Microphysics modelling with KROME

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Museum of Natural History / Niels Bohr Institute

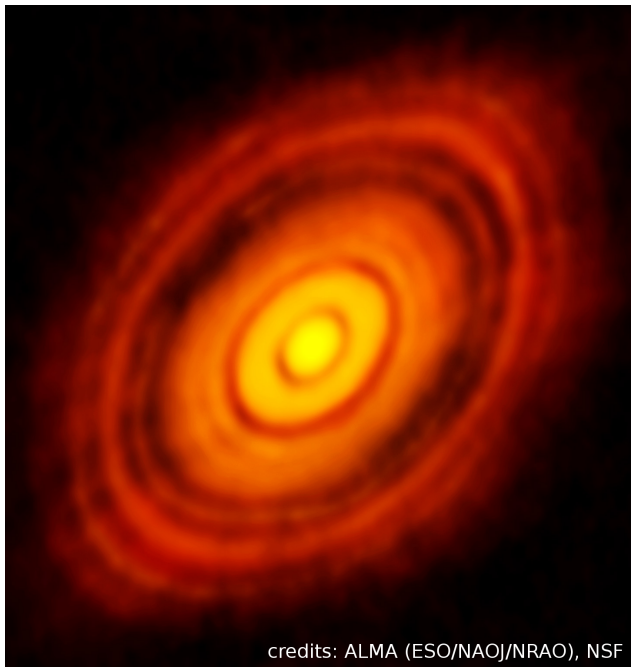
Note: actual sunny day in Copenhagen, no photoshop!

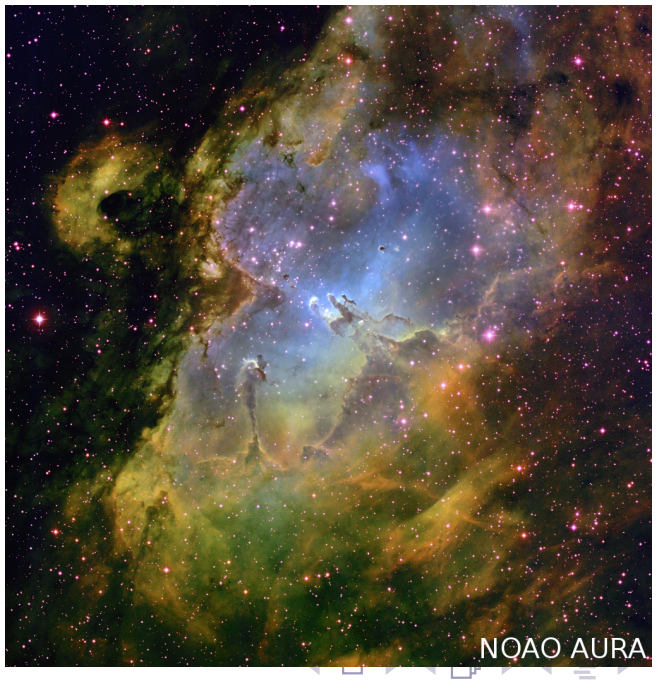
Museum of Natural History / Niels Bohr Institute

ISM chemistry/microphysics

Why chemistry/microphysics? (in numerical simulations)

- chemistry (and microphysics) is everywhere and plays a crucial role
- PDR, HII, disks, stars, planet atmospheres, ISM, WIM, CNM, HIM, MCs, ...
- controls gas thermal evolution
- controls opacity
- comparison with observations





ISM chemistry/microphysics

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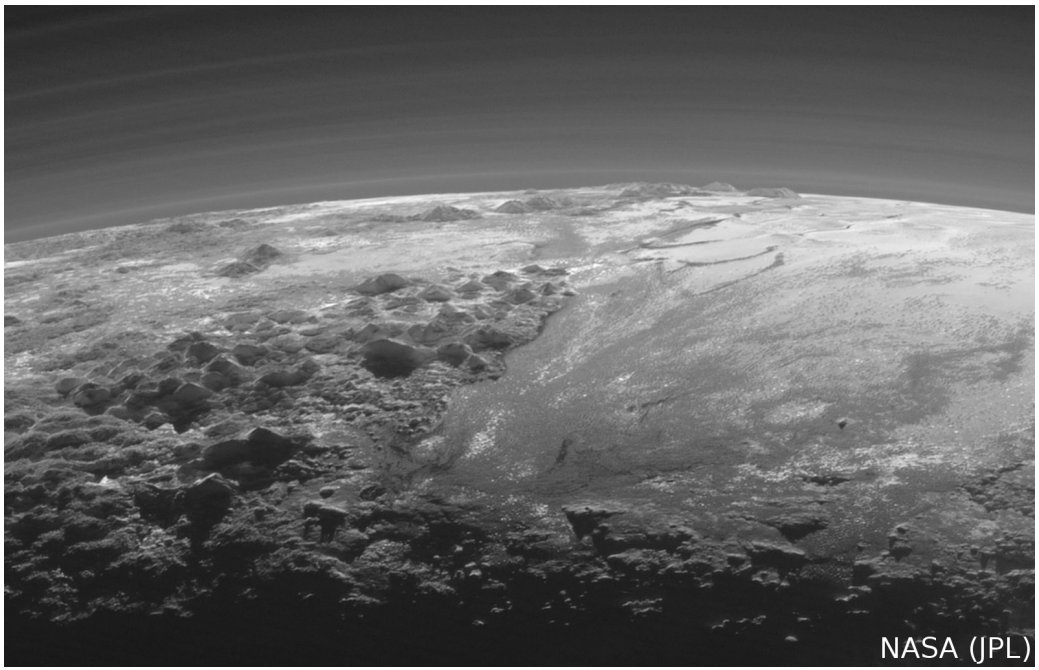
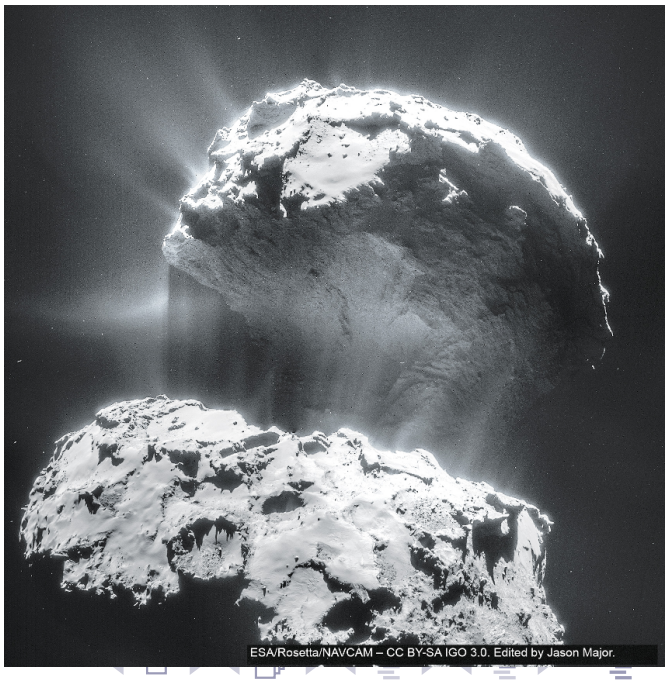




ISM chemistry/microphysics

Why chemistry/microphysics is troublesome (in numerical simulations)

- very CPU demanding (solving stiff ODEs)
- has a non-linear/complex behaviour (e.g. MC)
- connected with (and influenced by) many physical processes
- many atomic, molecular, thermochemical, . . . data required
- needs accurate rates for reaction rates (and xsecs)
- network completeness (include all species/reactions)

Chemistry, the full story (1/25)

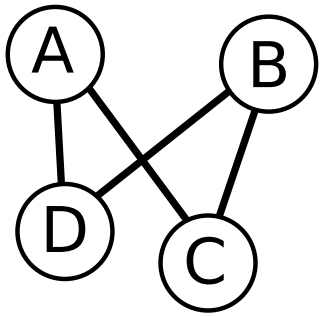
$$A + B \longrightarrow C + D$$

Chemistry, the full story (2/25)

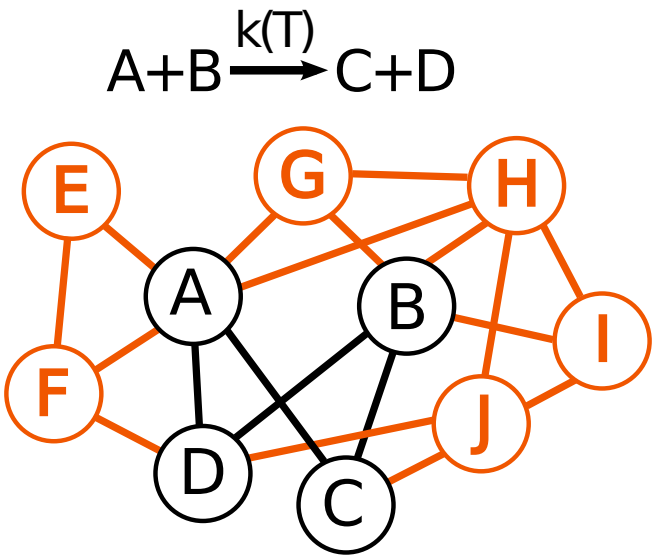
$$A + B \xrightarrow{k(T)} C + D$$

Chemistry, the full story (3/25)

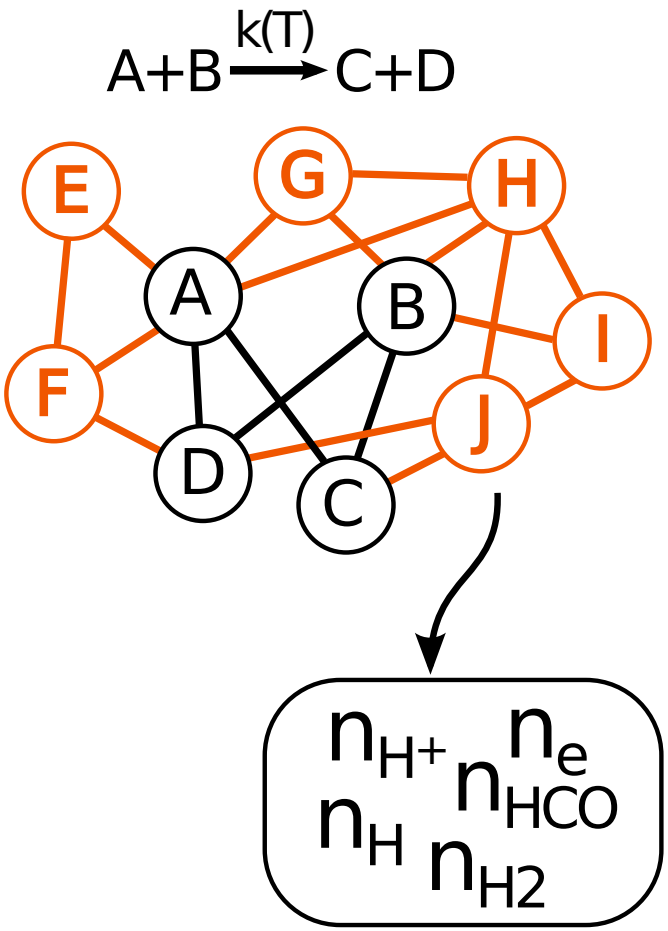
$$A + B \xrightarrow{k(T)} C + D$$



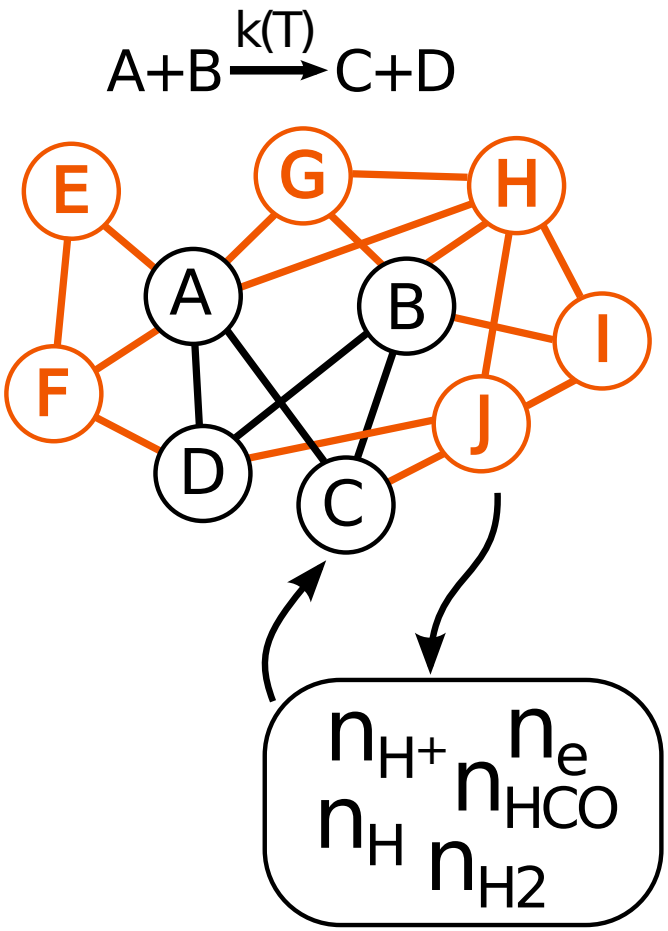
Chemistry, the full story (4/25)



