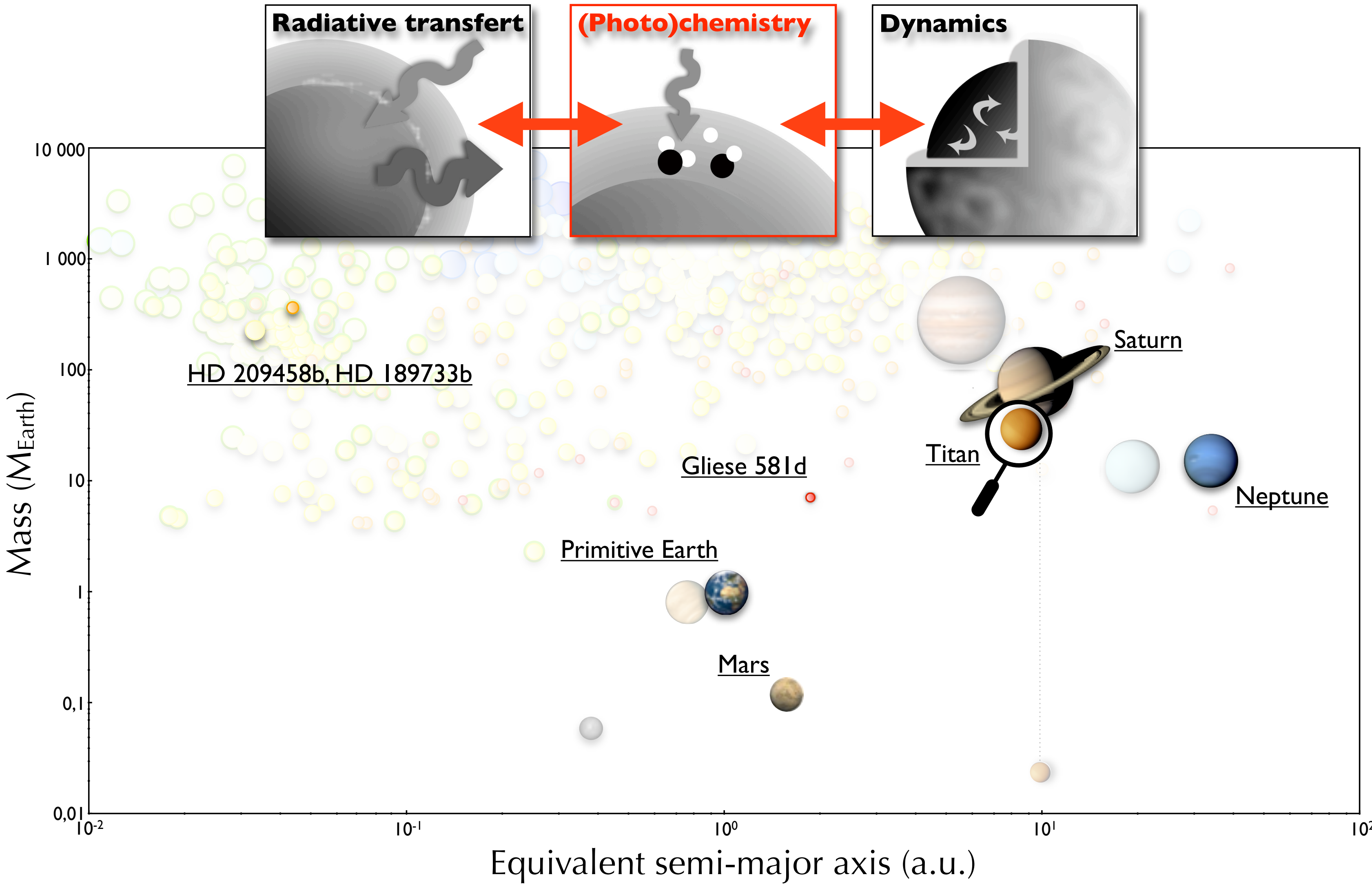


Need for a new generation of tools and databases for the physical/chemical study of (exo)planetary atmospheres



(Exo)planetary atmospheres chemical models

Eric Hébrard (LAB)



1D photochemical modeling of planetary atmospheres

- Photochemical models of interstellar or planetary atmospheres are complex ([0-3]D chemical-dynamical codes with thousands of highly coupled nonlinear equations)

- The chemical equations are based on **empirical parameters** :

$$\mathrm{AB} \xrightarrow{h\nu} \mathrm{A} + \mathrm{B} \qquad \mathrm{A} + \mathrm{B} \xrightarrow{(+\mathrm{M})} \mathrm{C} + \mathrm{D}$$

$$\sigma_i(\lambda, T) \quad q_{i,j}(\lambda, T) \qquad k_i(T) = \alpha_i(\frac{T}{300})^{\beta_i} \exp(-\frac{\gamma_i}{T})$$

Photodissociations — Neutral-neutral reactions

- These empirical parameters are obtained from experiments, calculations and/or **extrapolations** :

  ☞ They are always evaluated with **[[very] large] uncertainty**

  ☞ In some conditions, estimated parameters are numerous

  Ex : in Titan photochemical models, less than 10% of reaction rates are measured at relevant temperatures.

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Neutral-neutral reactions

- These empirical parameters are obtained from experiments, calculations and/or [more or less [but most often less]] educated-guessed estimations :

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  ☞ Most of the cases, **extrapolations** of these parameters are mandatory

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(Exo)planetary atmospheres chemical models

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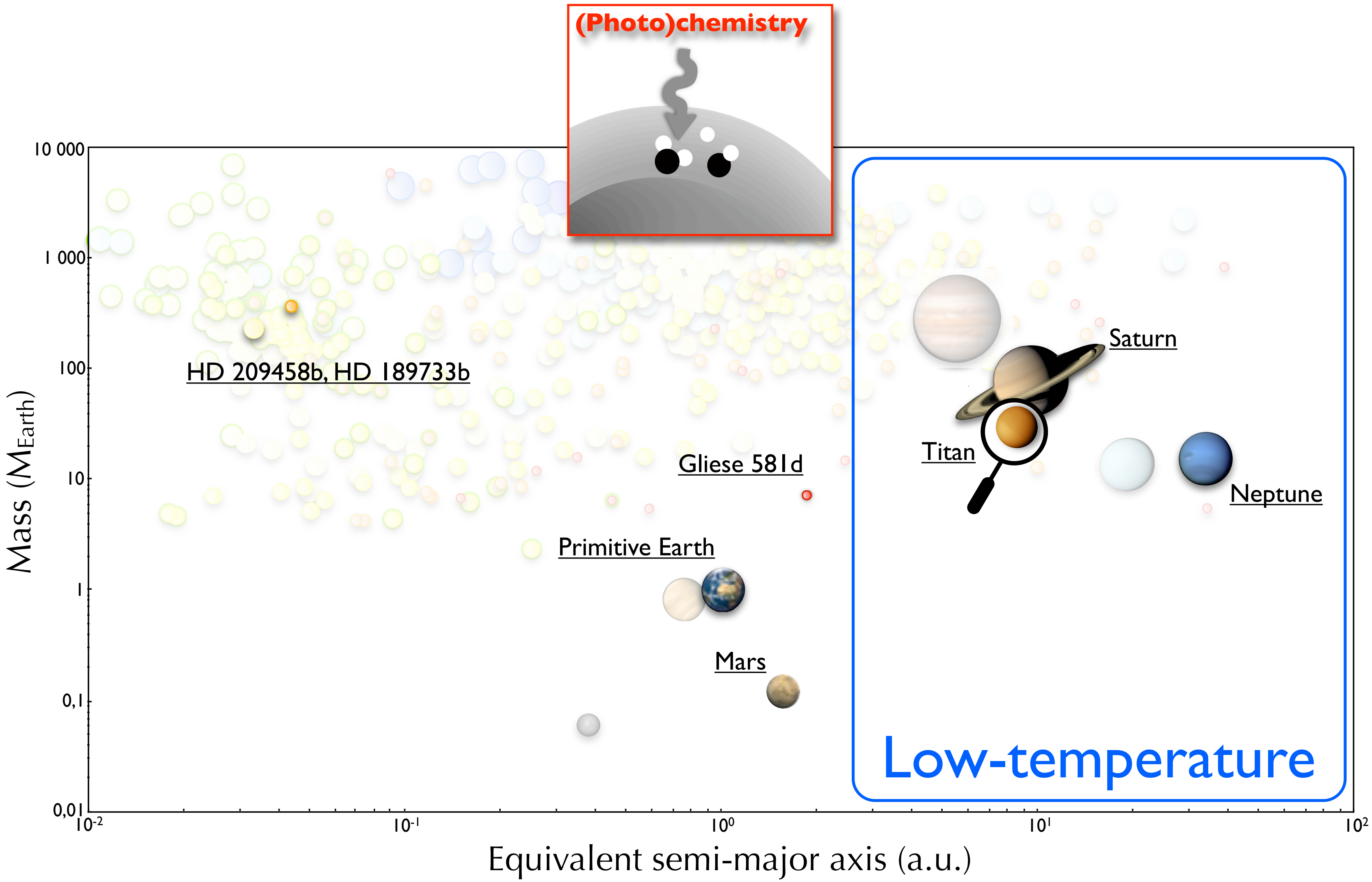

1D photochemical modeling of planetary atmospheres

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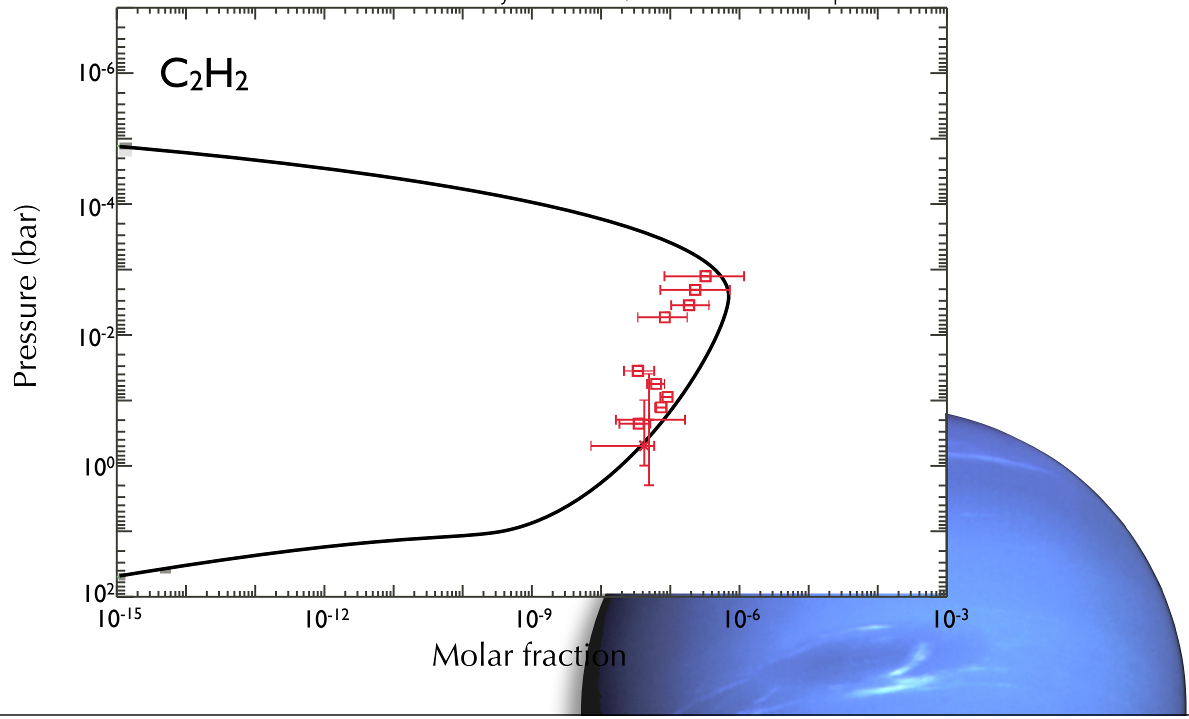
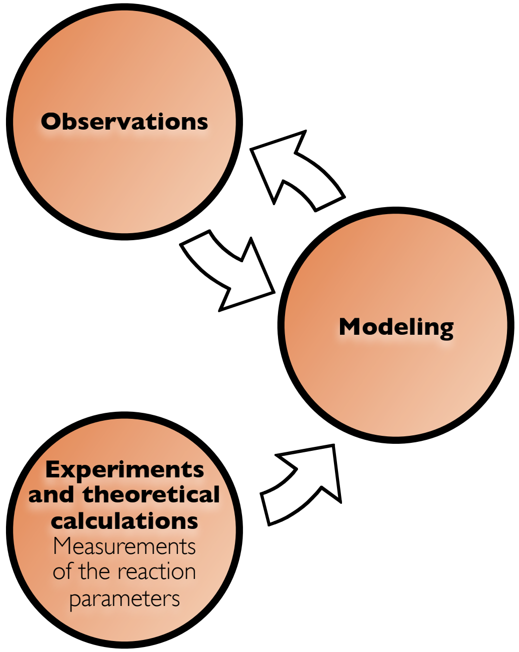
Neutral-neutral reactions

Dobrijevic et al., 2010 - Planet. Space Sci.