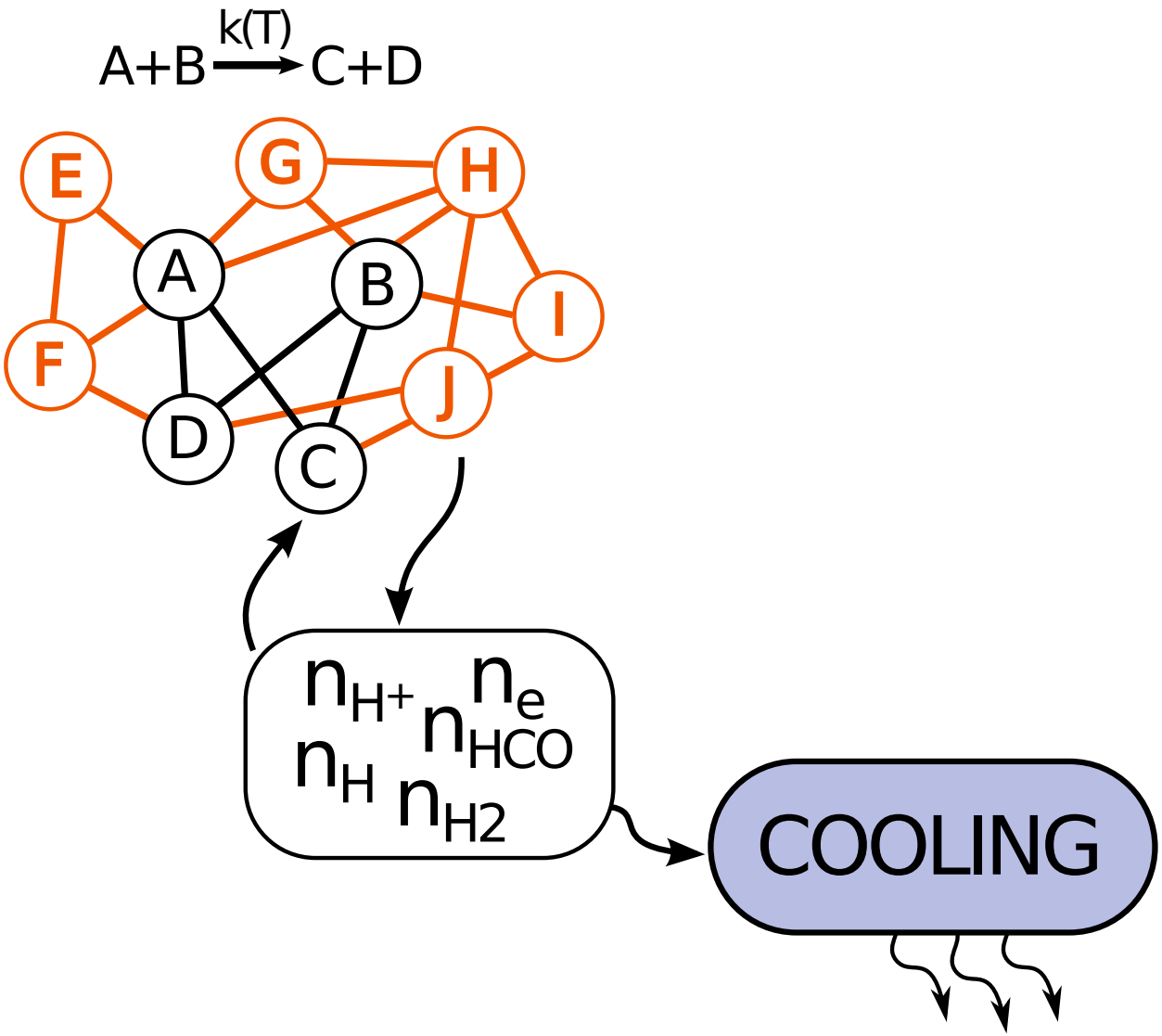
Chemistry, the full story (5/25)



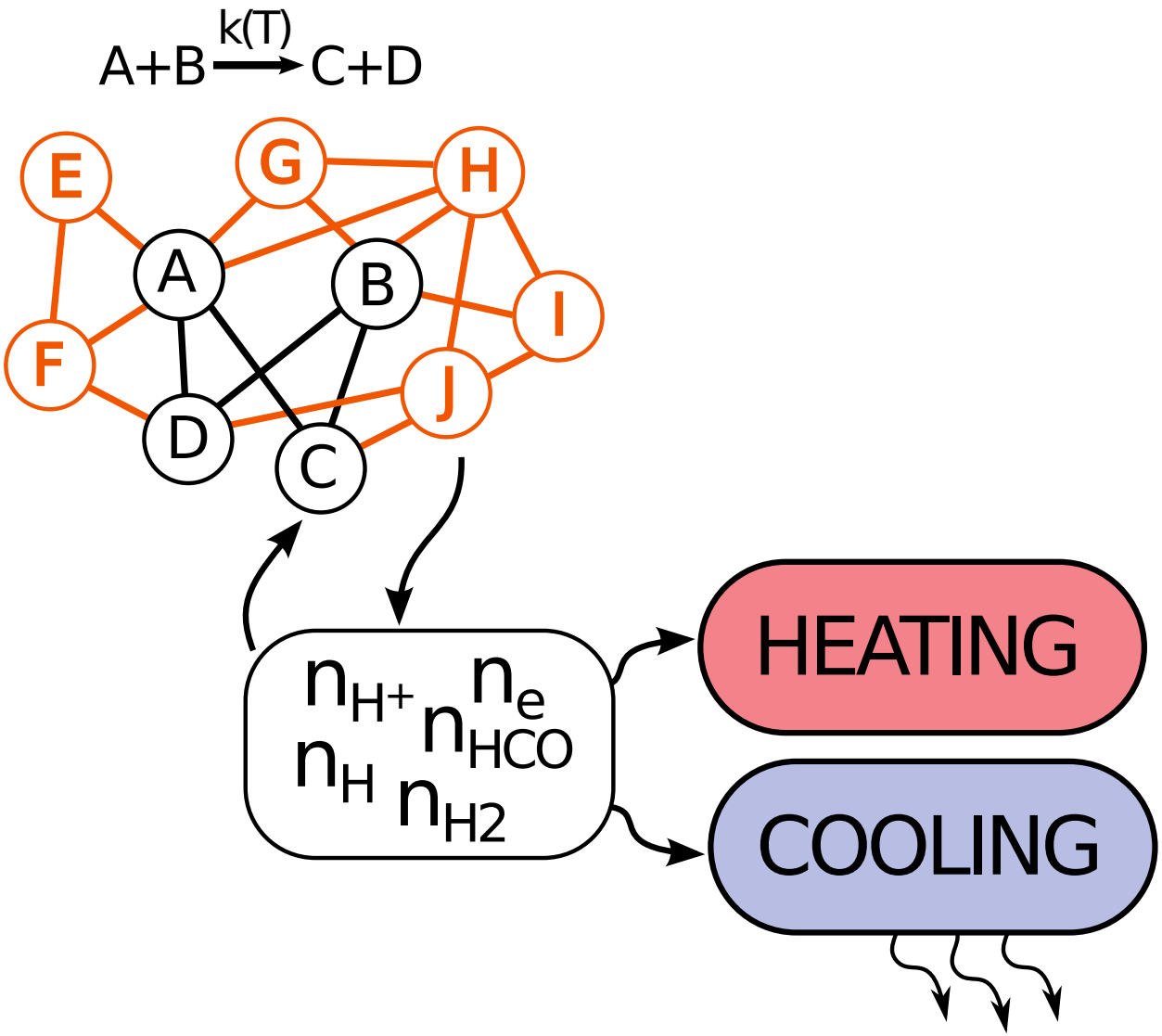
Chemistry, the full story (6/25)



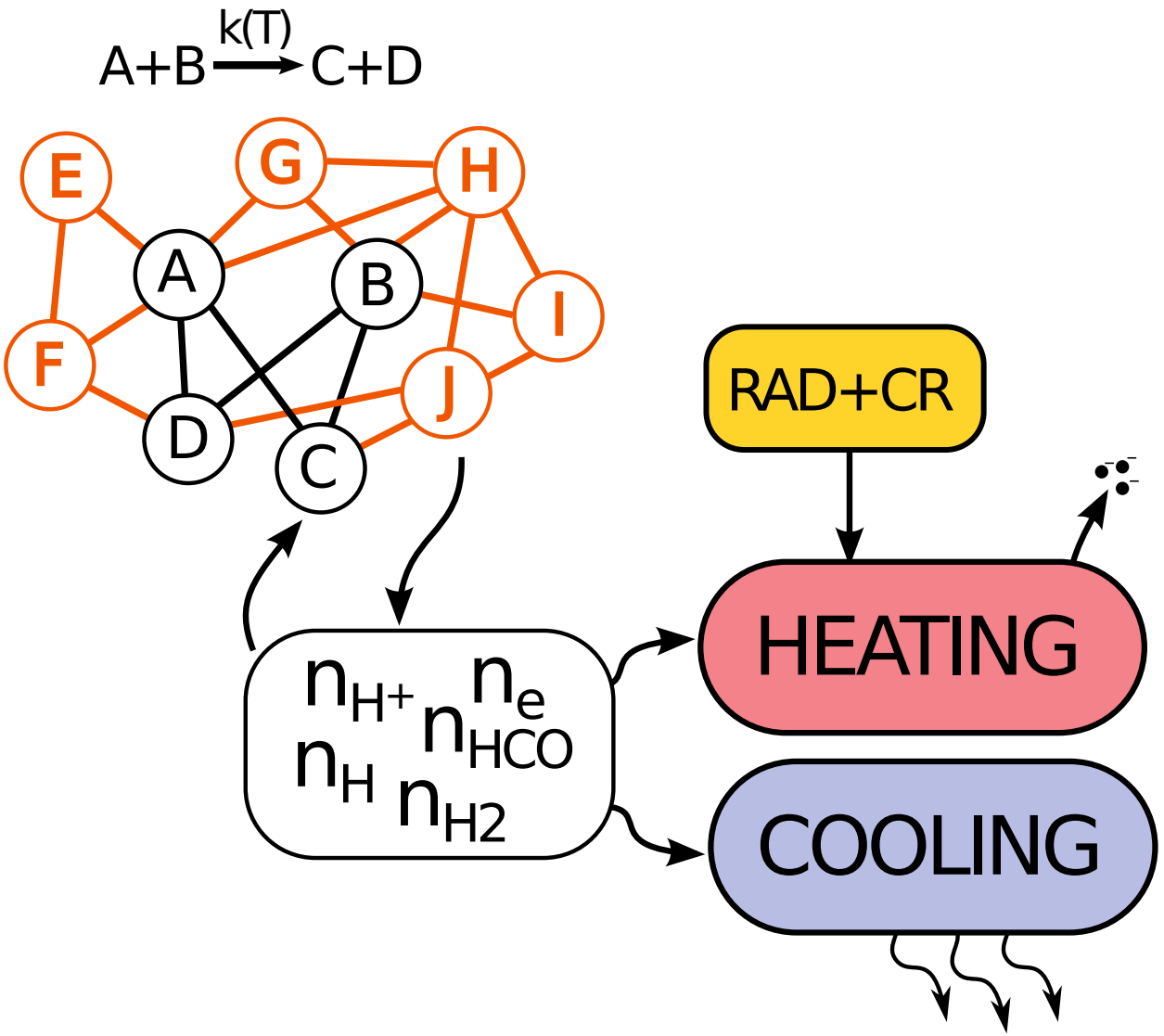
Chemistry, the full story (7/25)



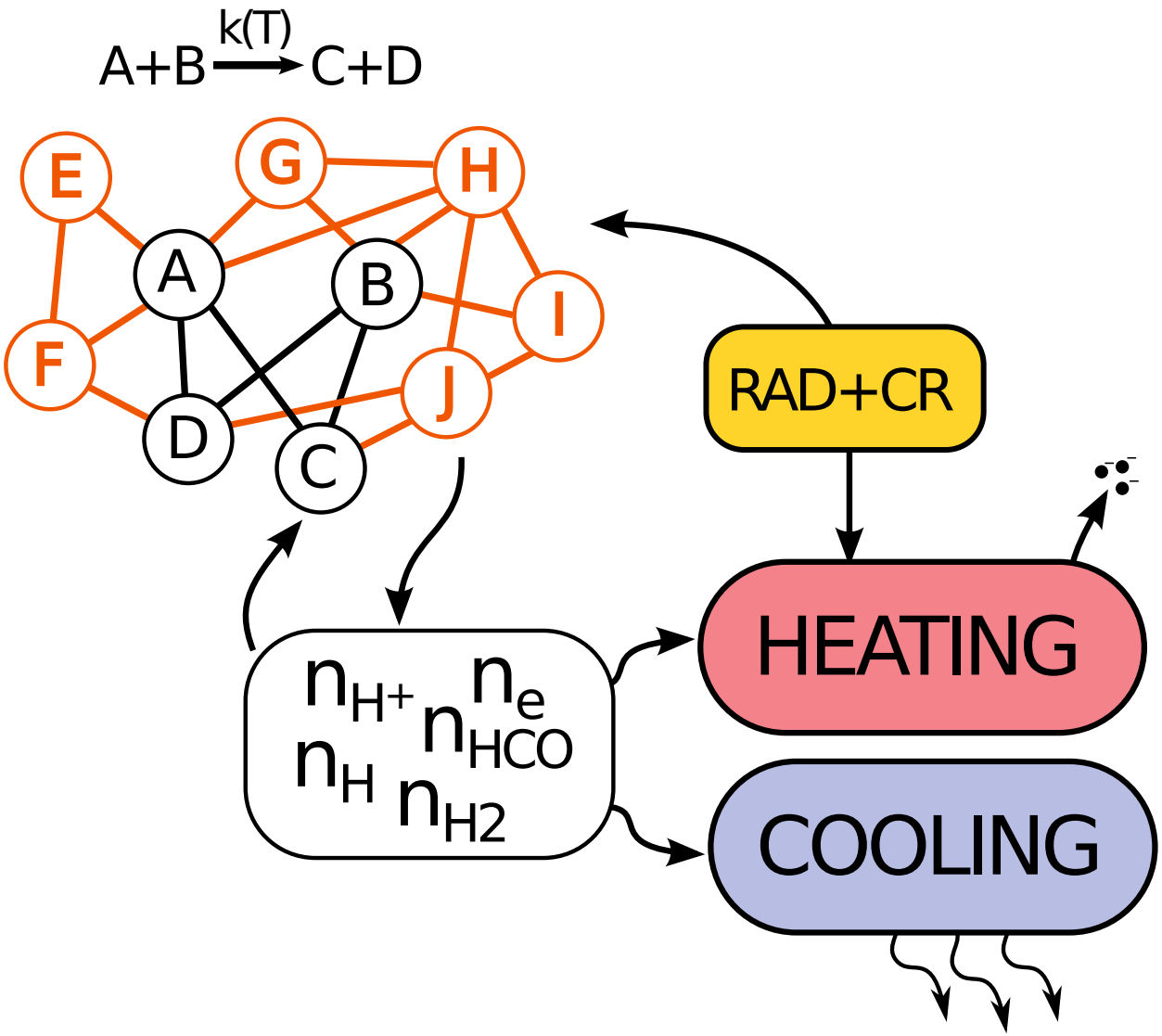
Chemistry, the full story (8/25)



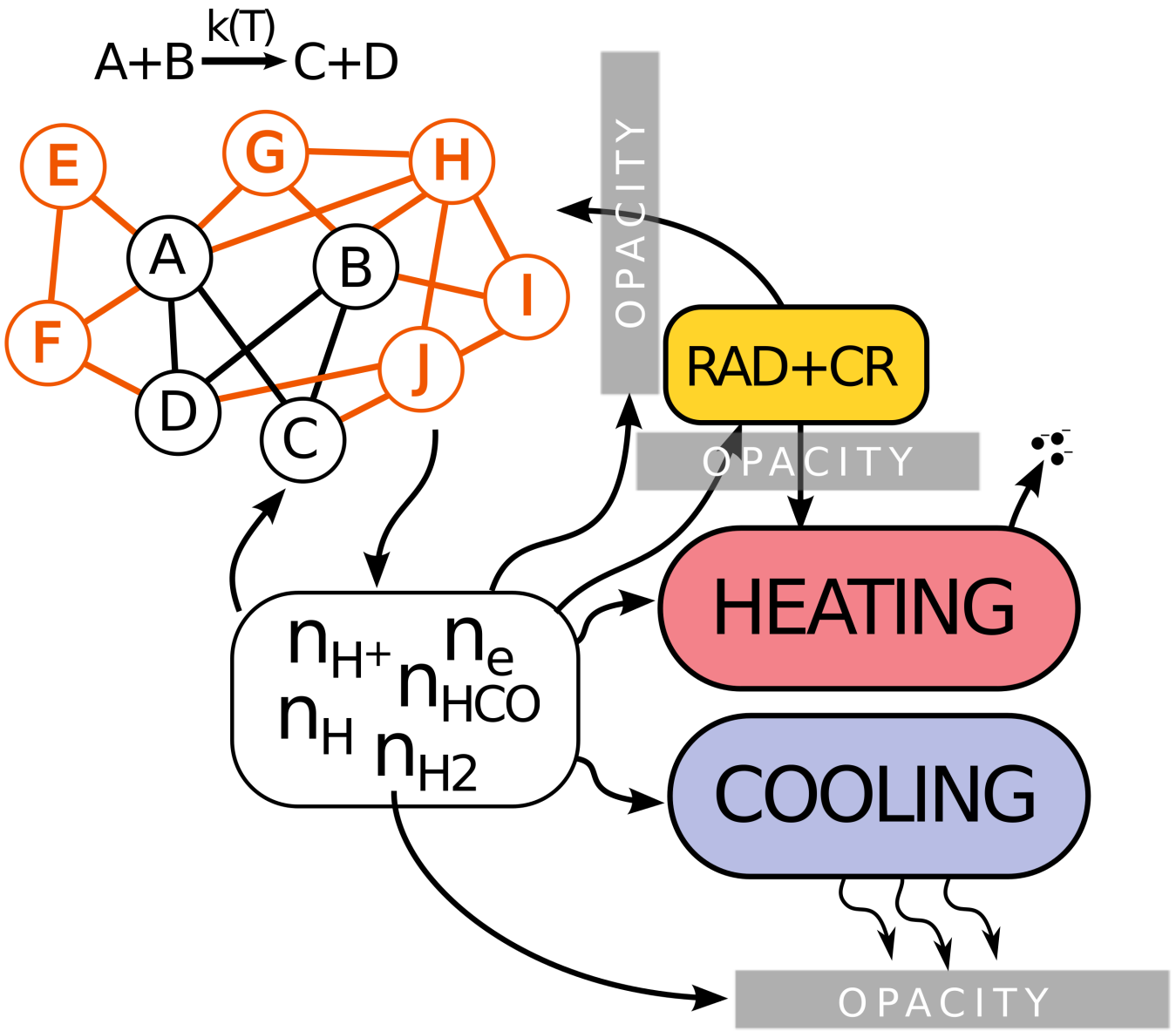
Chemistry, the full story (9/25)



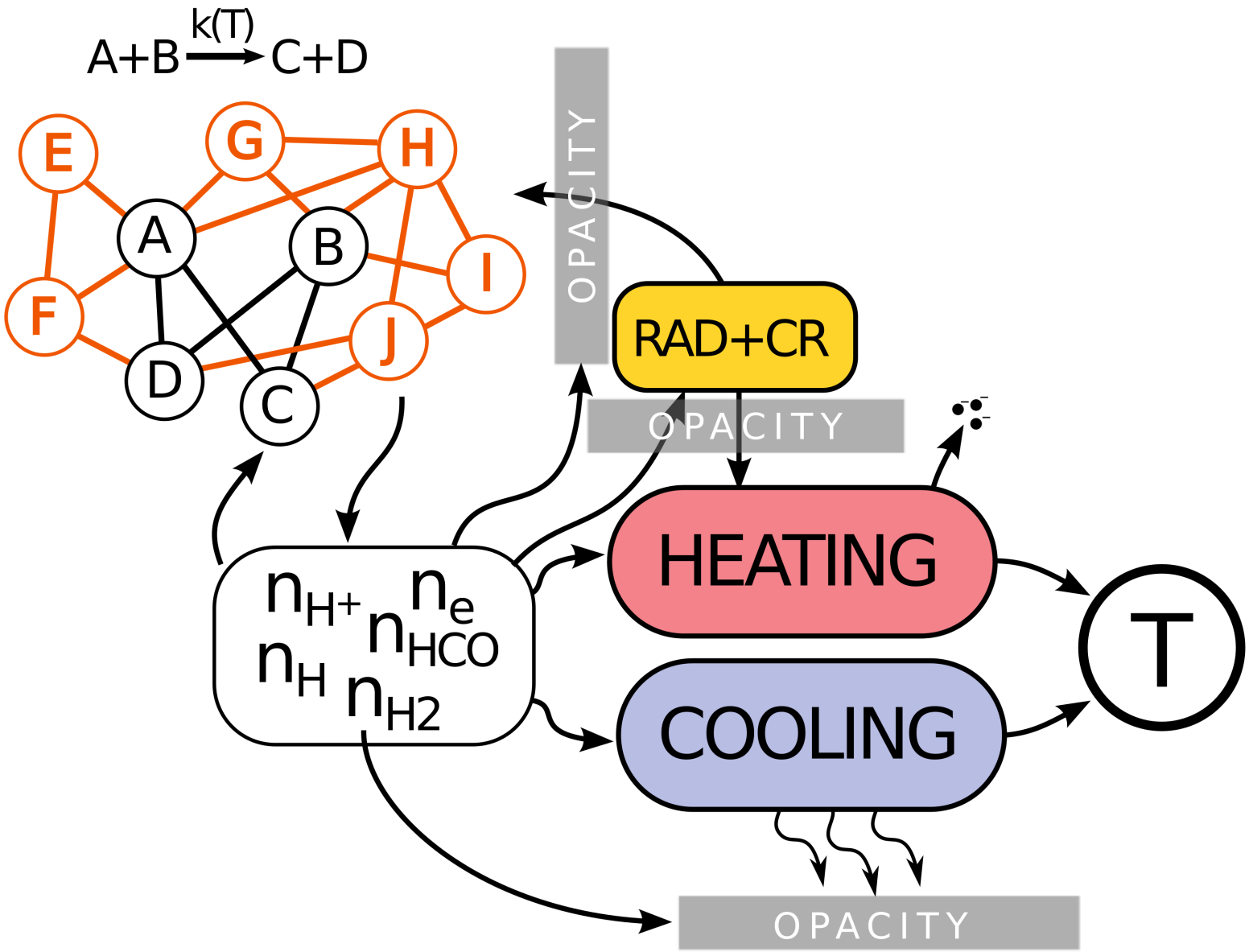
Chemistry, the full story (10/25)



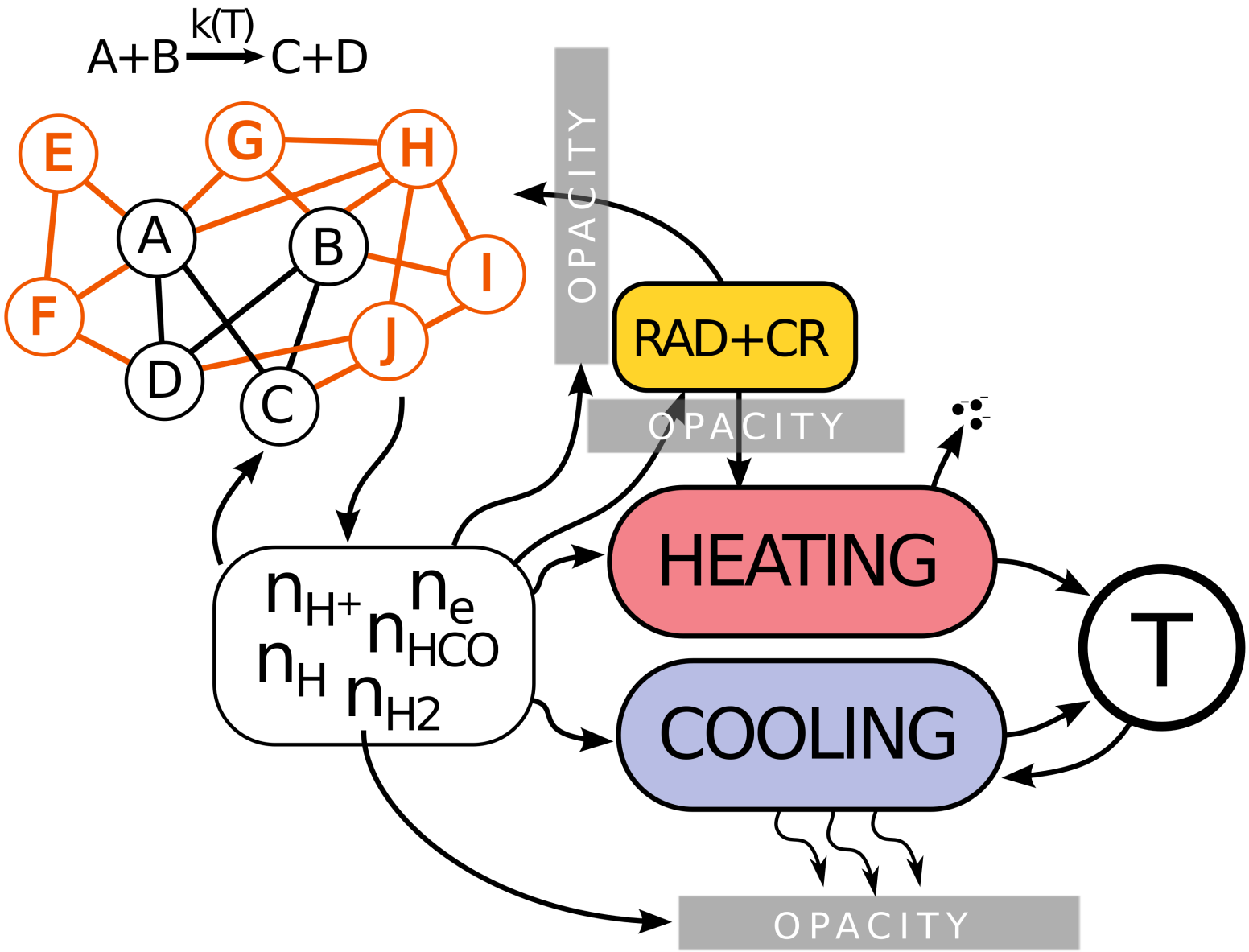
Chemistry, the full story (11/25)



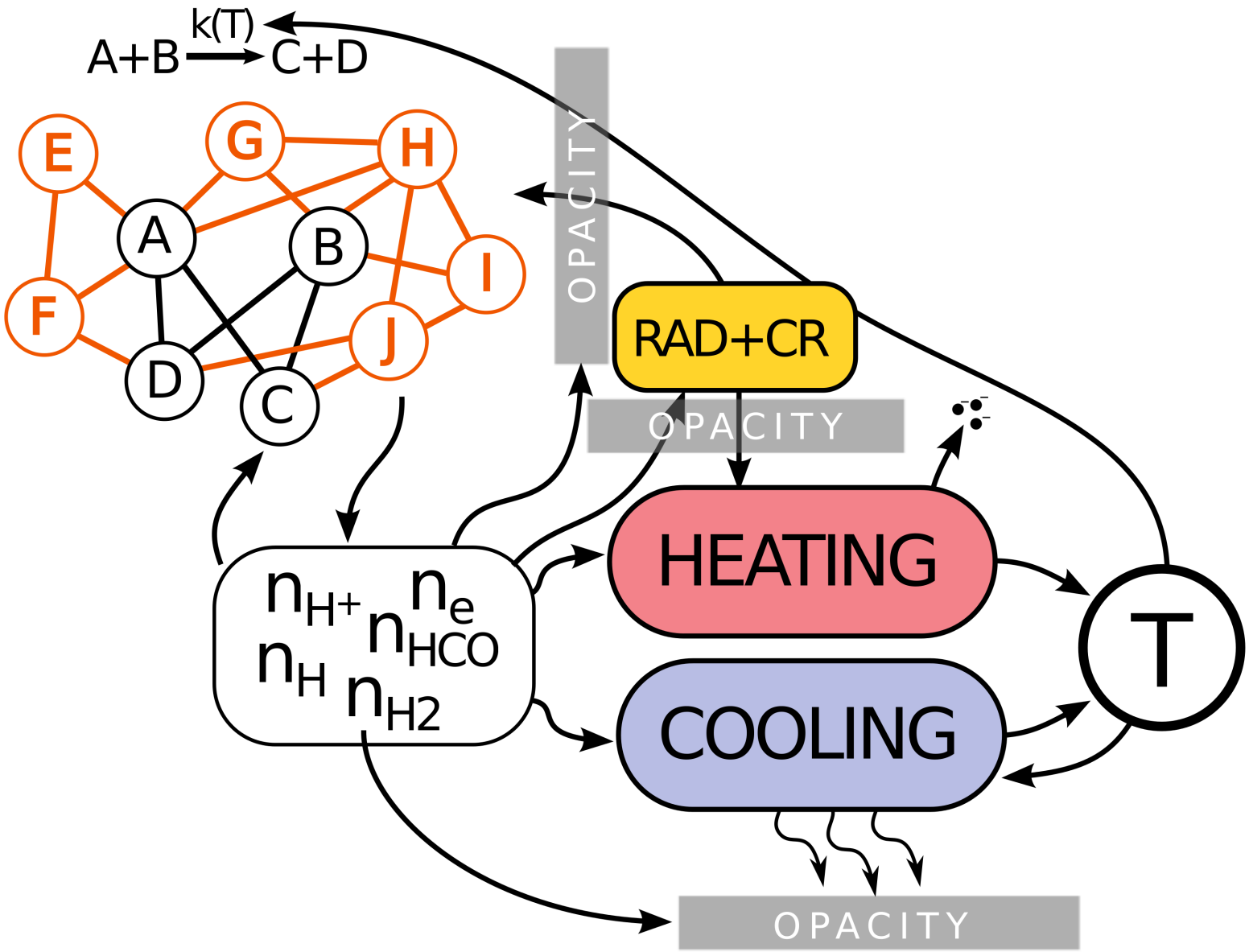
Chemistry, the full story (12/25)