1D photochemical modeling of planetary atmospheres

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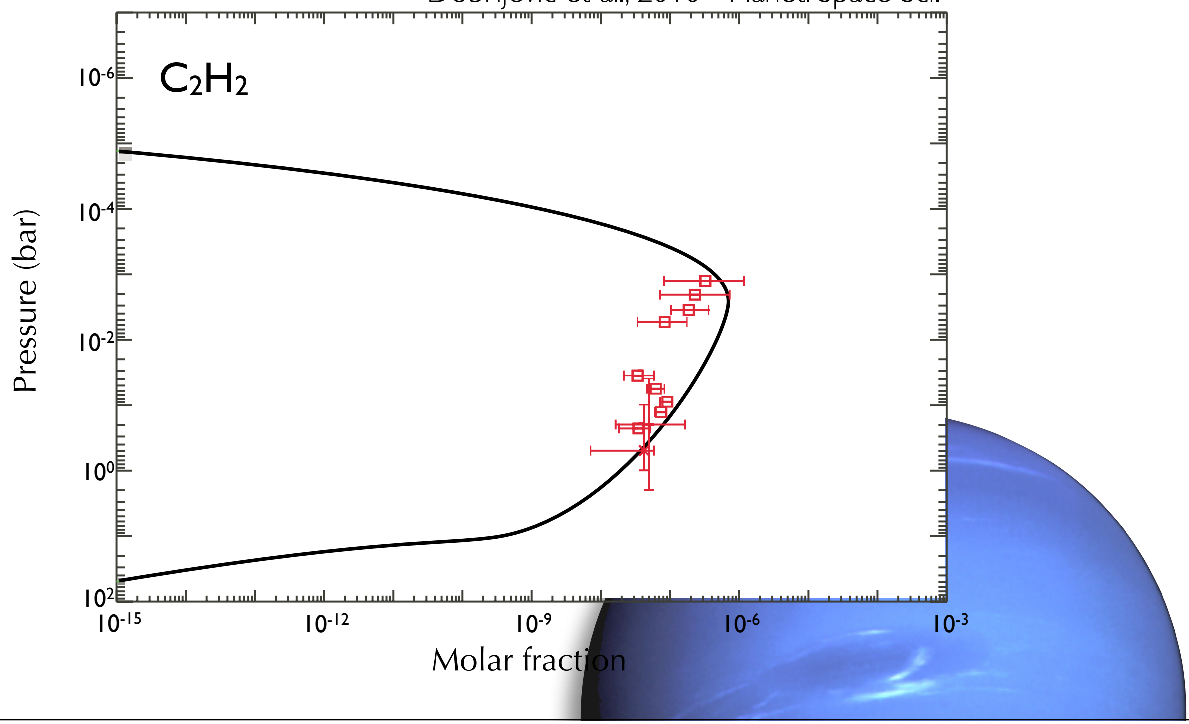

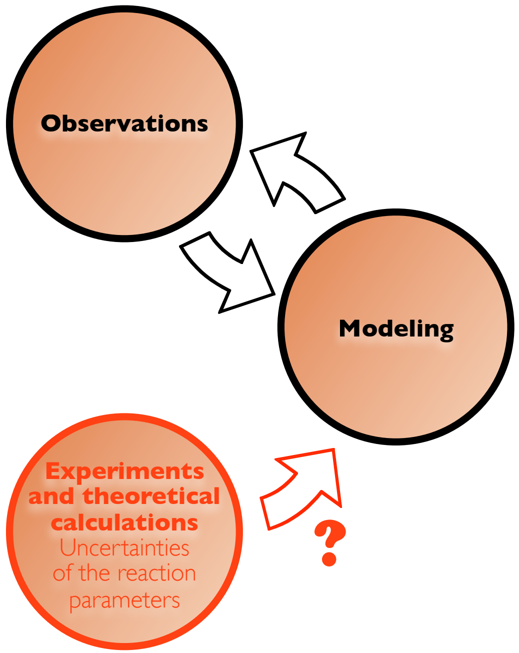

« Next-generation » photochemical modeling

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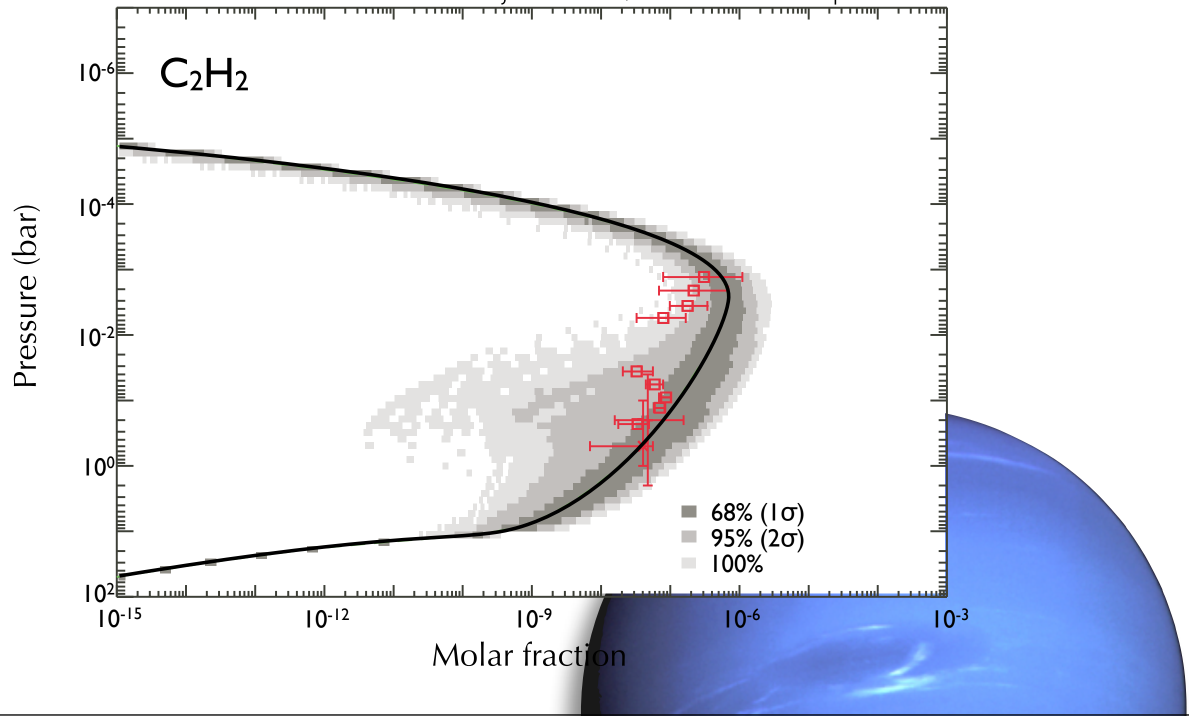

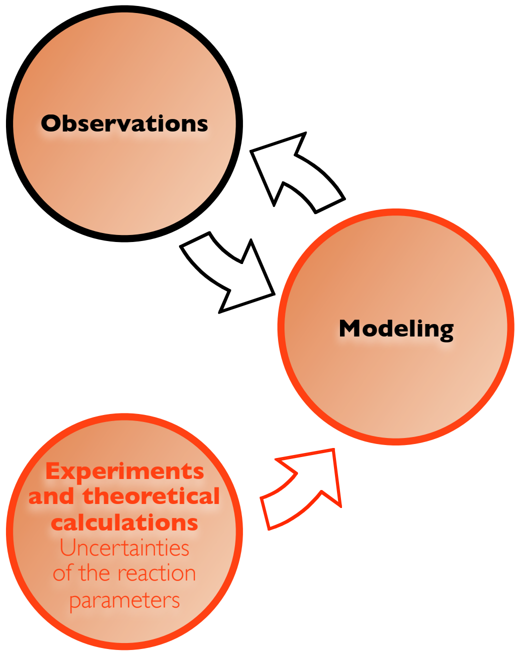

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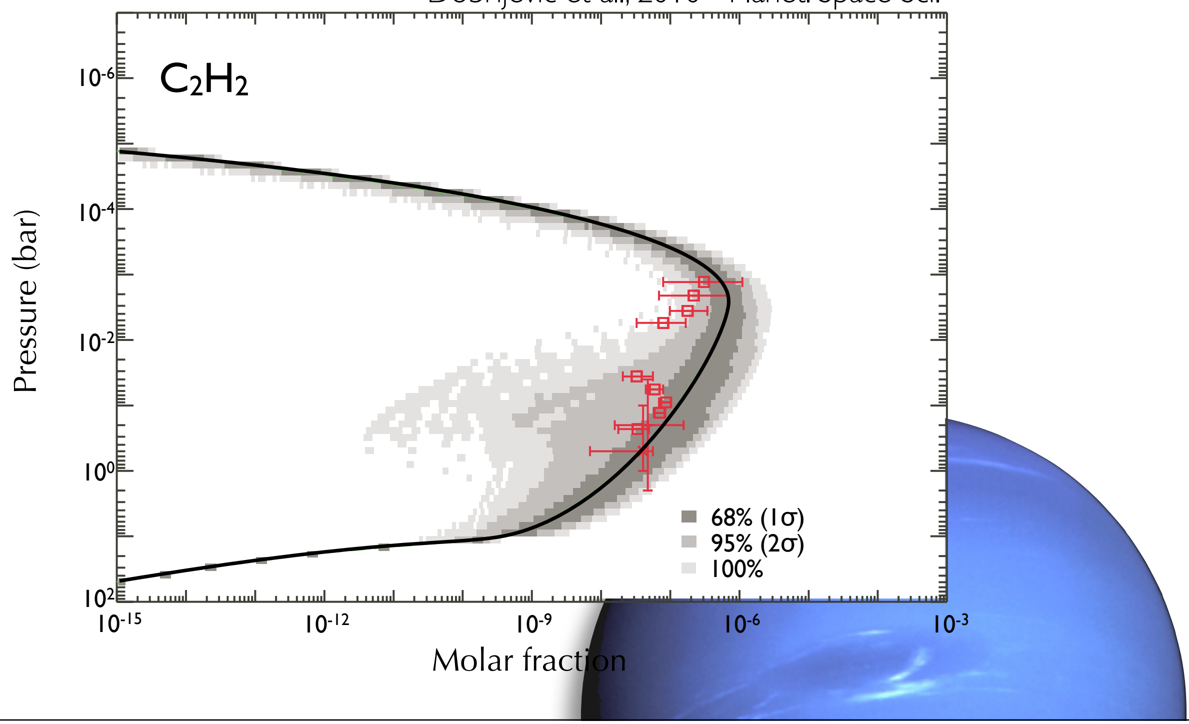

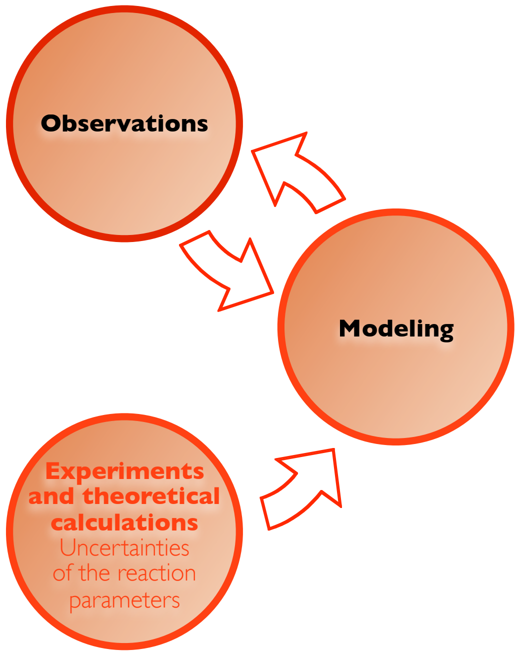

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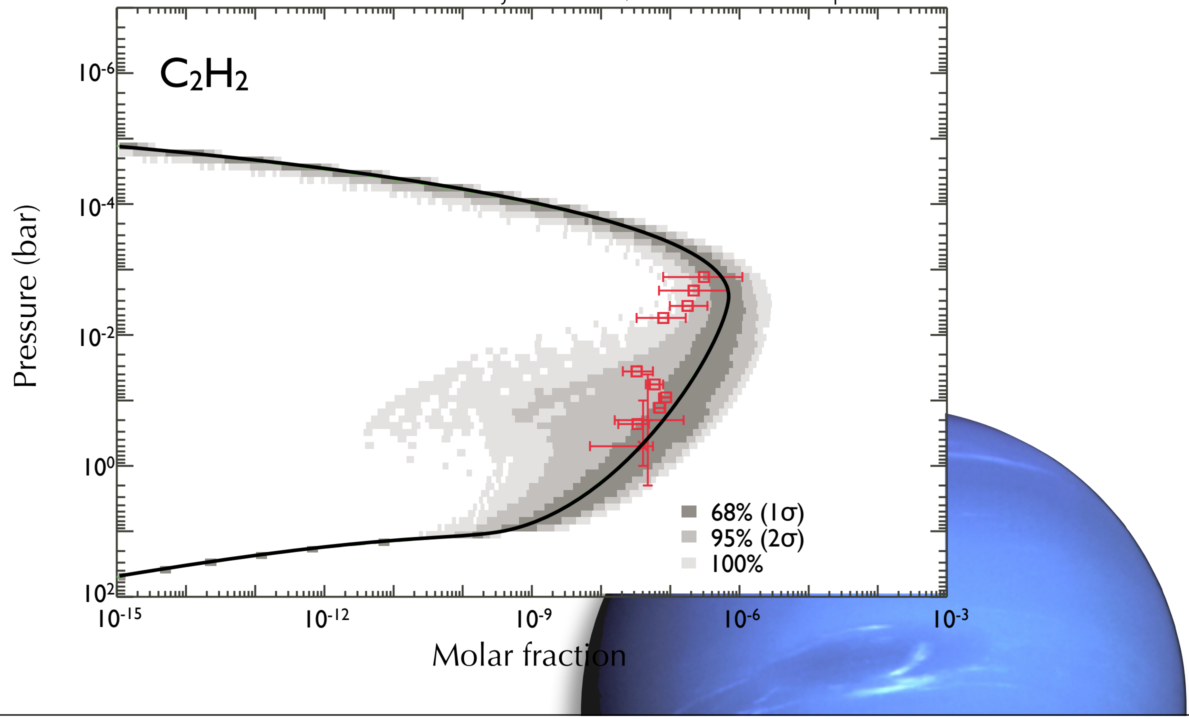

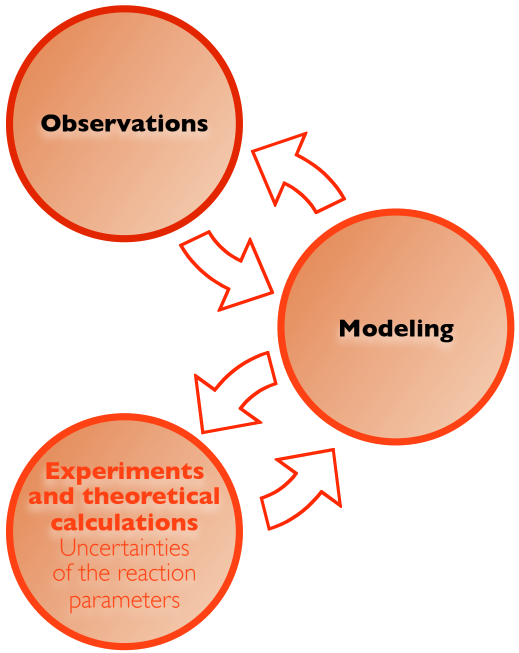

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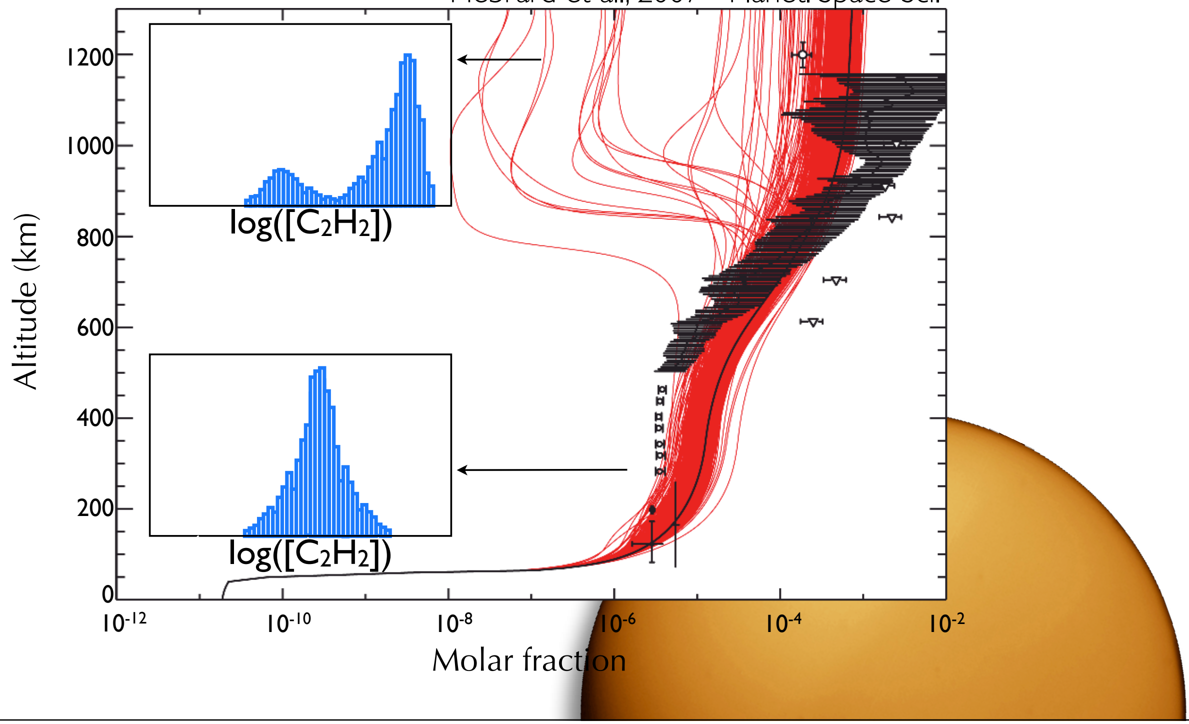
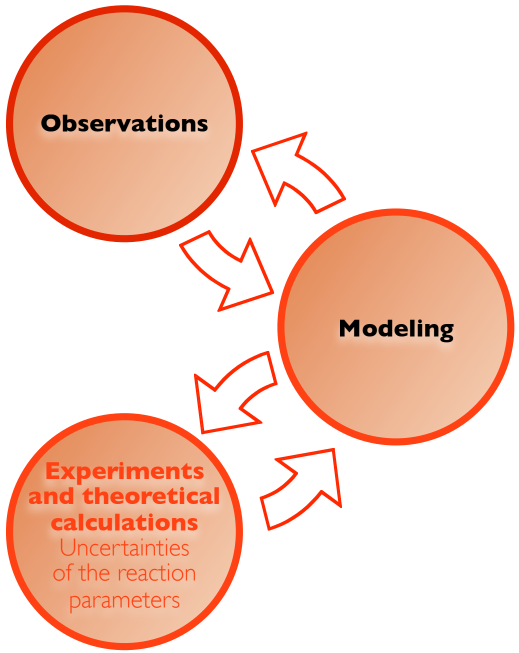
Hébrard et al., 2007 - Planet. Space Sci.





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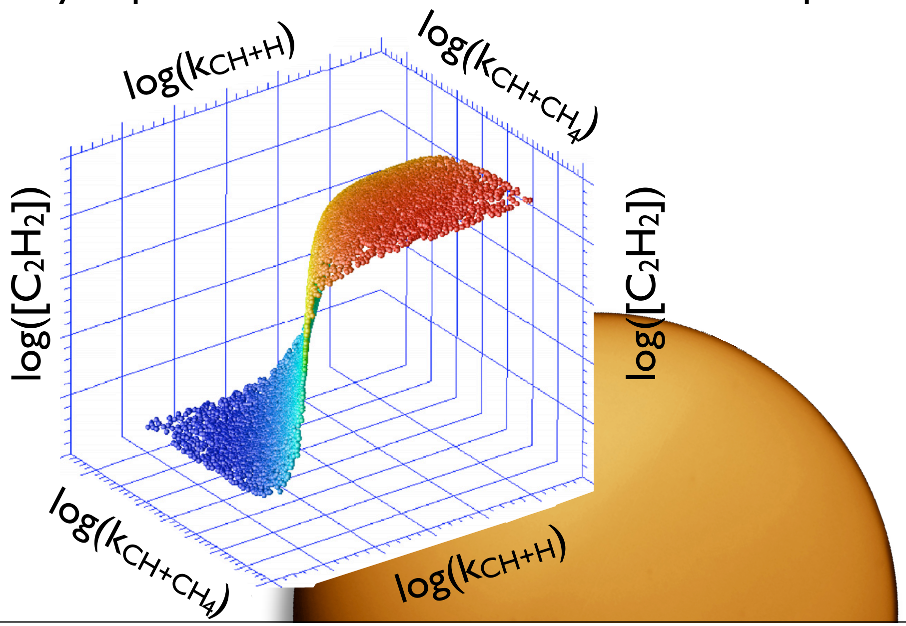
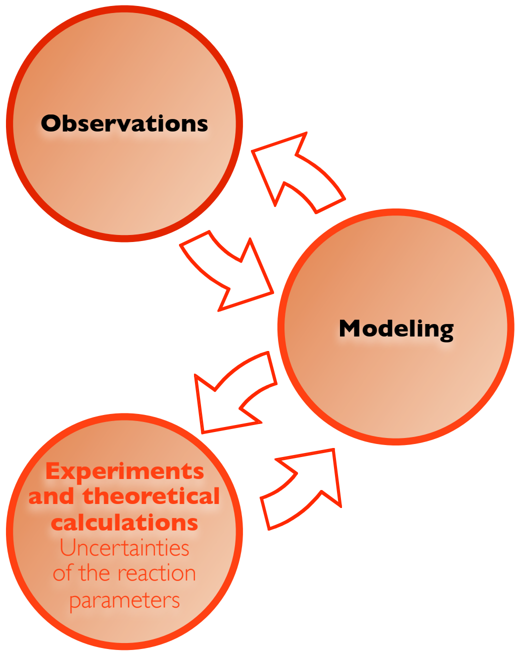
Epistemic bimodality in photochemical models of Titan's atmosphere





Evaluation and extrapolation of the uncertainties of (photo)chemical parameters

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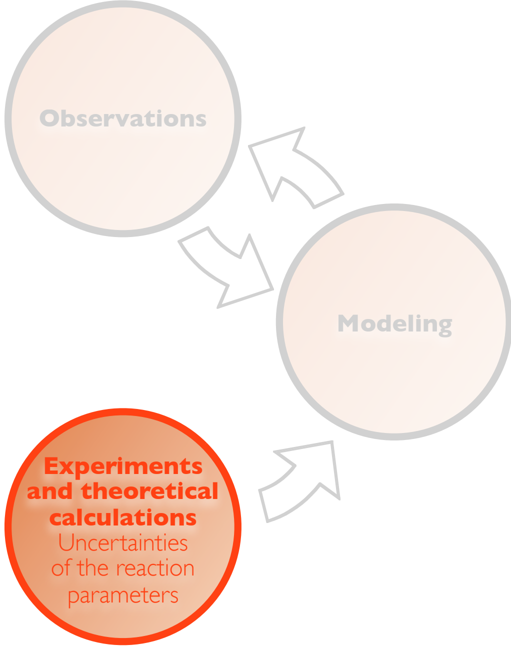