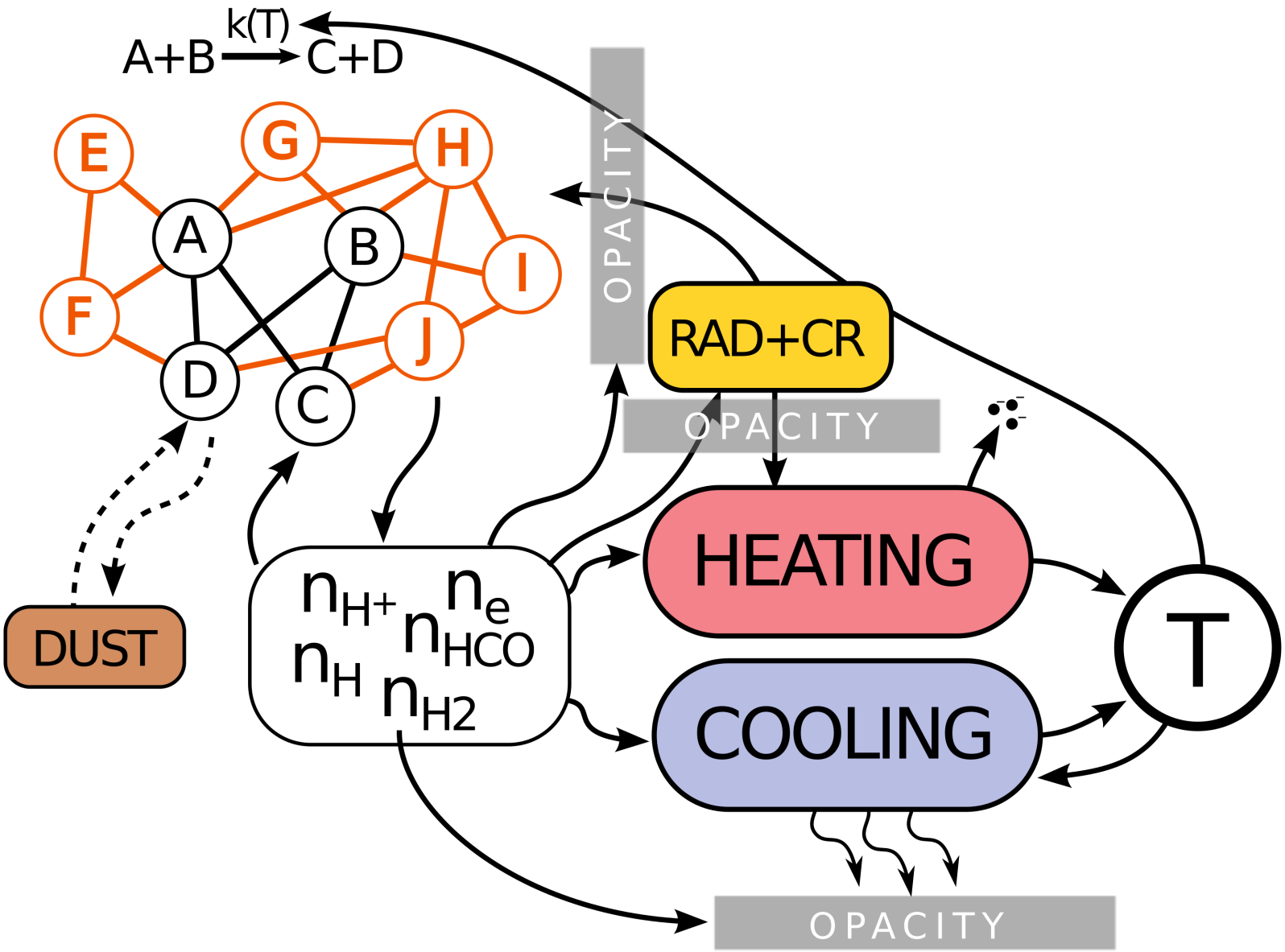
Chemistry, the full story (13/25)



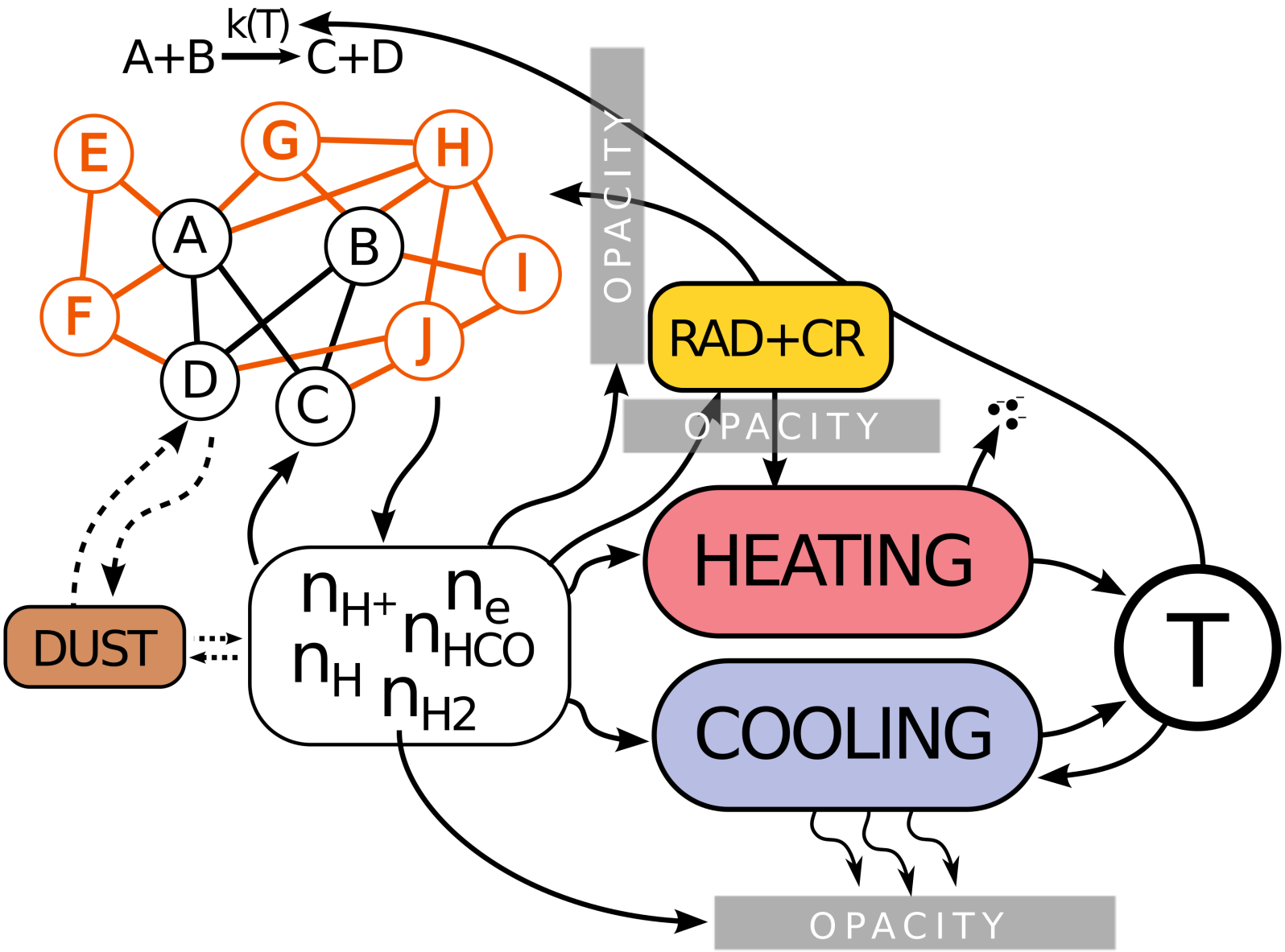
Chemistry, the full story (14/25)



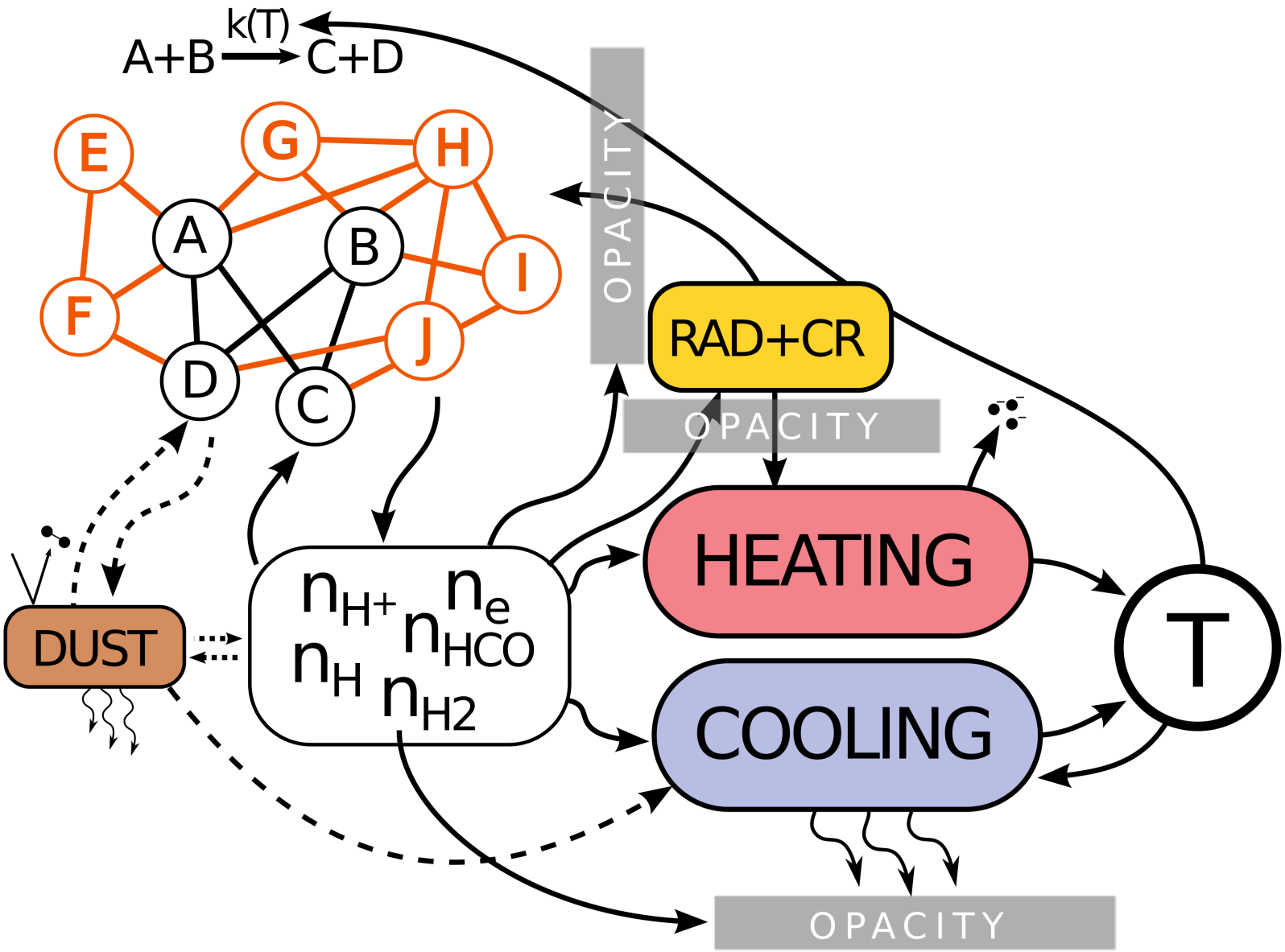
Chemistry, the full story (15/25)



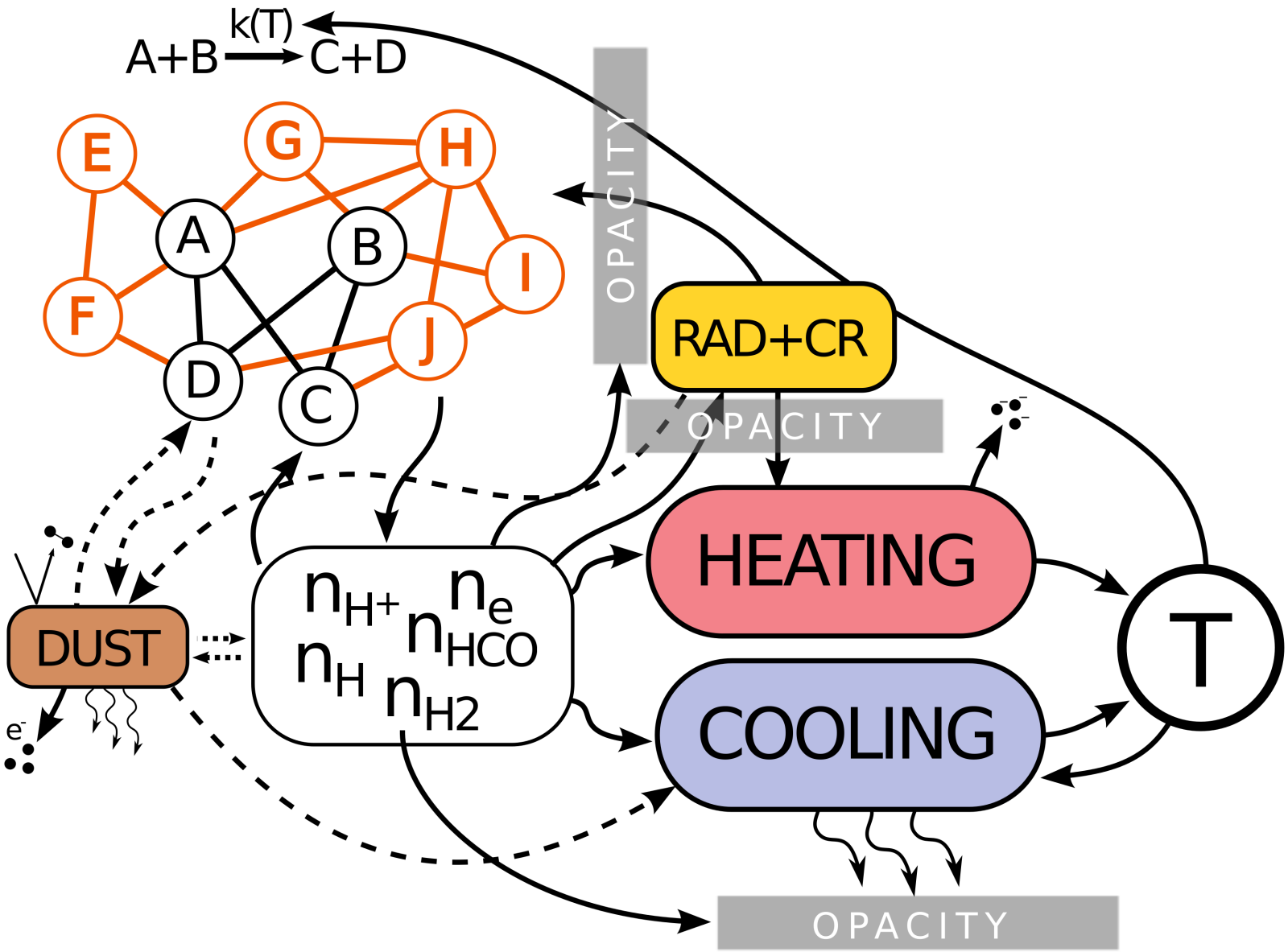
Chemistry, the full story (16/25)