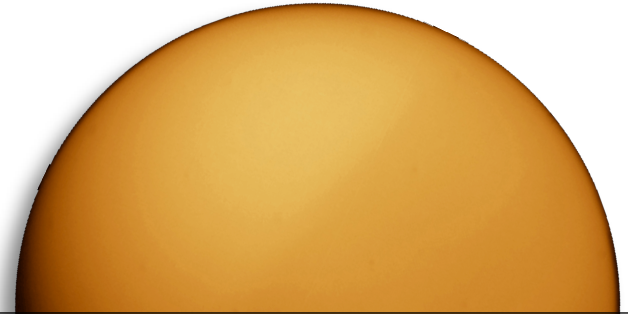

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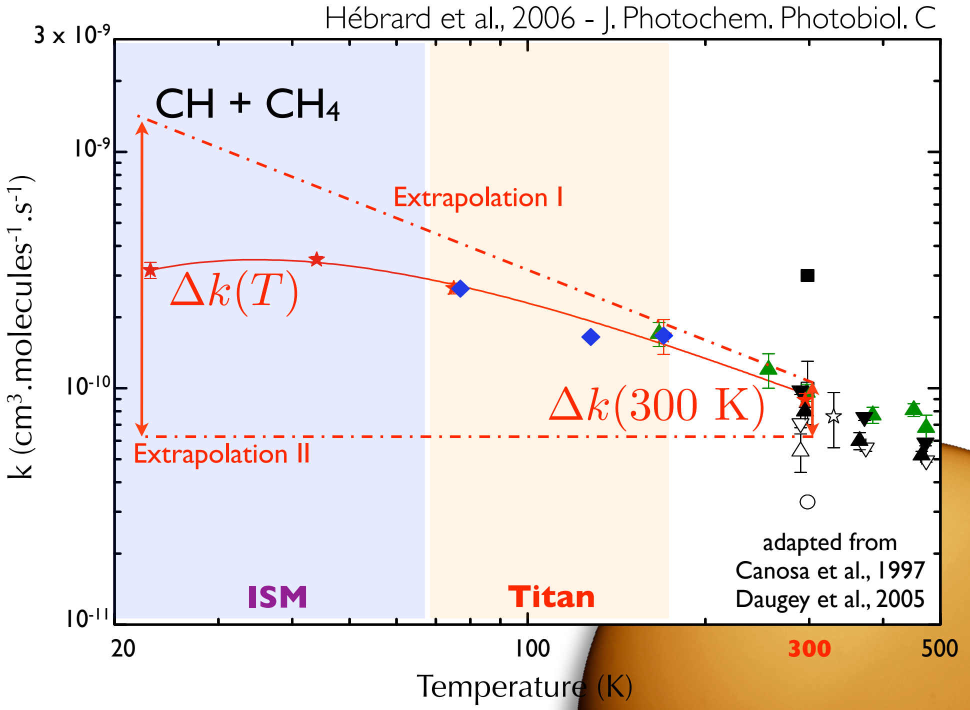

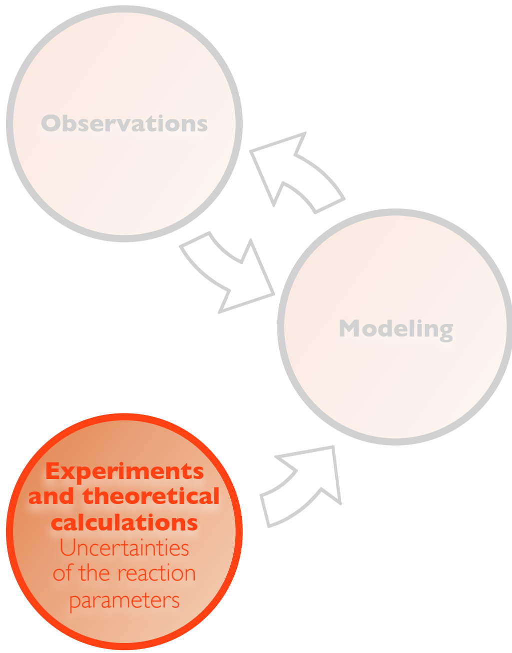

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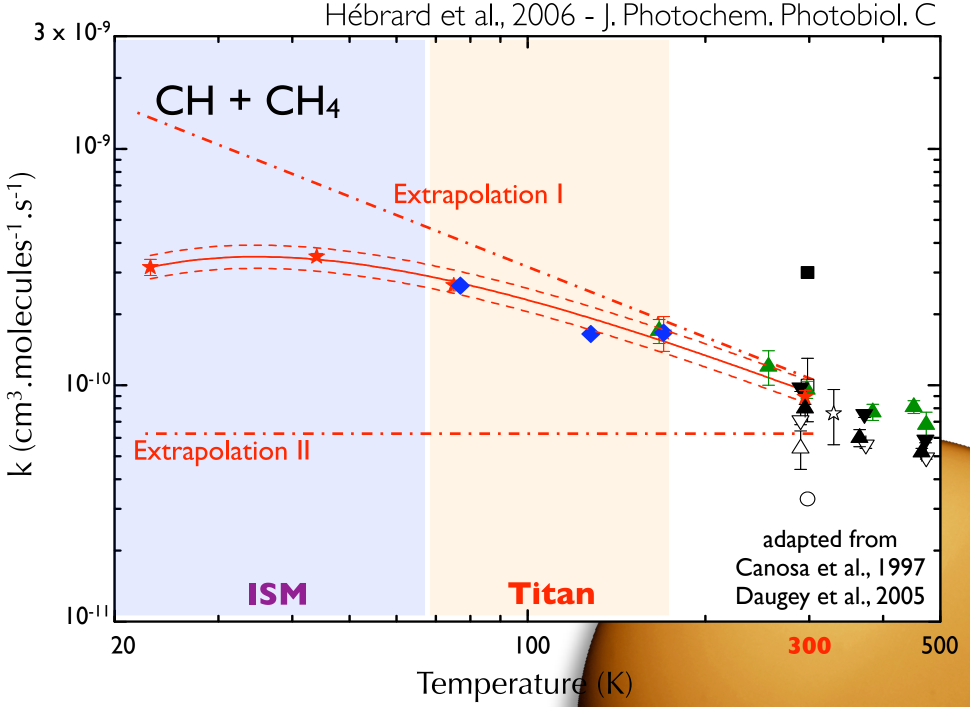
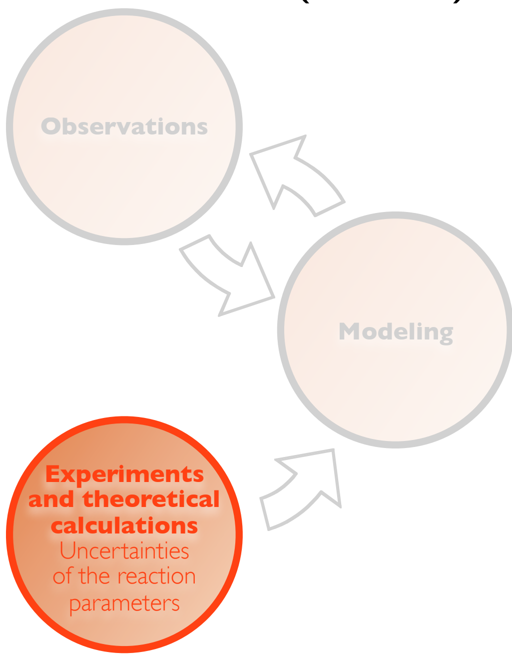
$$F_{k_i(T)} = F_{k_i(300\,K)} \times \exp\left|g\left(\frac{1}{T} - \frac{1}{300}\right)\right|$$

Poster 3.105
Valentine Wakelam
(LAB/OASU)

Hébrard et al., 2006 - J. Photochem. Photobiol. C





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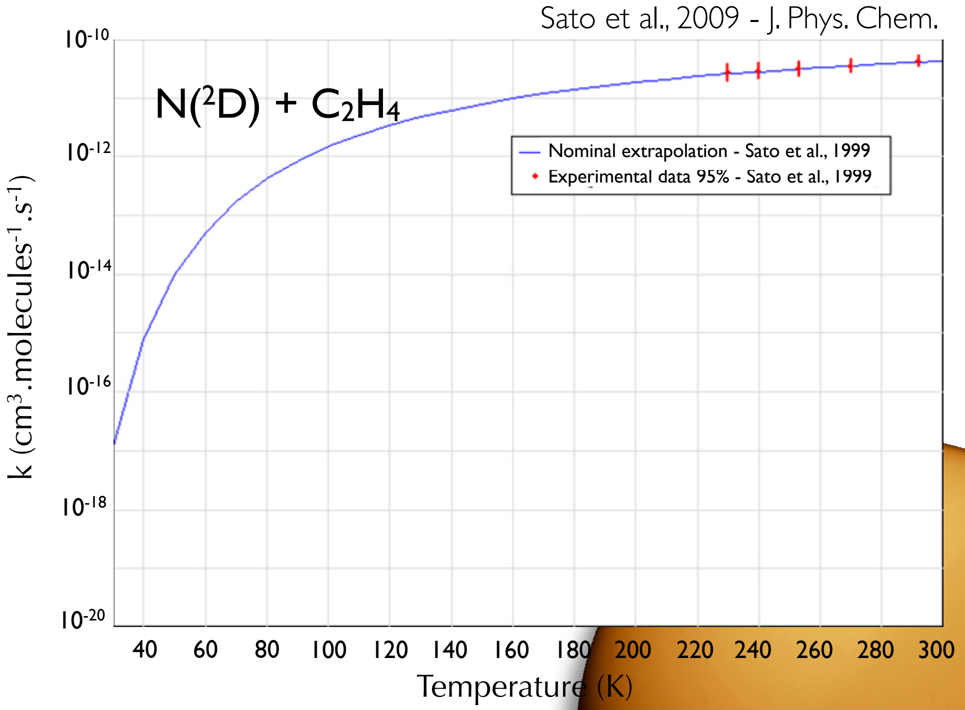

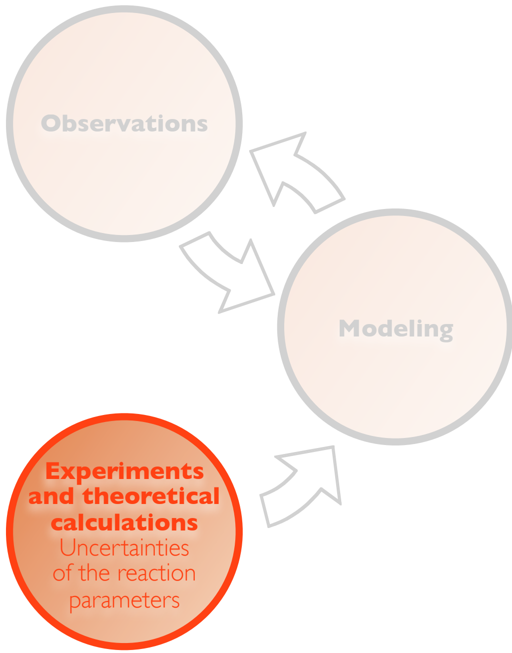

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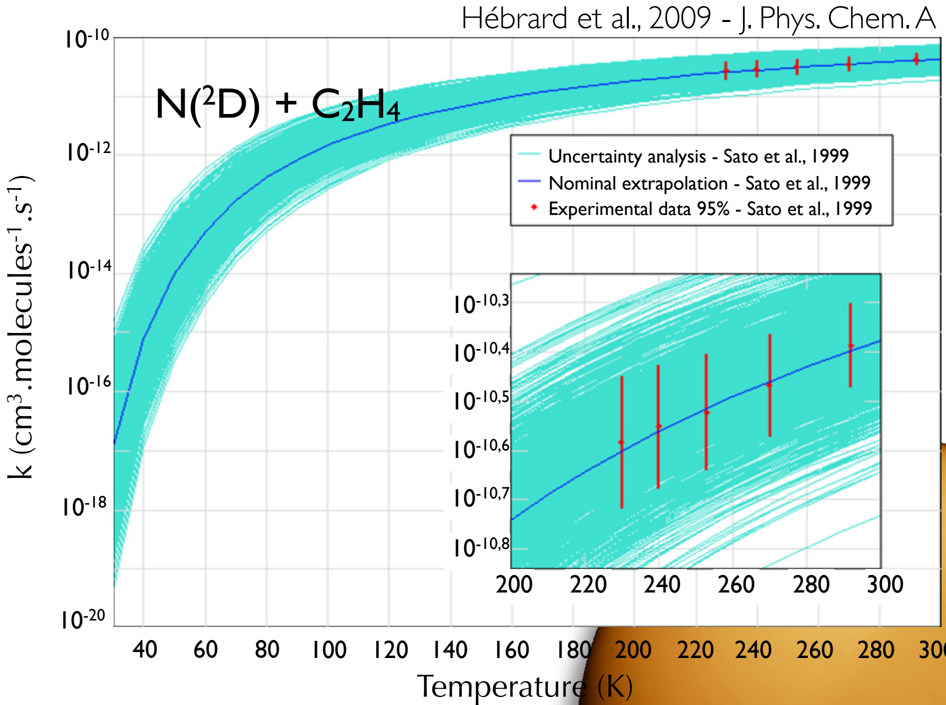

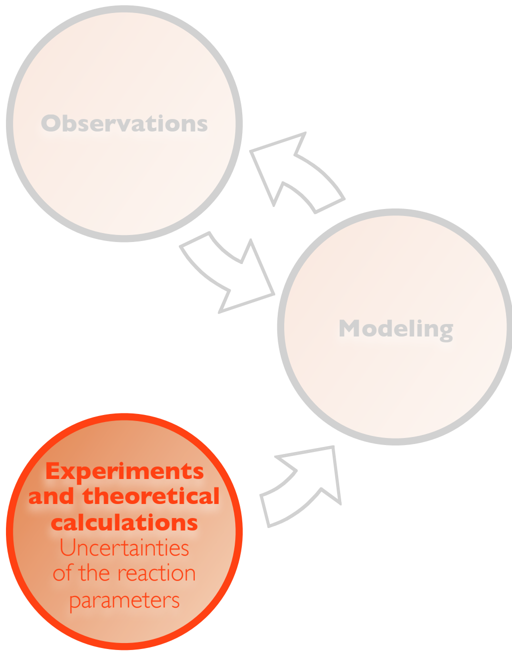

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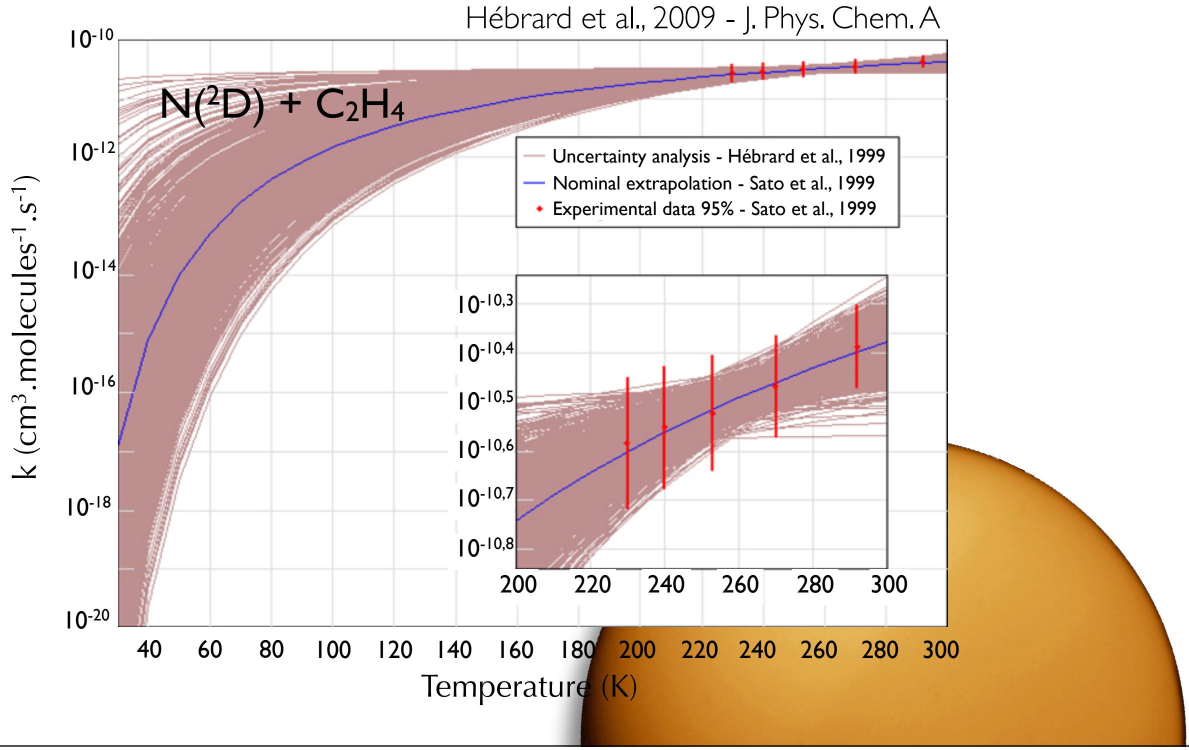
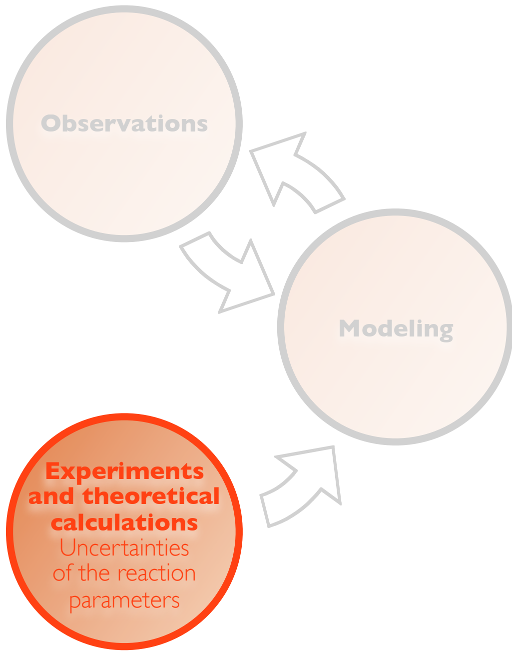
Hébrard et al., 2009 - J. Phys. Chem. A





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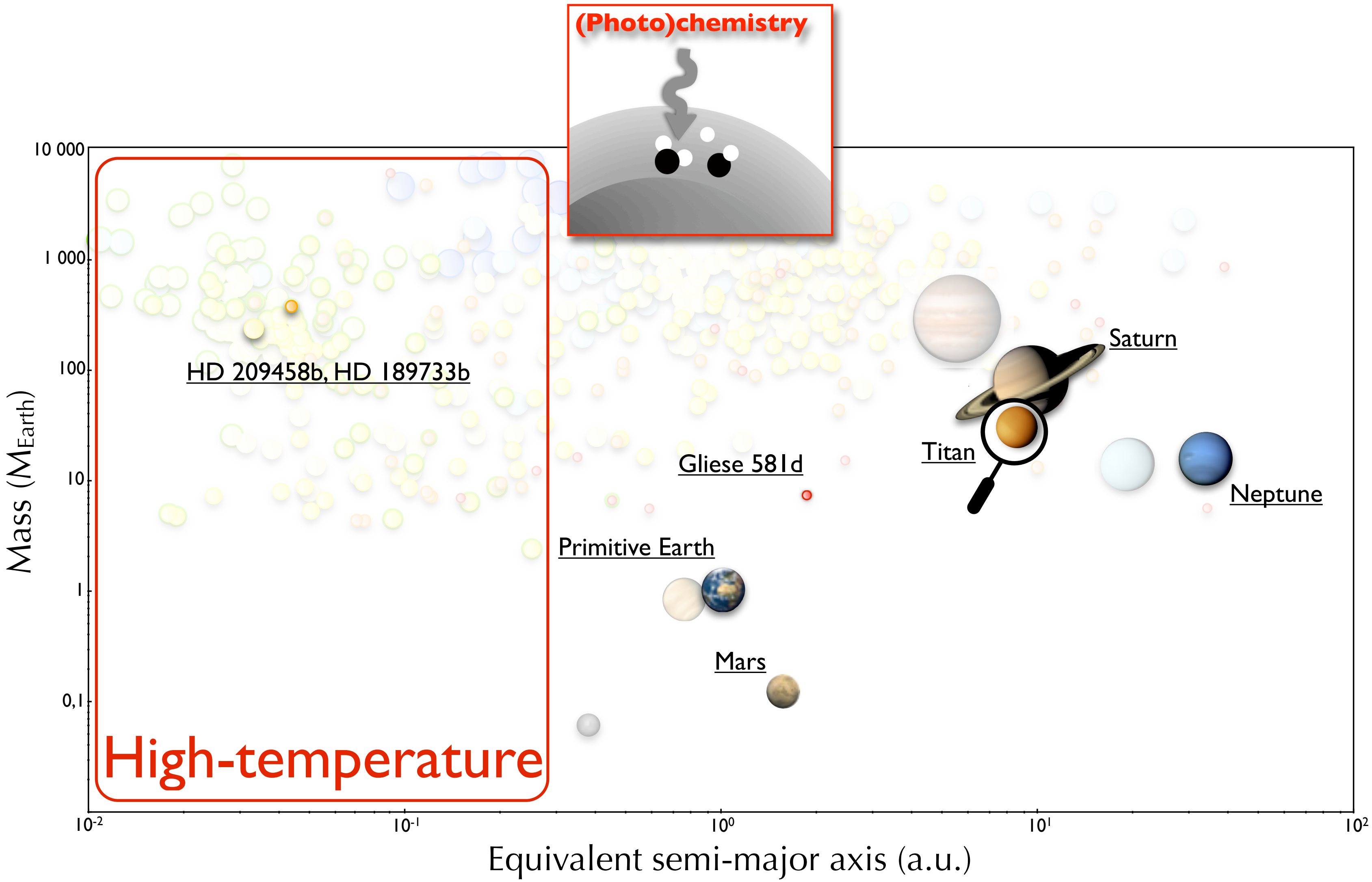


PhotoChemistry

In the upper/cold atmospheres of the Solar System, chemical reactions are initiated by radicals UV-induced production.

$$A + h\nu \longrightarrow A^*$$

Only exothermic reactions are included.

$$A + B \rightleftarrows C + D$$

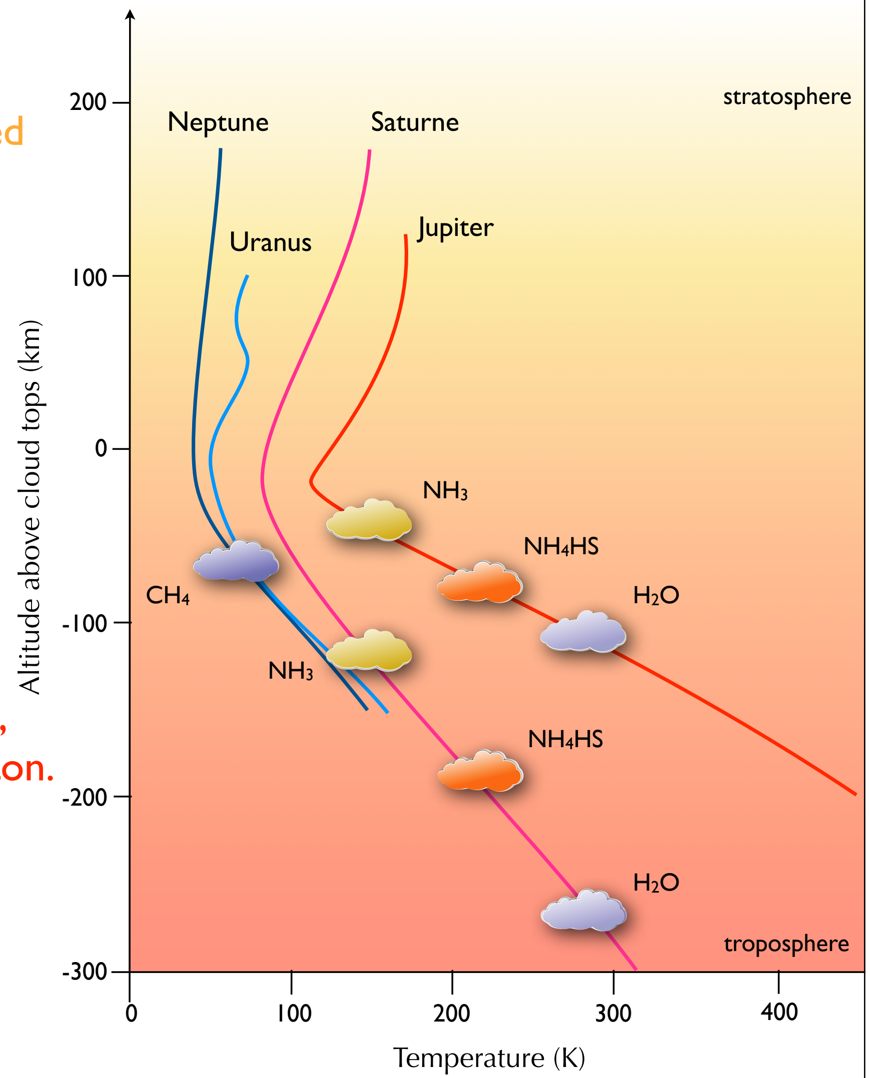
Photochemical networks are wrong at high temperatures

ThermoChemistry

In the deep/hot layers of the giant planet atmospheres of the Solar System, endothermic reactions take place. There is no UV photon.

$$A + B \rightleftarrows C + D$$

Thermochemical networks are unable to take into account non-equilibrium processes (photodissociations, circulation)



Photo/Thermochemistry

In hot dense atmospheres subjected to high UV fluxes,
a new situation arises, in which
both photodissociations and endothermic reactions matter:

$$A + h\nu \longrightarrow A^*$$

$$A + B \rightleftarrows C + D$$

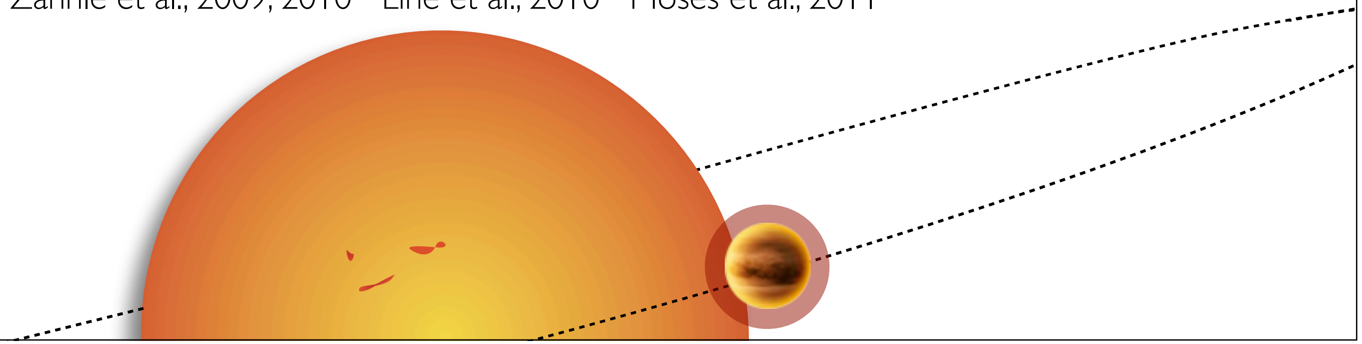
Photothermochemical networks evolve towards thermodynamic equilibrium when photodissociations and circulation are turned off.