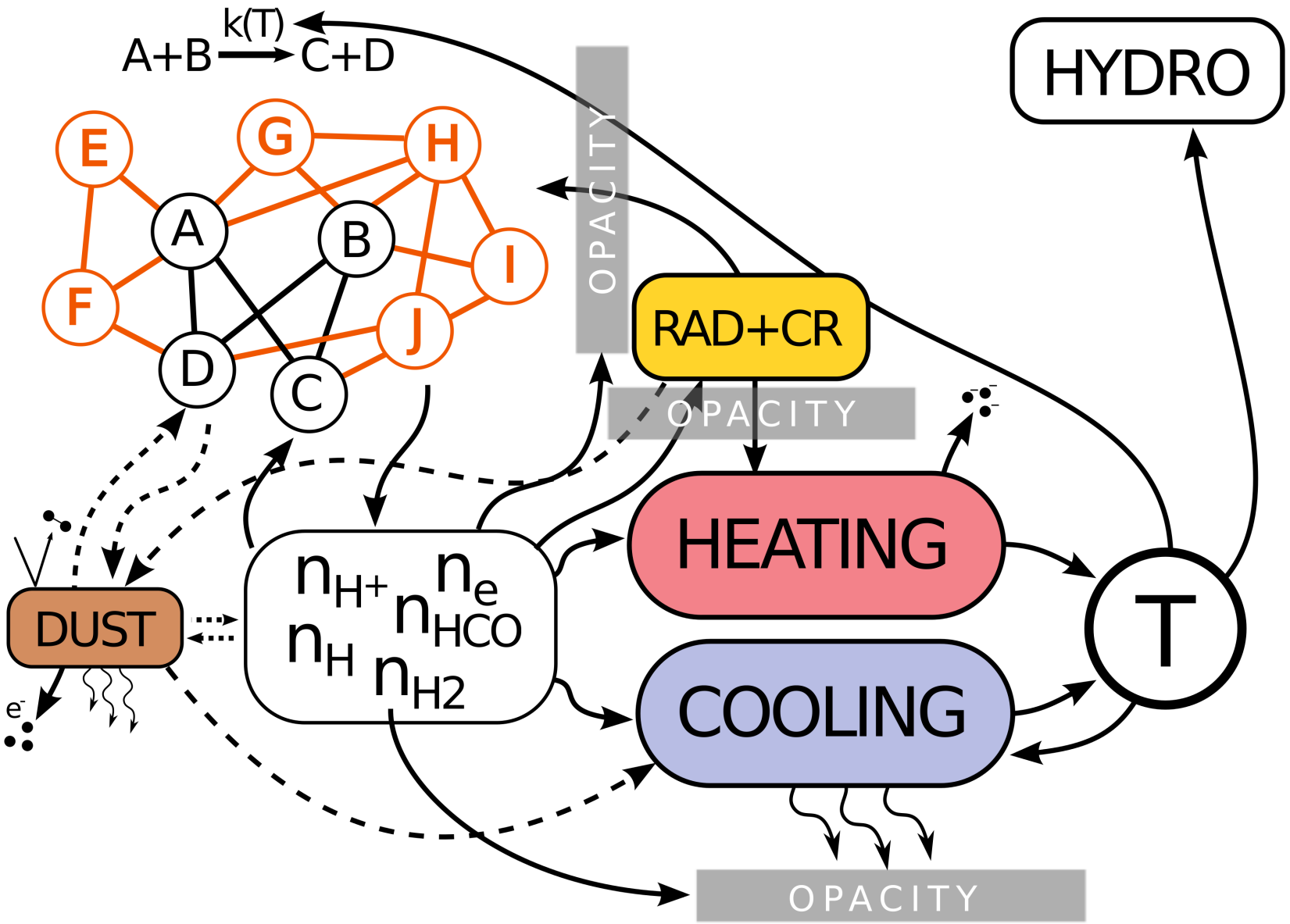
Chemistry, the full story (17/25)



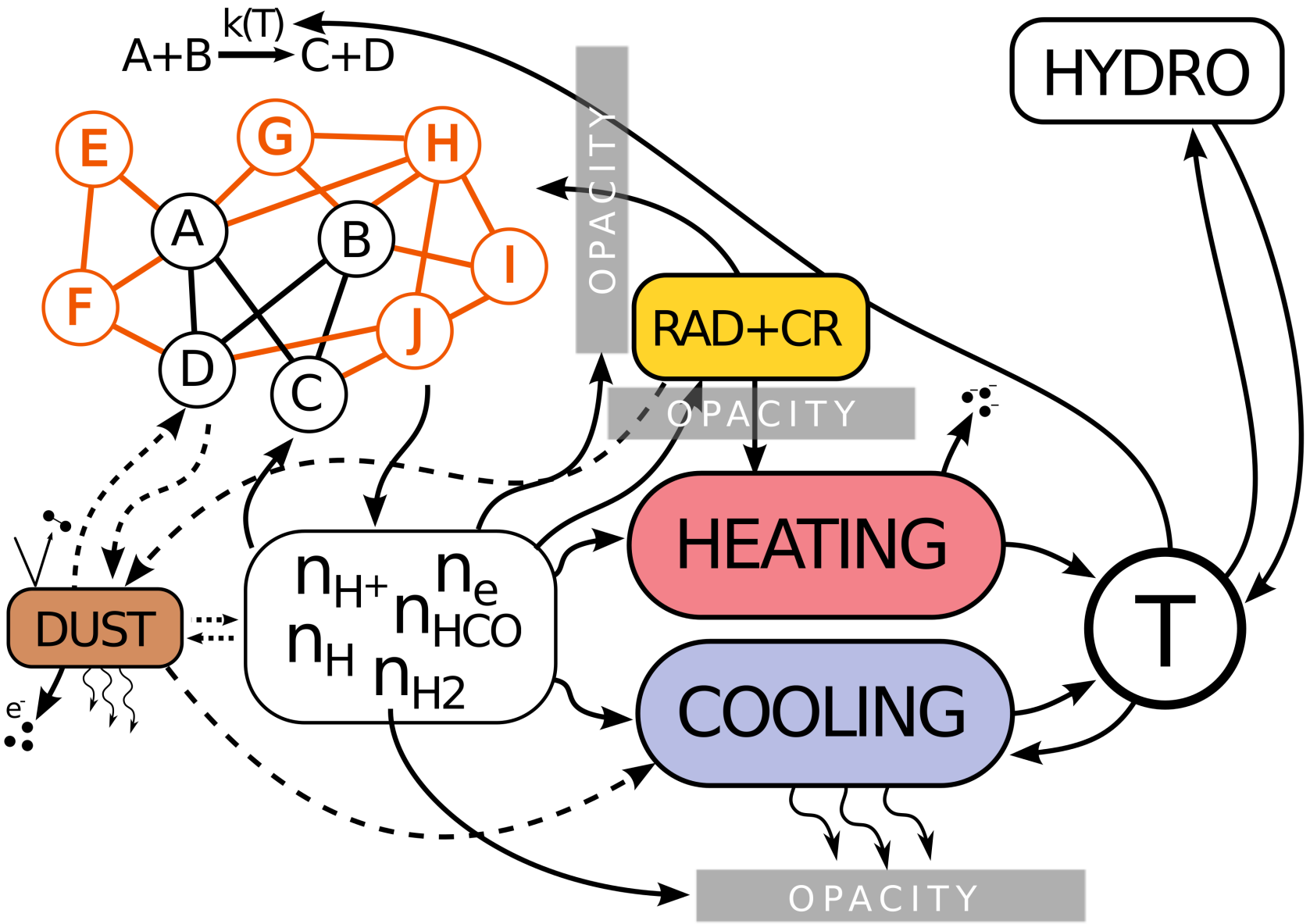
Chemistry, the full story (18/25)



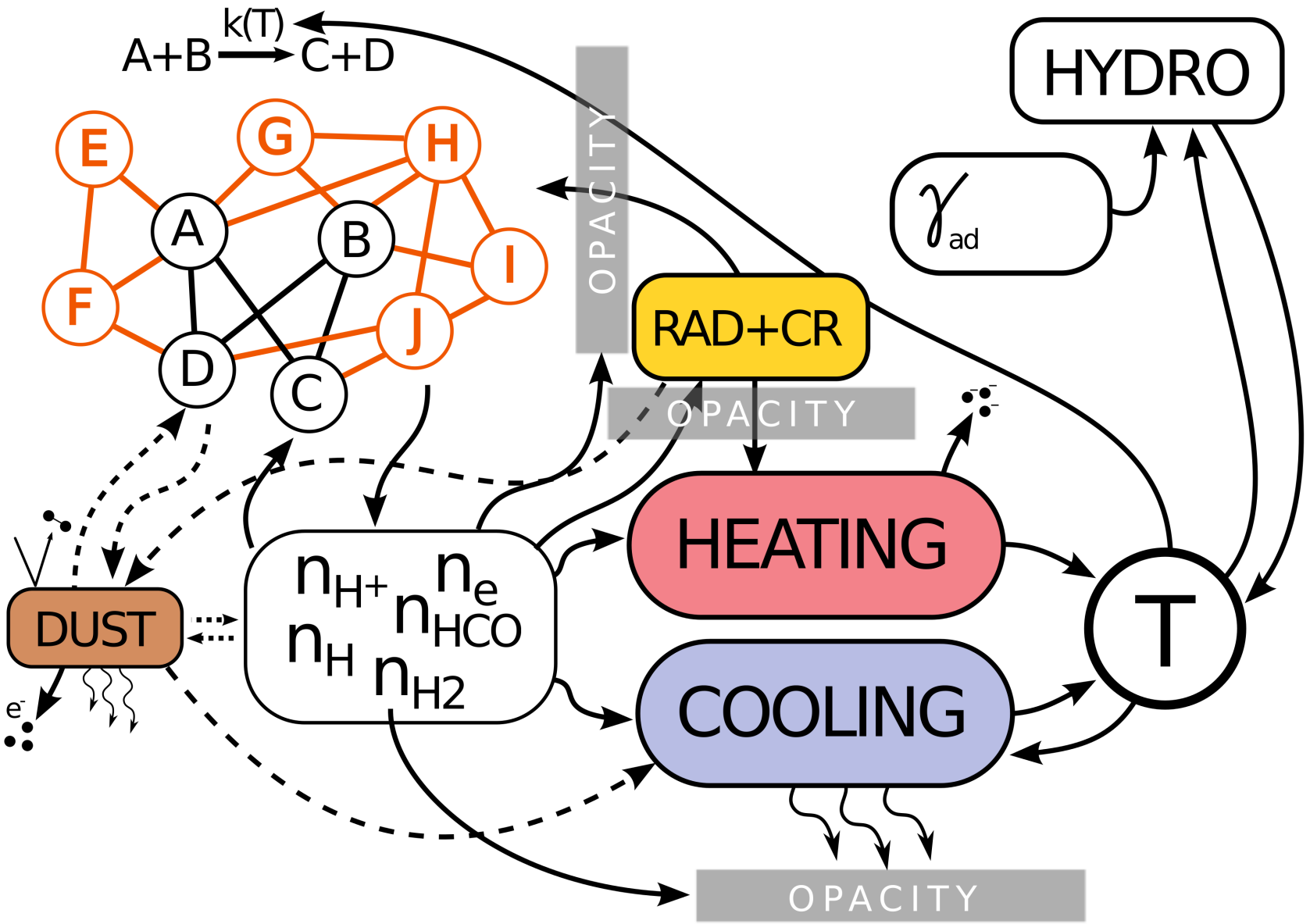
Chemistry, the full story (19/25)



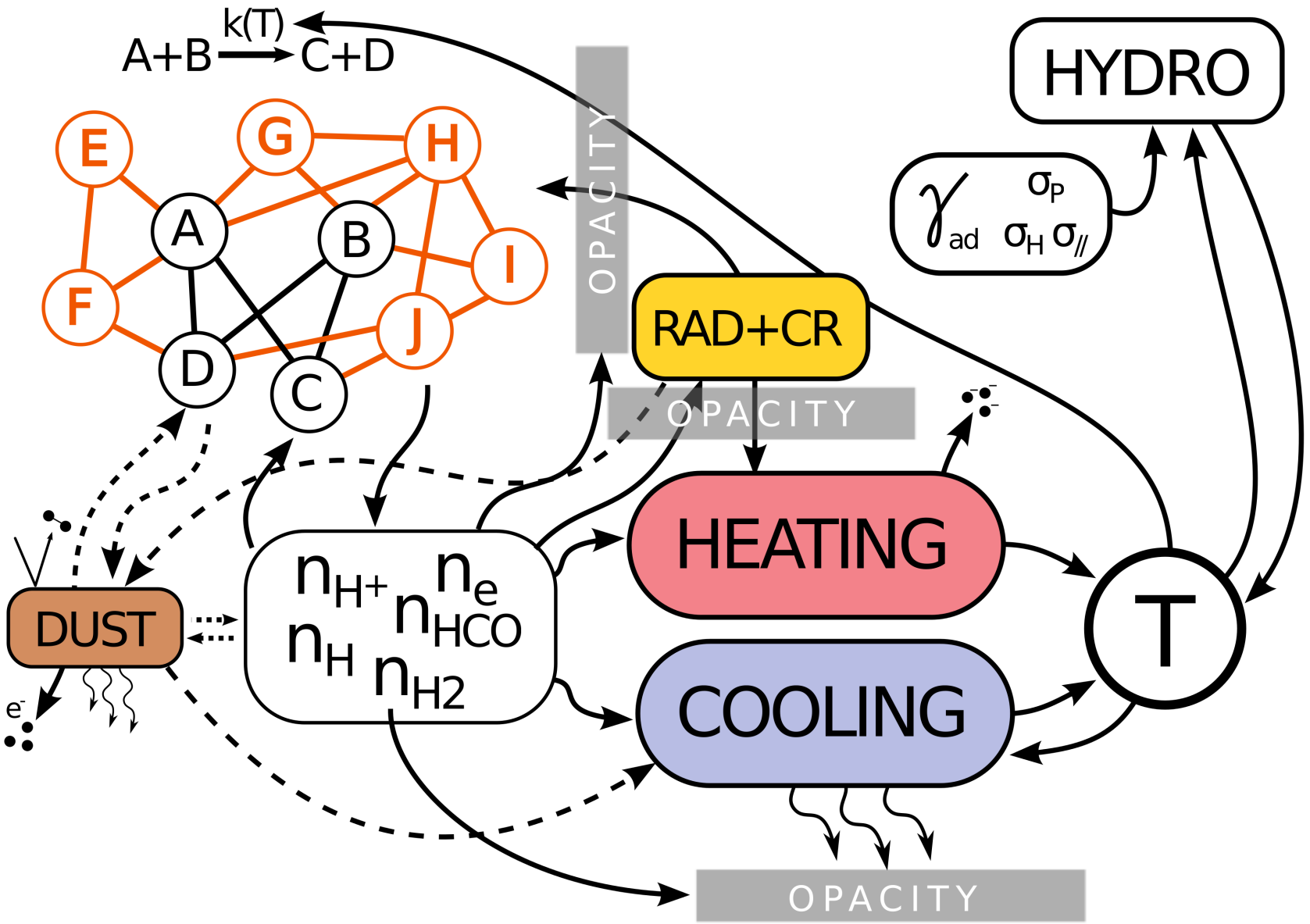
Chemistry, the full story (20/25)