All reactions must be balanced

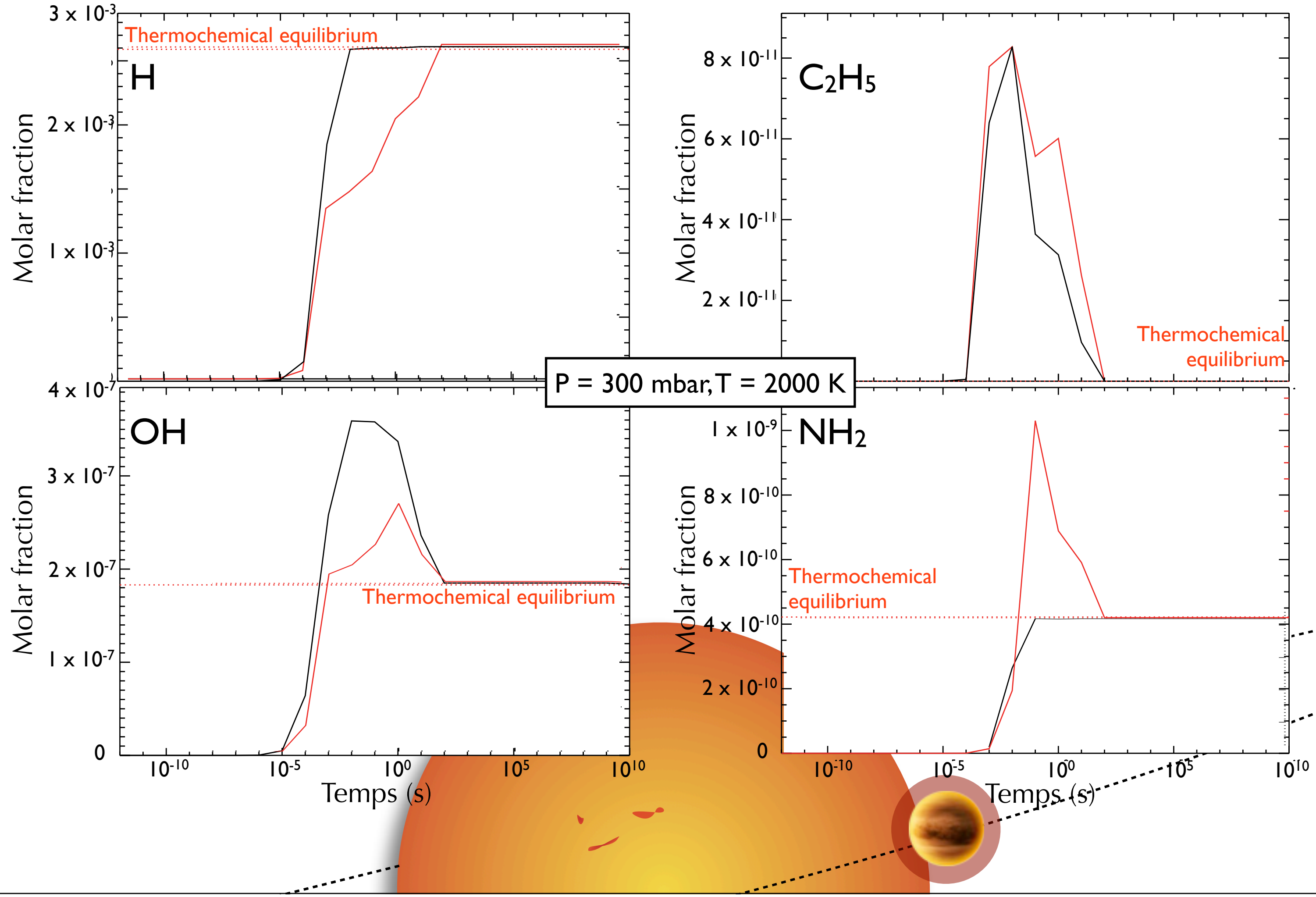
$$A + B \underset{k_{-1}(T)}{\overset{k_1(T)}{\rightleftarrows}} C + D$$

$$\begin{cases} k_1(T) = \alpha_1 (\frac{T}{300})^{\beta_1} \exp(-\frac{\gamma_1}{T}) \\ K_{eq} = \dfrac{k_1(T)}{k_{-1}(T)} = \exp\left(-\dfrac{\Delta_r G_T^0}{RT}\right) \end{cases}$$

Zahnle et al., 2009; 2010   Line et al., 2010   Moses et al., 2011



Hot Jupiter Photo/Thermochemical modeling

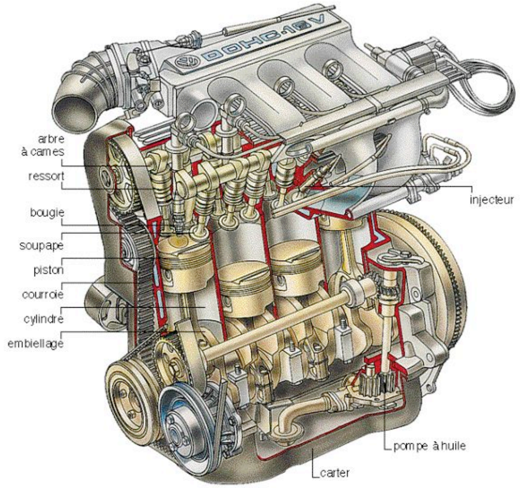


Hot Jupiter Photo/Thermochemical modeling

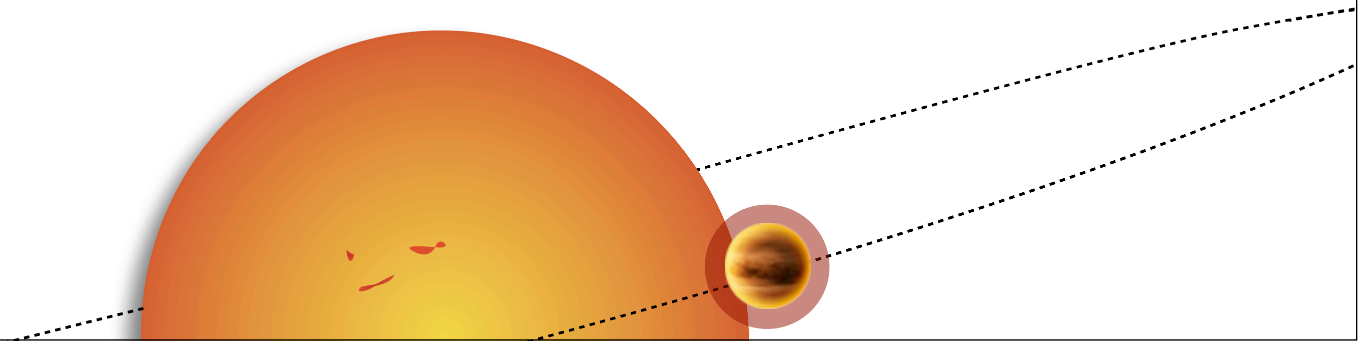
C + H + O + N + He + ...

=

+

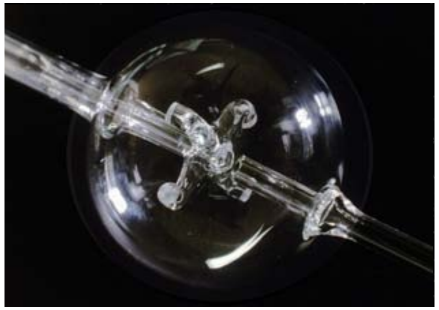


C_0-C_2 and/or C_0-C_6
+ NO_x + PAHs



(Exo)planetary atmospheres chemical models

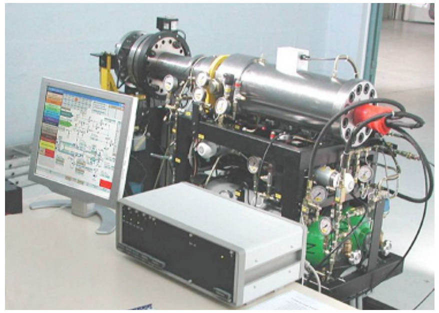
Eric Hébrard (LAB)



Perfectly Stirred Reactor

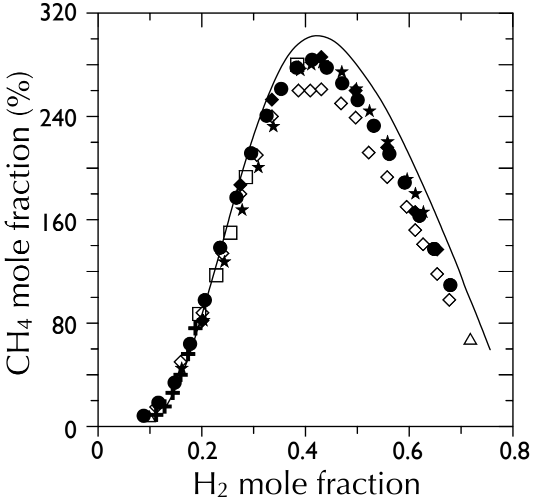
Shock Tube

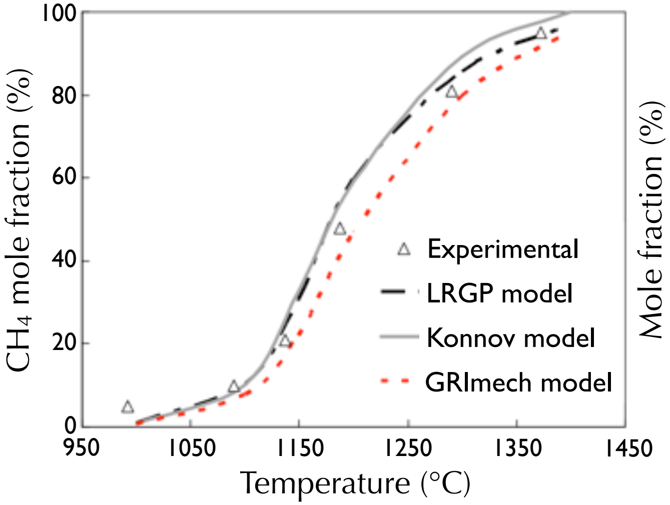
Flame speeds

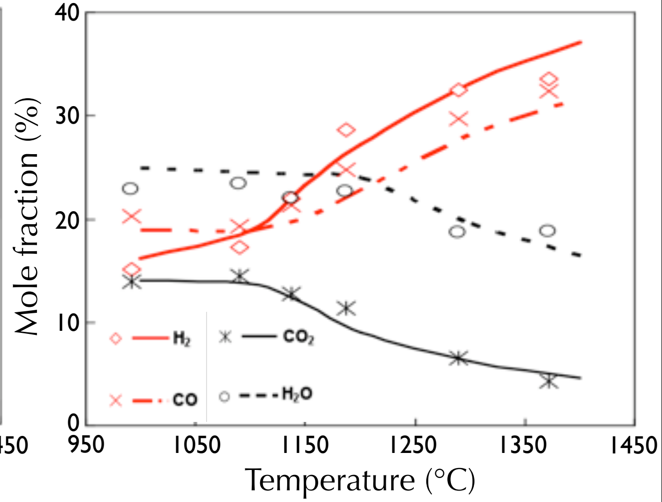


Rapid Compression Machine

LAB
Laboratoire d'Astrophysique de Bordeaux
+
LRGP
Laboratoire Réactions et Génie des Procédés

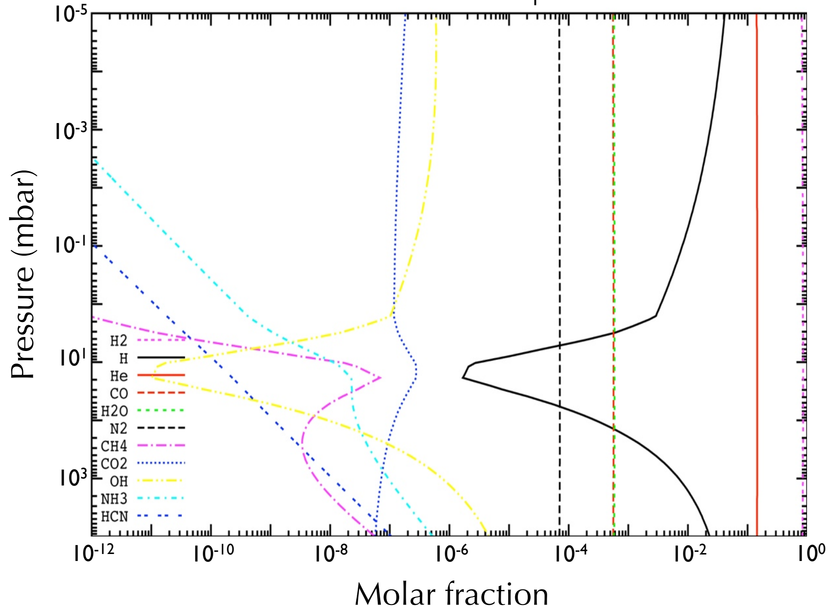




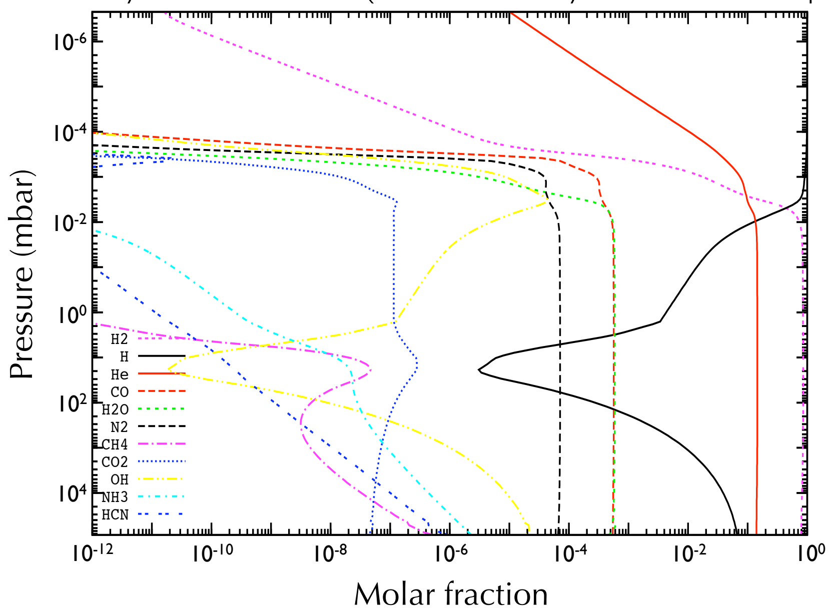


Hot Jupiter Photo/Thermochemical modeling

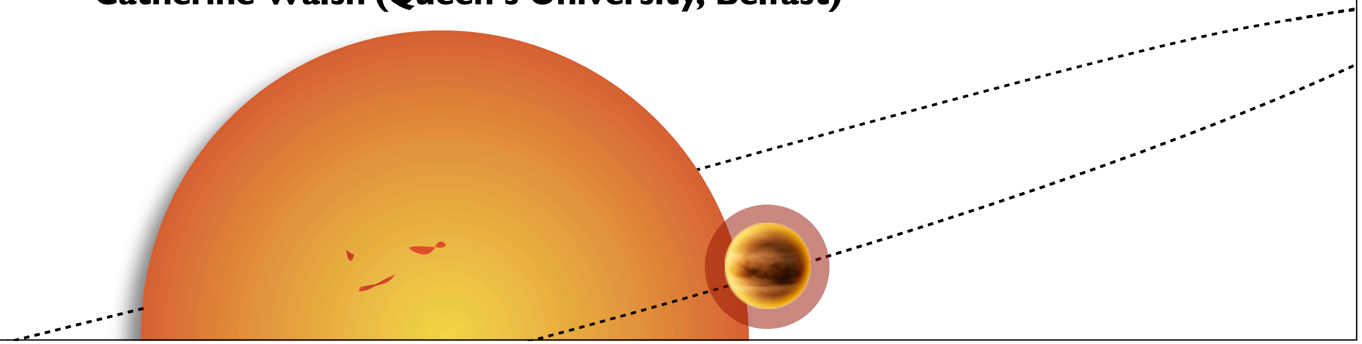
Thermochemical equilibrium



Steady-state kinetics (HT chemistry + UV + transport)



See following talk
Catherine Walsh (Queen's University, Belfast)

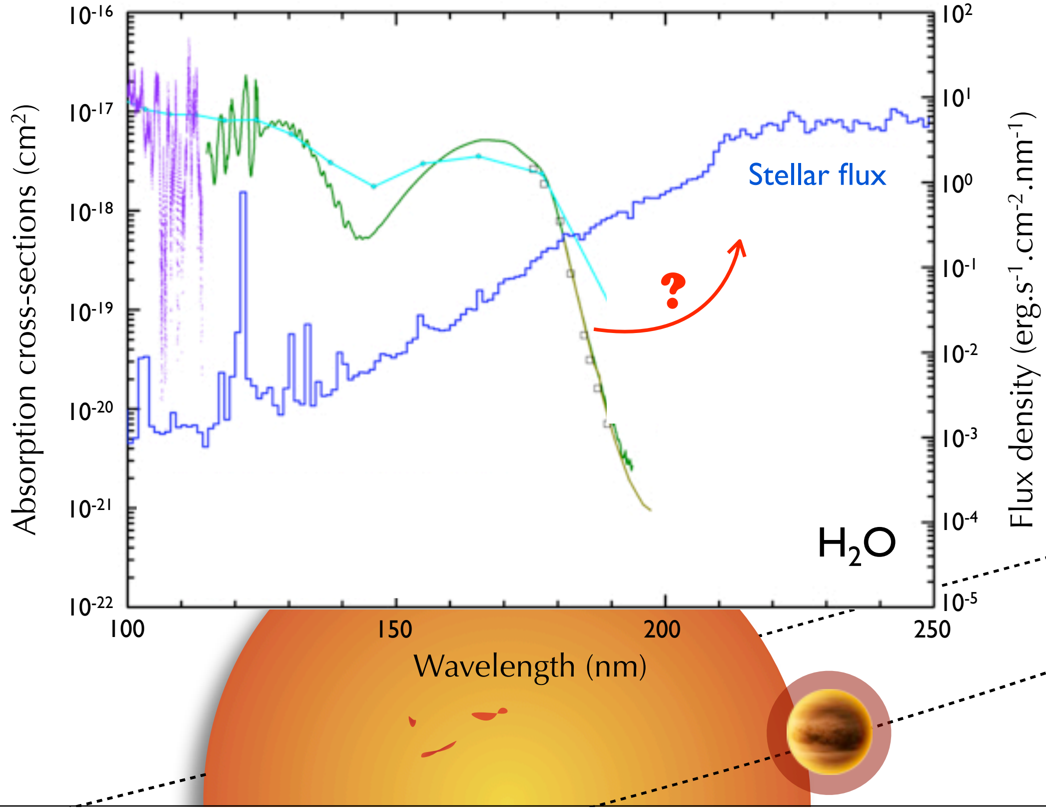


Hot Jupiter Photo/Thermochemical modeling

$$AB \xrightarrow{h\nu} A + B$$

$$\sigma_i(\lambda, T) \quad q_{i,j}(\lambda, T)$$

Need for high temperature molecular photoabsorption cross-sections



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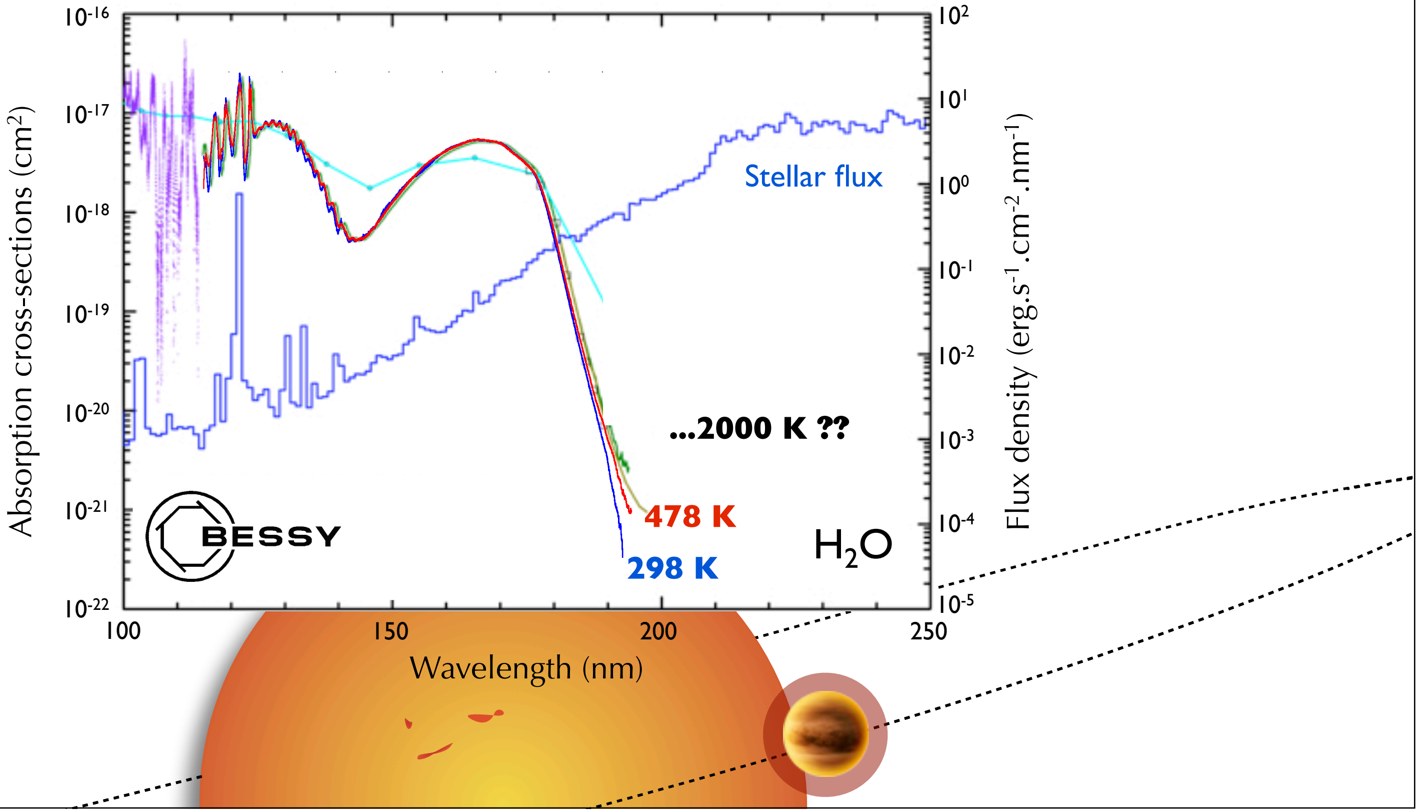