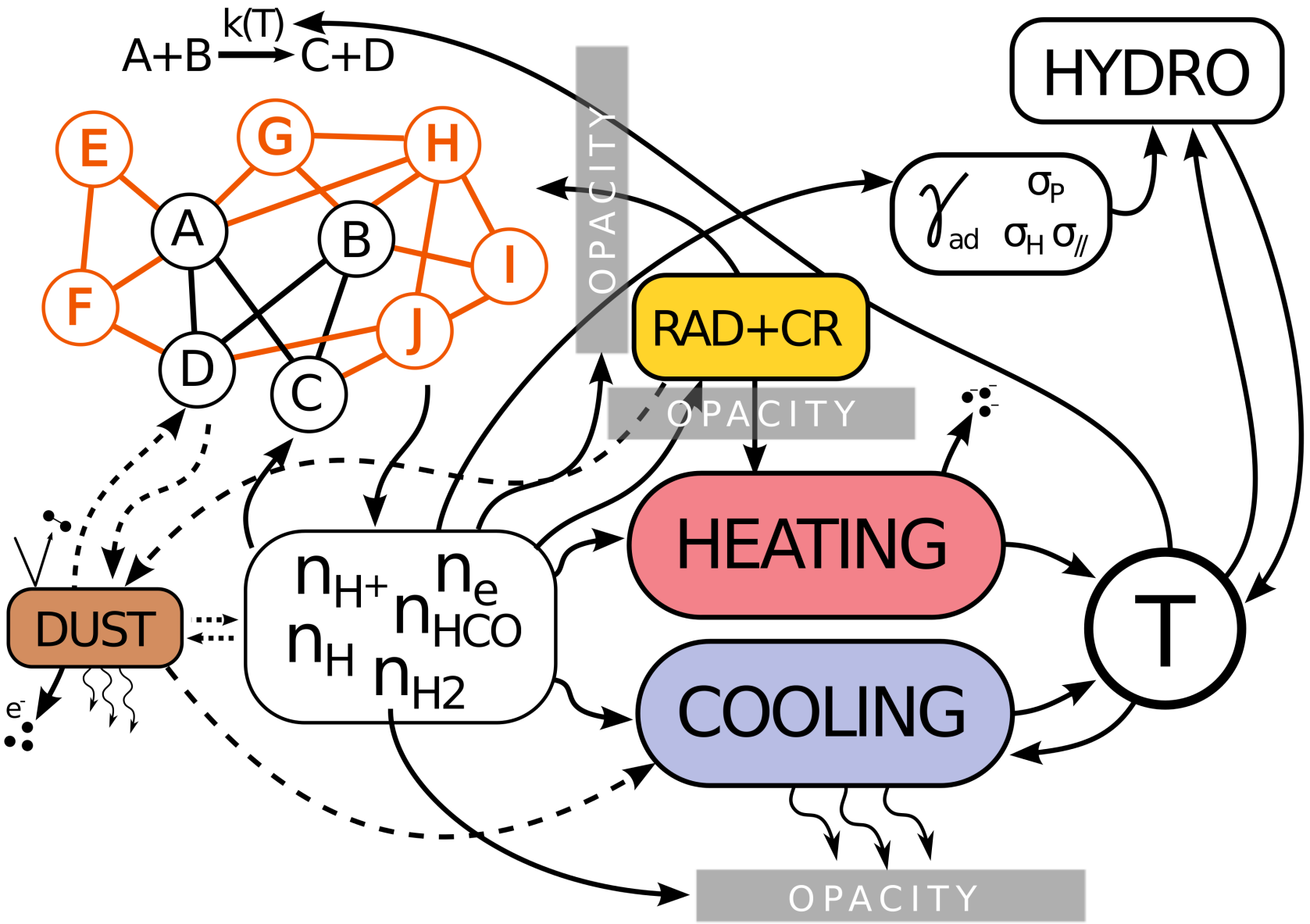
Chemistry, the full story (21/25)



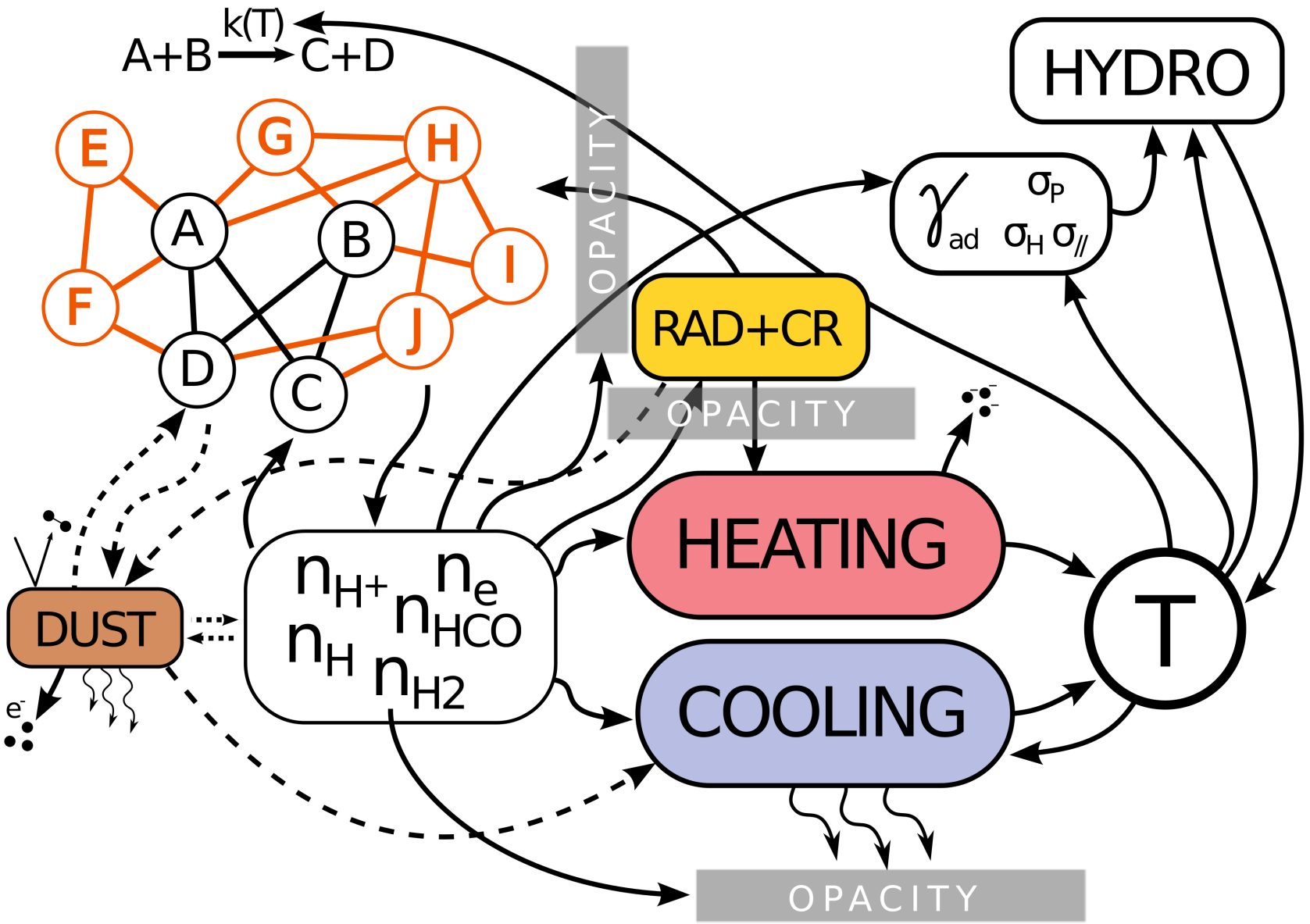
Chemistry, the full story (22/25)



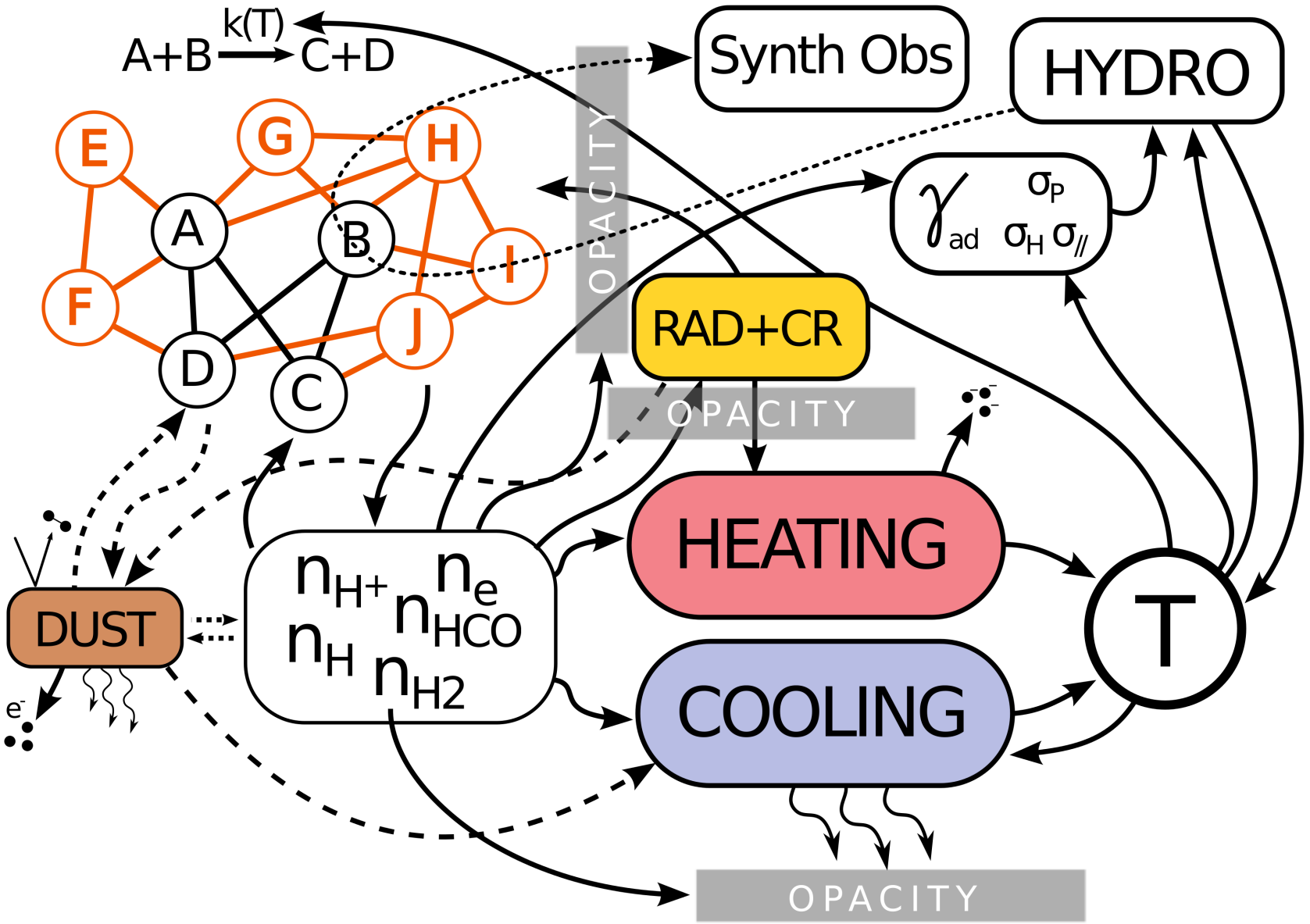
Chemistry, the full story (23/25)



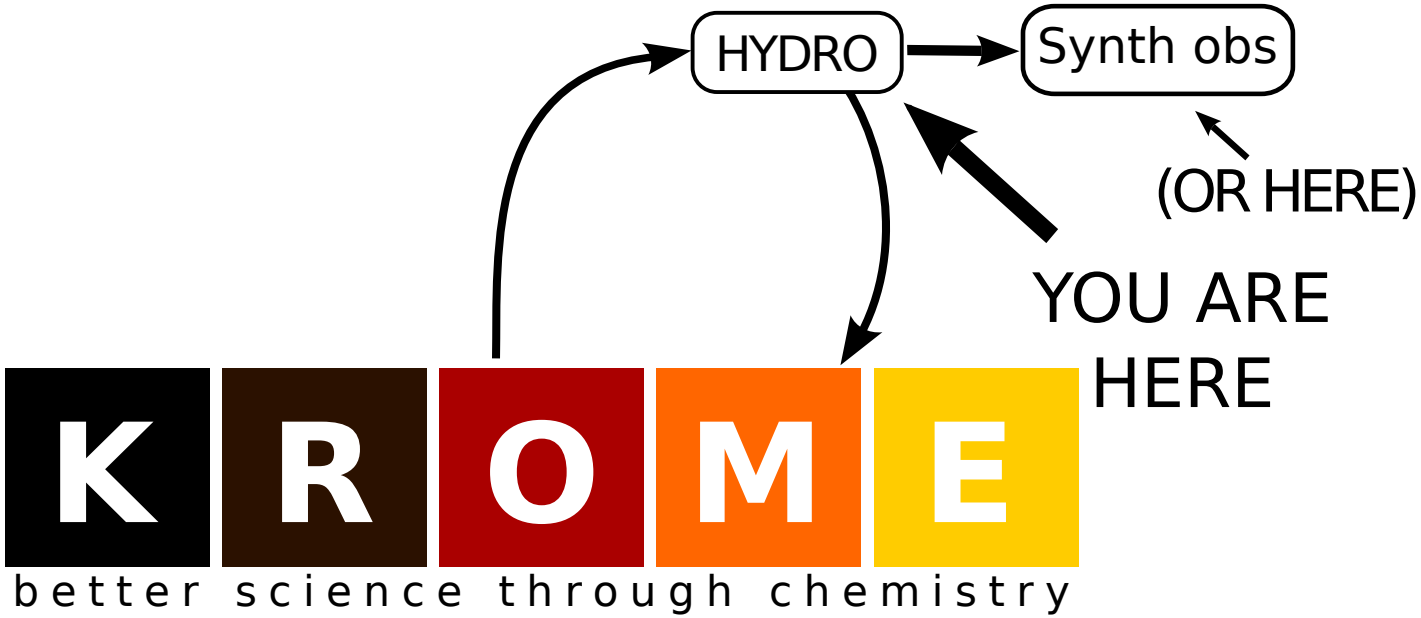
Chemistry, the full story (24/25)



Chemistry, the full story (25/25)