Hot Jupiter Photo/Thermochemical modeling

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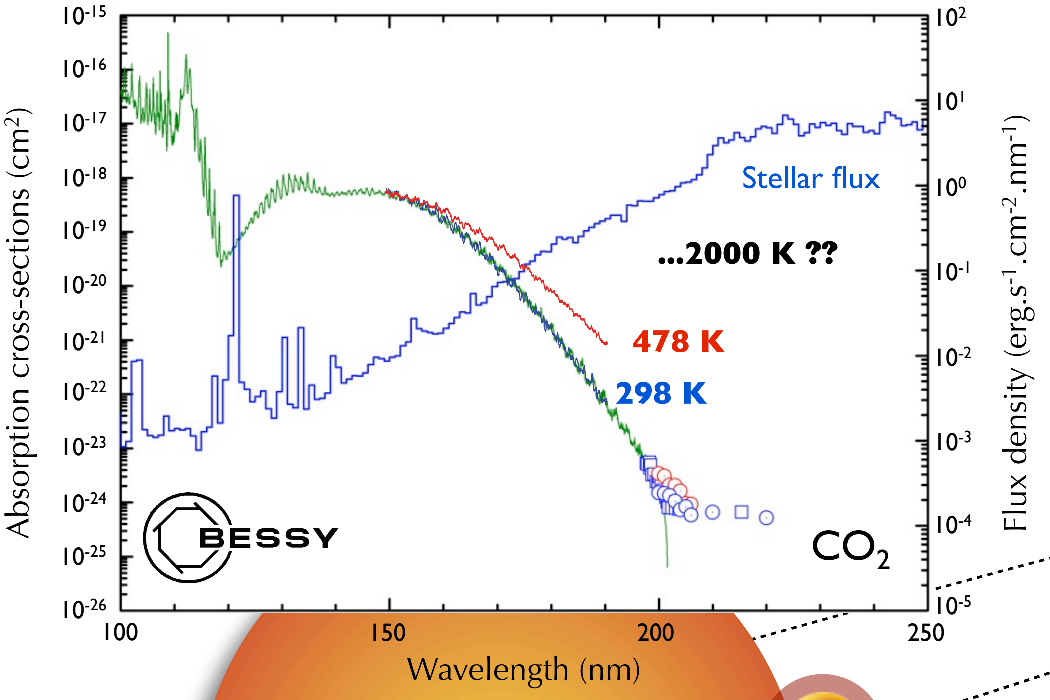
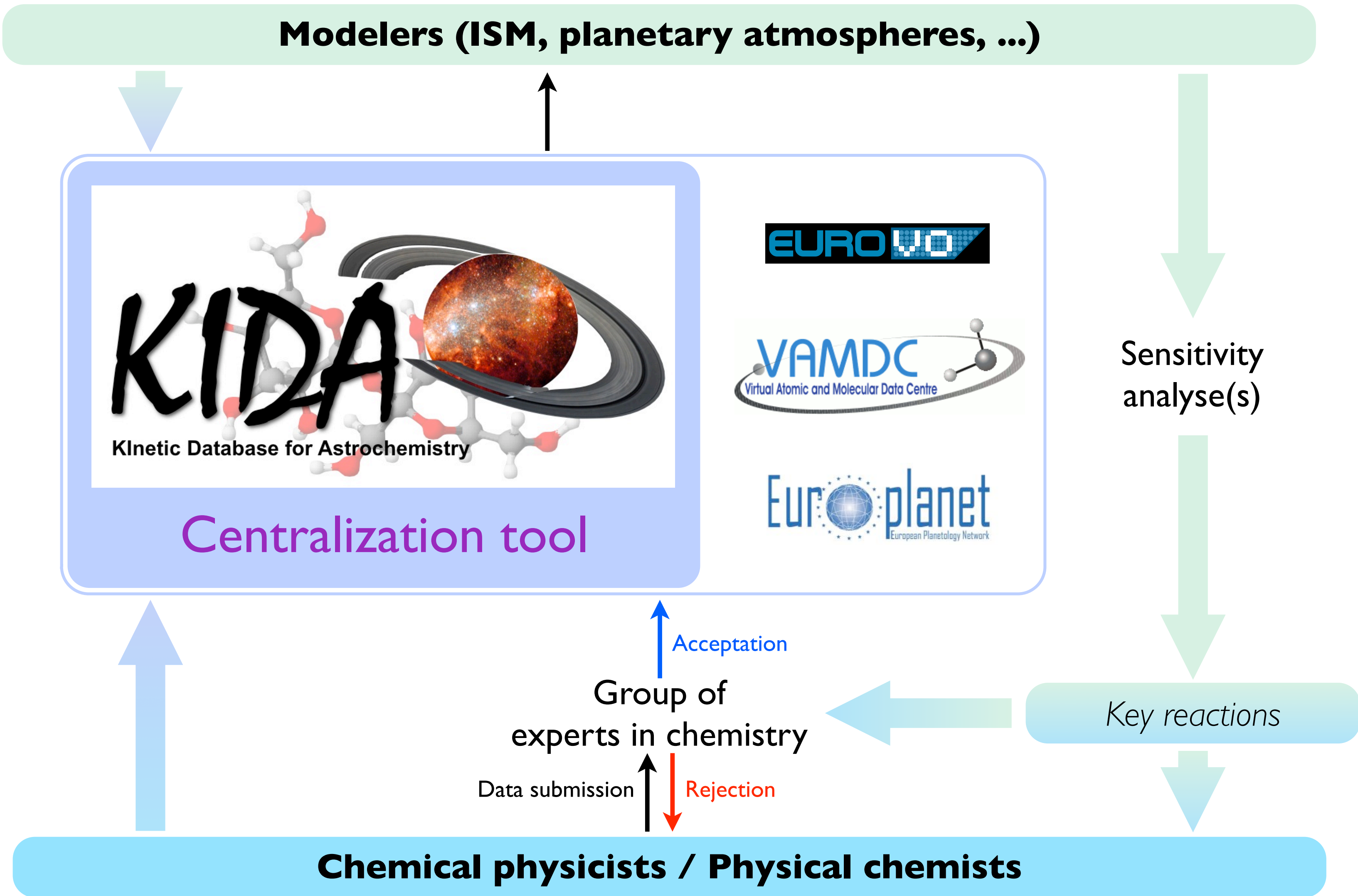


(Exo)planetary atmospheres
chemical models

Eric Hébrard (LAB)

http://kida.obs.u-bordeaux1.fr/

Poster 3.105 - Valentine Wakelam (LAB/OASU)

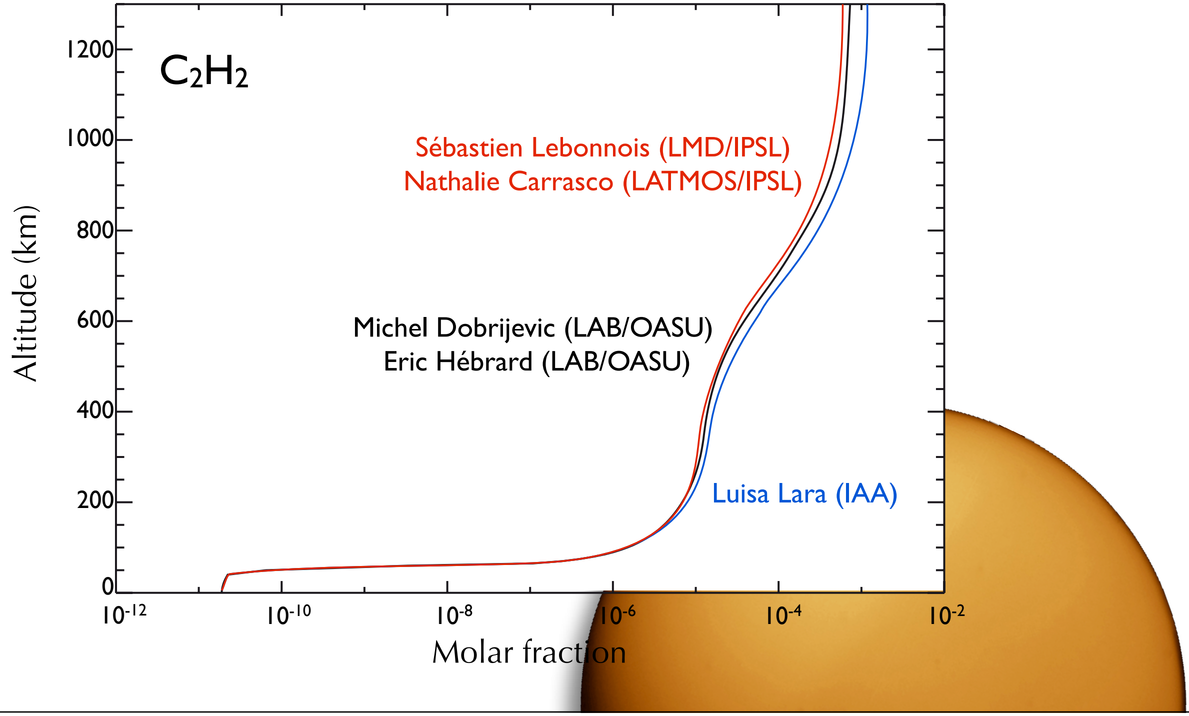


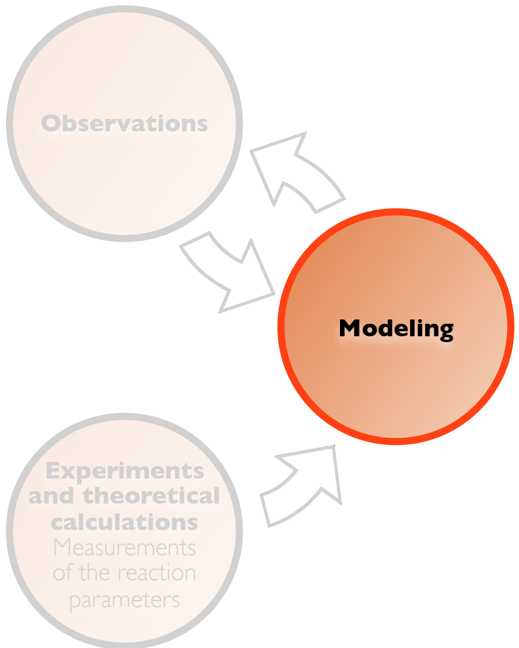
1D photochemical modeling of planetary atmospheres

Intercomparison of 1D photochemical models of Titan's atmosphere

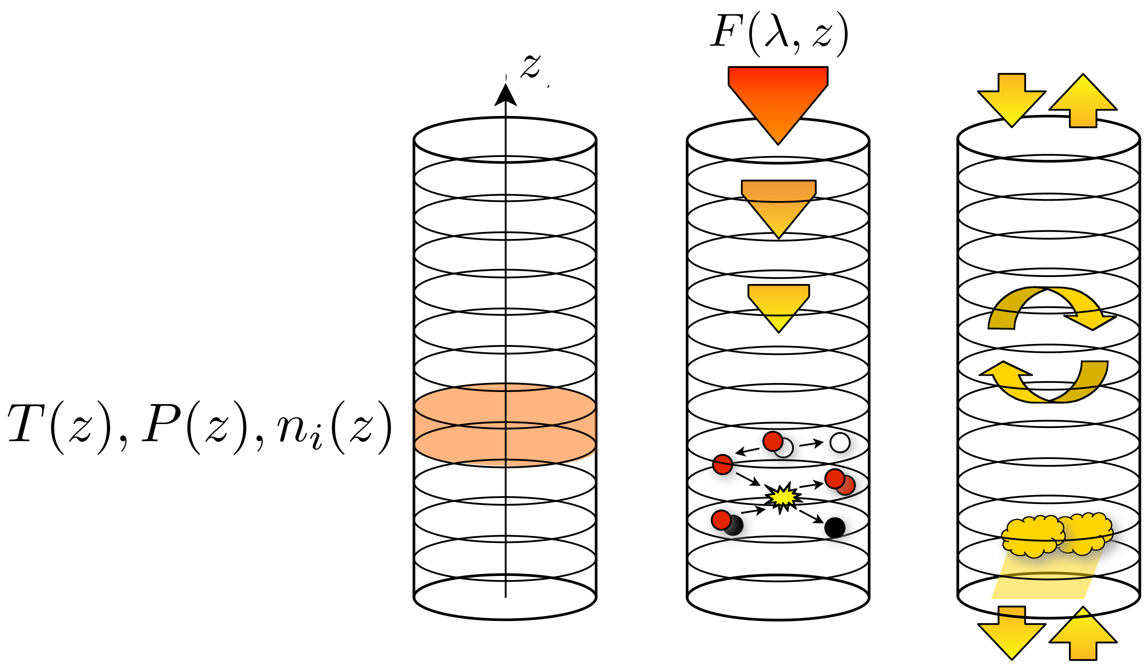
Pascal Pernot (LCP)

INTERNATIONAL SPACE SCIENCE INSTITUTE





1D photochemical modeling of planetary atmospheres



For each compound *i*,
at each altitude level *z*:

$$\frac{dn_i}{dt} = \underbrace{P_i - n_i L_i}_{\text{Chemical coupling between coumpounds}} - \underbrace{div(\Phi_i)}_{\text{Dynamical coupling between altitude levels}} - C_i$$

Chemical coupling between coumpounds

Dynamical coupling between altitude levels