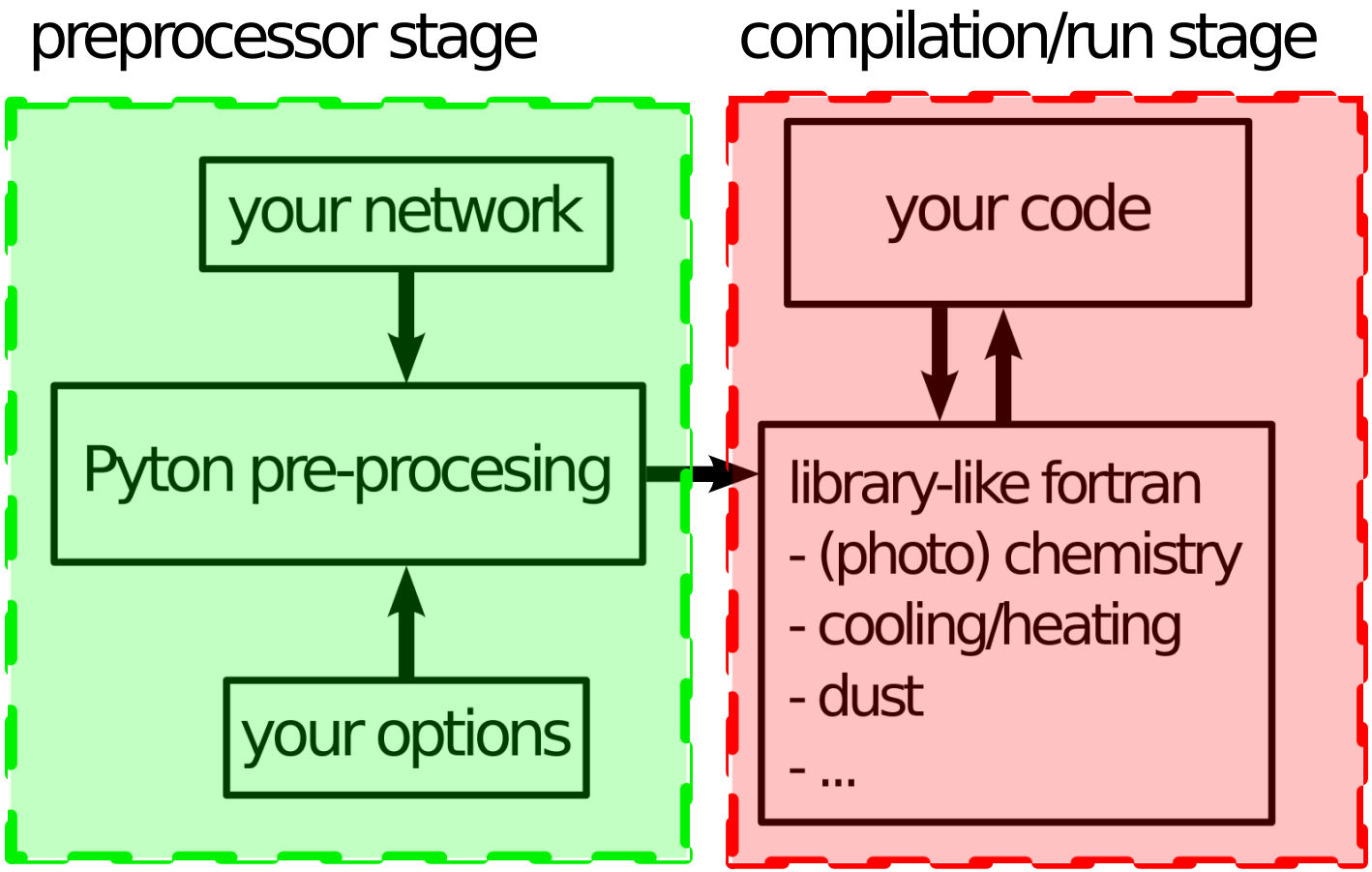
KROME



What is KROME?

- Python pre-processor creates *ad hoc* F90 modules
- Chemistry, dust-related physics, cooling, heating, photoionization, ...
- Open source, `kromepackage.org`, Grassi+2014 (MNRAS)
- Highly optimized, "fast" solver (DLSODES)
- Can be coupled to hydrocodes, RAMSES, Enzo, FLASH, Gasoline, ...
- growing comunity, 19 papers, 2 schools (`kromepackage.org/bootcamp`)

KROME - Basic design



Minimum example

```
!init krome (once for all)
call krome_init()

!init species (1/cm3)
x(:) = 0d0
x(krome_idx_H2) = 1d4
x(krome_idx_O) = 1d0
x(krome_idx_C) = 0.5d0

!set Tgas (K)
Tgas = 5d1
```

```
!set time-step (s)
dt = 1d6*seconds_per_year

!call KROME
call krome(x(:), Tgas, dt)

!print results
print *,x(:)
print *,Tgas
```

Simple chemical network (example)

$H^+ + e^-$	$\rightarrow$	$H + \gamma$	recombination
$H + e^-$	$\rightarrow$	$H^- + \gamma$	radiative attachment
$H^+ + H^-$	$\rightarrow$	$H + H$	mutual recombination
$H + e^-$	$\rightarrow$	$H^+ + 2e^-$	collisional ionization
$H^- + H$	$\rightarrow$	$2H + e^-$	collisional detachment

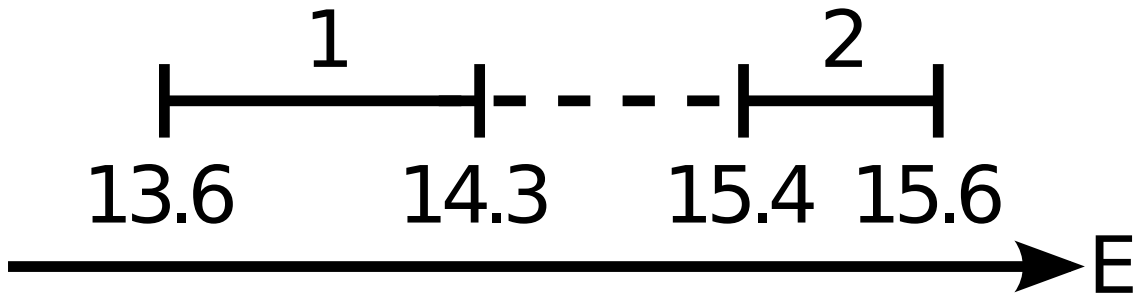
```
##############################
@format:idx,R,R,P,rate
1,H+,E,H,3.5d-12*(Tgas/3d2)**(-0.7)
2,H,E,H-,myLovelyFunction(Tgas)

@format:idx,R,R,P,P,rate
3,H+,H-,H,H,auto

@format:idx,R,R,P,P,P,rate
4,H,E,H+,E,E,auto
5,H-,H,H,H,E,auto
```

Photochemistry (example)

```
./krome -n network.ntw -usePhotoBins=2
```

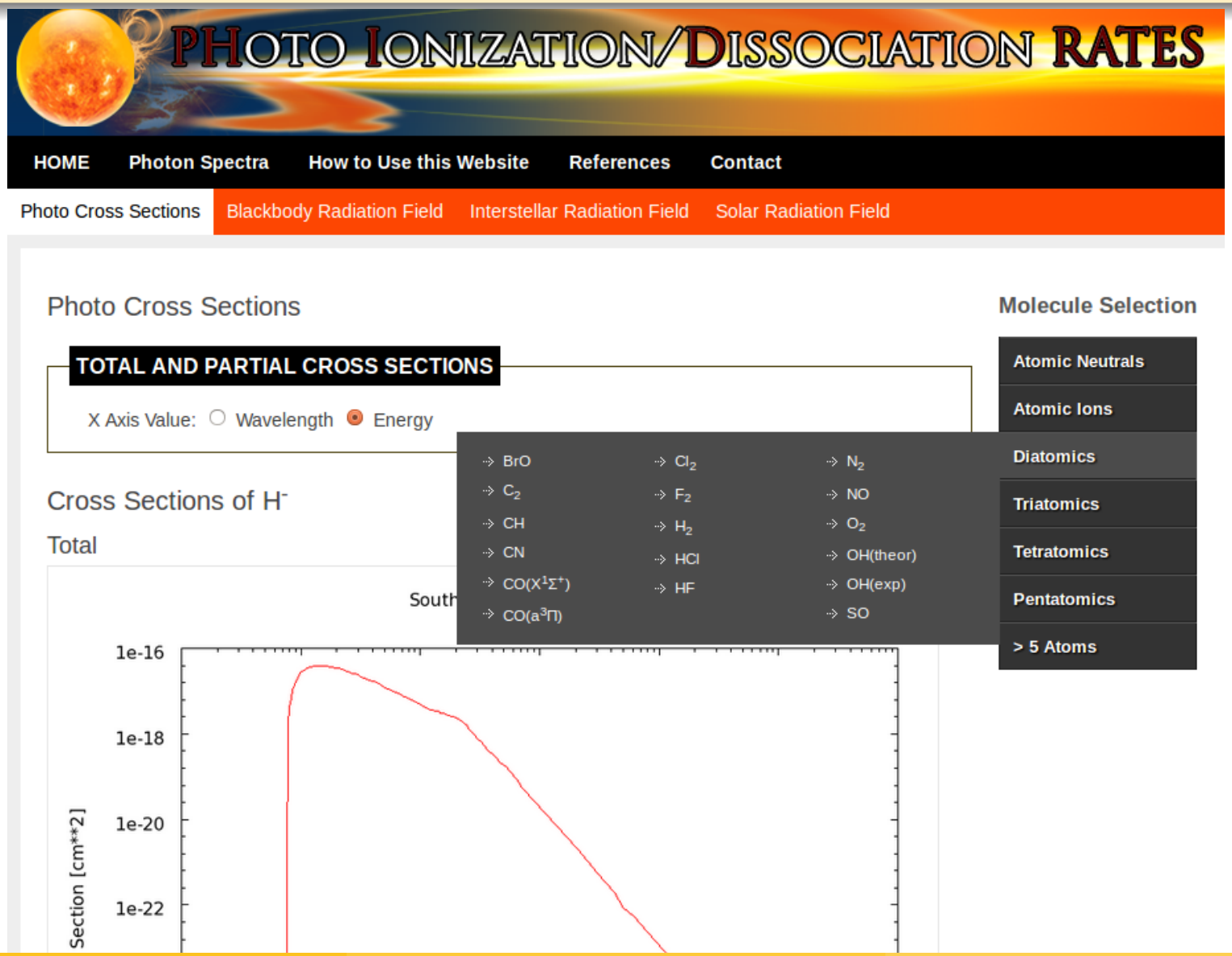



```
real*8::arrayL(krome_nPhotoBins)
real*8::arrayR(krome_nPhotoBins)
arrayL(:) = (/13.6d0, 15.4d0/) !eV
arrayR(:) = (/14.3d0, 15.6d0/) !eV
call krome_set_photobinE_lr(arrayL(:), arrayR(:))
mid(:) = krome_get_photoBinE_mid()
print *,mid(:)
```

```
13.9500000000000    15.5000000000000
```

Photochemistry/2 (SWRI database)

http://phidrates.space.swri.edu/



External cross section (network), e.g. $H^- + \gamma \rightarrow H + e^-$

```
@photo_start
 1,H-,H,E,@xsecFile=SWRI
@photo_end
```

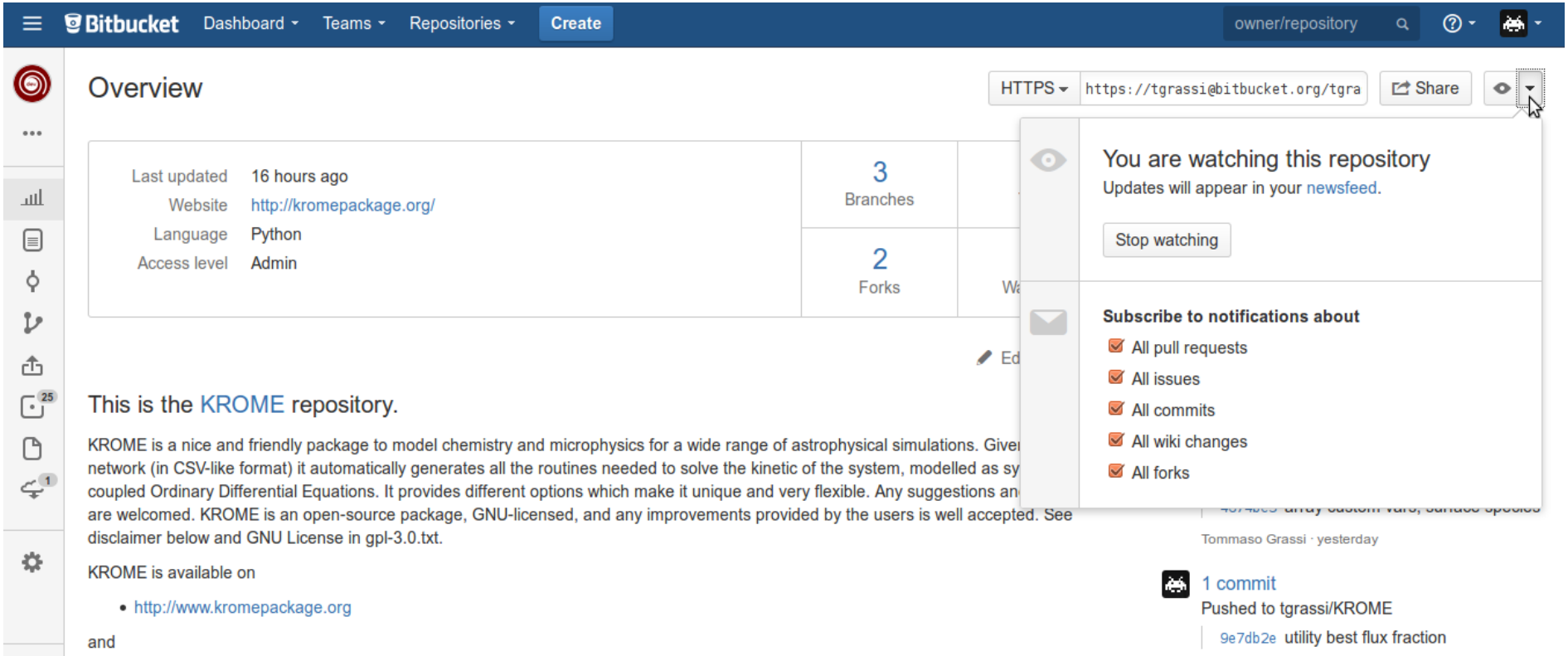
```
data/database/swri_xsecs/H-.dat
```

External cross section (data file)

```
 Branching ratio for H-    Total    2 branches
 Lambda   Total       H+/2e       H/e
    1.0   2.00E-27    0.00E+00    2.00E-27
    5.2   6.11E-25    4.58E-28    6.11E-25
   10.0   5.60E-24    9.00E-27    5.59E-24
   15.5   2.40E-23    6.22E-26    2.39E-23
   20.0   5.53E-23    1.87E-25    5.51E-23
    ...
```

KROME - bitbucket

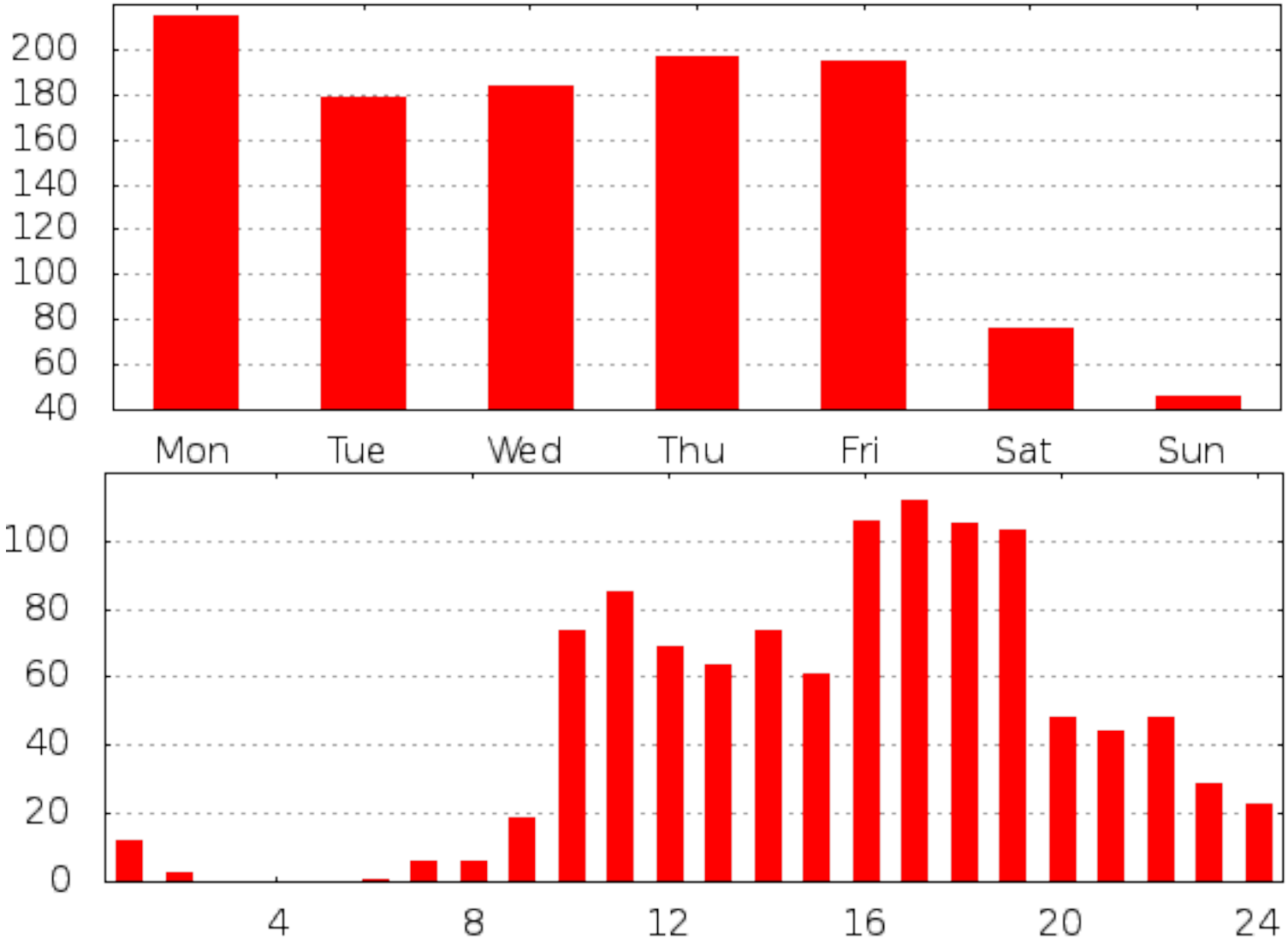
`bitbucket.org/tgrassi/krome`



Just google: kromeuser google groups

KROME - gitstat

sourceforge.org/gitstats



Prototypical problem

Context
Turbulent Molecular Clouds (w T.Haugbølle)

- Star-forming regions
- Complex structures at all scales
- Molecular richness (mainly H-C-O, but also F-S)
- Large CO variability
- CH^+ and SH^+ unexpected abundances
- CO-to-H_2 conversion factor still under investigation

Caveats and bottlenecks (computational)

- Multi-scale interaction
- Chemistry/microphysics at different scales (“hierarchical chemical legacy”)
- Non-trivial coupling between “pure” chemistry, microphysics, and dynamics
- Radiative-transfer and other amenities

Prototypical problem/2

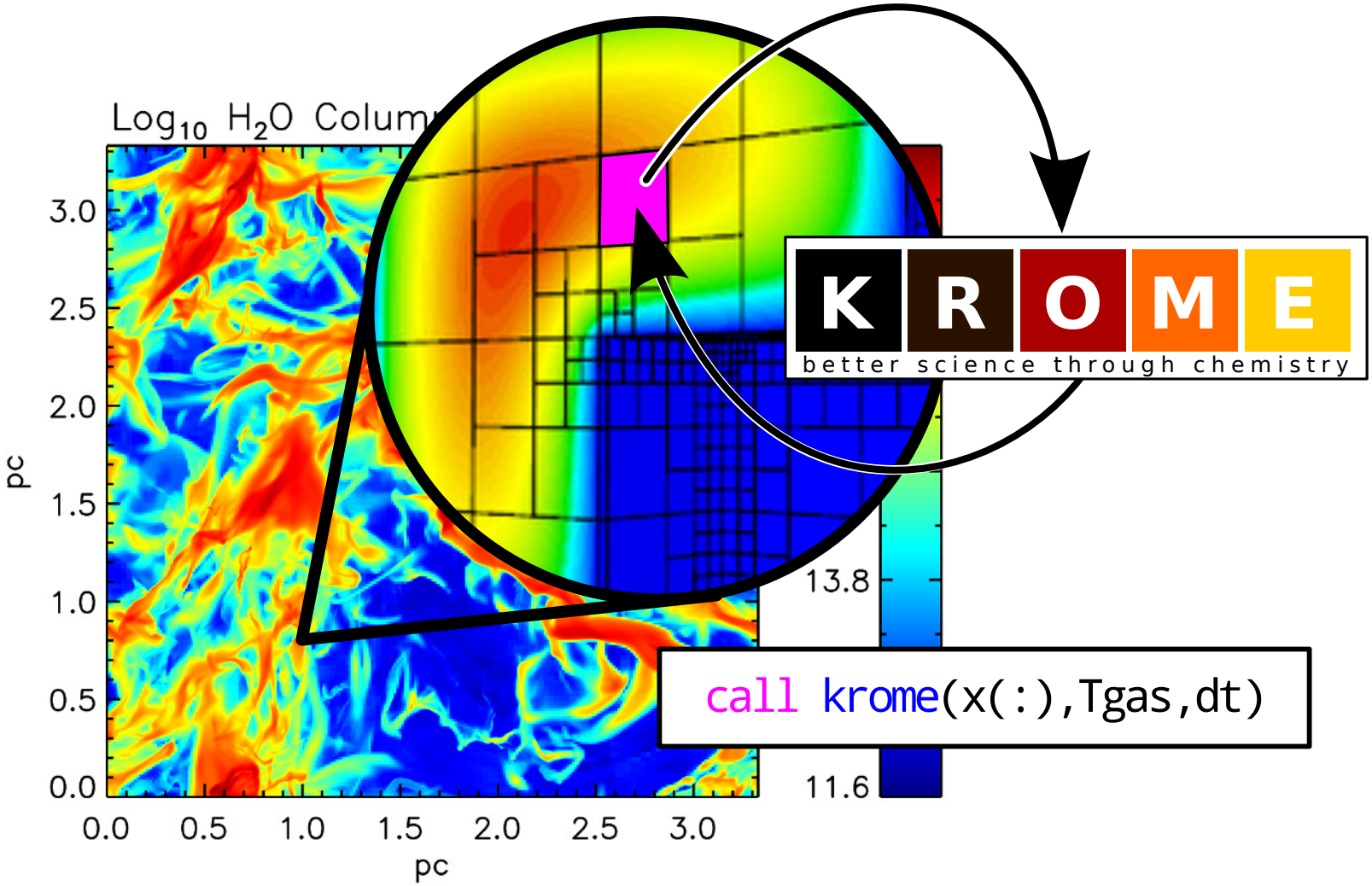
RAMSES-CPH (+KROME, w T.Haugbølle)

- Non-equilibrium H-C-O chemistry (+CRs, +photo, ∼Glover+2009)
- Fully coupled thermochemistry (on-the-fly fine-structure +tables, ∼Maio+2007)
- Consistent adiabatic index (partition functions, Boyle+2007)
- Dust chemistry (H_2,Cazaux+2009), dust cooling/photoheating (Dopcke+2011)
- Workaround: local density-based photochemisty, i.e. $A_v = f(n_{\rm tot})$
- Optional: access to photochemistry-based opacity (RT-ready)
- Testing: more dust chemistry (Hocuk+2015) + dust tables (Grassi+2015 in prep.)

Molecular cloud model details

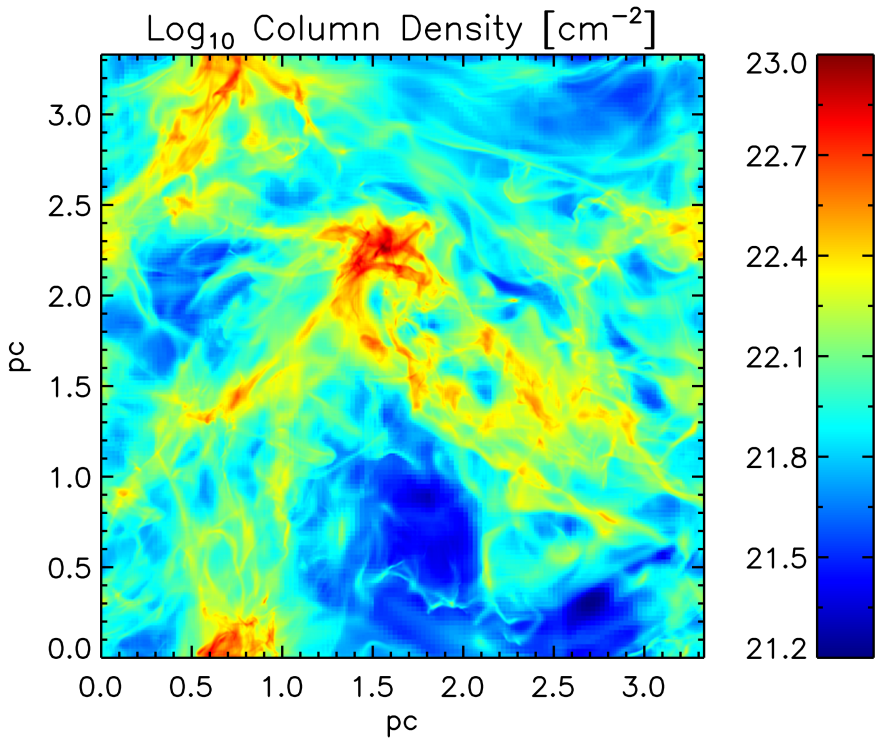
- MHD
- $\simeq 3.3 \times 3.3 \times 3.3$ pc
- Turbulence: Mach 11 @ 10 K
- $\langle n_{\rm tot} \rangle \simeq 10^3$ cm^{-3}
- $\langle B \rangle \simeq 7\ \mu$G
- > 18 Mcells
- 4.7 Myr $\simeq 3.5\,\tau_d \simeq 4.5\,\tau_{ff}$
- ~ 300 rates, ~ 40 species

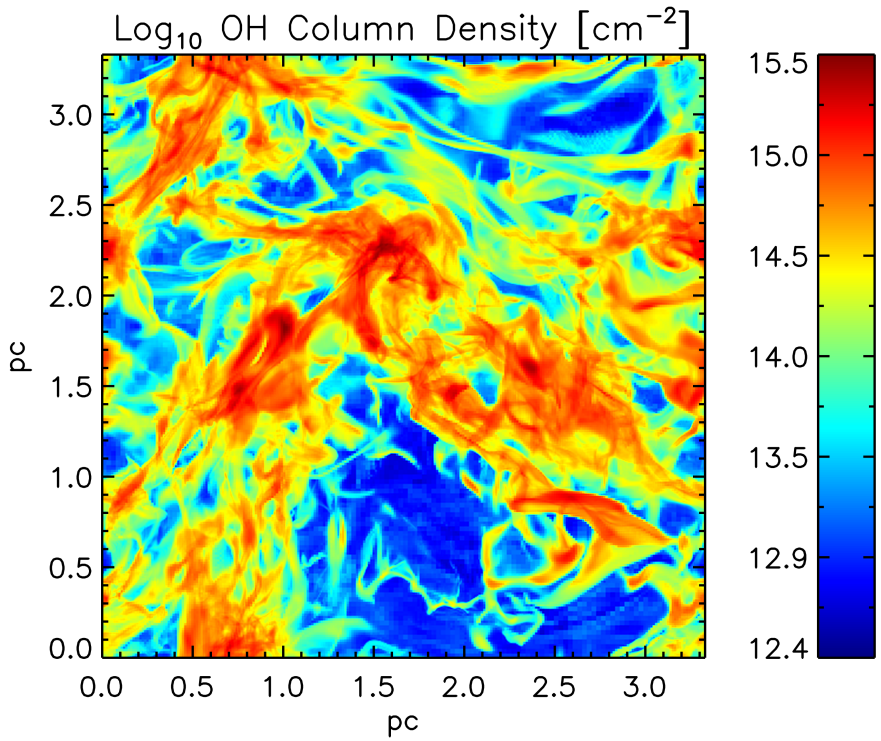
Cell-by-cell



- A set of one-zone models: one for each cell (this case $\gtrsim 18$M).

RAMSES+KROME results





Modelling: getting started/1

Problem 1 - nodes (species)

atoms (H, He, C, N, O, Si, Ne, S, P, F, Al, ...)?
species (H, H2, CO, CH, ...)?
cations and anions (H^-, H^+, C^{3+}, CH^- ...)?
isomers (HOC^+, HCO^+, ...)?
isotopes ($^{12}C^{16}O$, $^{13}C^{16}O$, ...)?
"fancy" stuff (dust, PAH, ...)?

Problem 2 - edges (reactions)

bimolecular ($OH^+ + e^- \rightarrow O + H$)?
photochemsitry ($H^- + \gamma \rightarrow H + e^-$)
cosmic rays ($CO + CR \rightarrow C + O$)
cosmic rays secondary ($CO + CRP \rightarrow C + O$)
3-body ($H + H + H_2 \rightarrow H_2 + H_2$)

you can always expand a chemical network

Modelling: getting started/2

Problem 3 - rate coefficients

$$\mathrm{A+B} \xrightarrow{k} \mathrm{C+D}$$

$$\dot{n}_{\mathrm{A}}(t) = -k(T)\, n_{\mathrm{A}}(t)\, n_{\mathrm{B}}(t)$$

Methods to determine $k(T)$

- Experimental (lucky, often single T)
- Langevin (estimate, constant T, could be completely off!)
- Physical considerations (e.g. HD==H_2, extremely dangerous!)
- *ab initio* calculations (not always available, small systems only)

How to retrieve $k(T)$?

- Databases (KIDA, UMIST, . . .)
- Literature search (best, but time-consuming)
- Do it yourself! (strongly discouraged)
- Educated guess (also strongly discouraged)
- Ask a (theoretical) chemist!

Modelling: getting started/3

Problem 4 - initial conditions

- metallicity
- individual metallicity ratios (e.g. C/O is critical)
- ionization level
- temperature(s)
- dust content
- . . .

Problem 5 - ambient

- density range
- temperature range
- radiation flux (mainly UV, X)
- extinction (opacity, self-shielding)
- cosmic ray ionization flux
- dust type, size, distribution, . . .
- . . .

Think first, code later

Summary/Outlook

- KROME is a state-of-the-art and growing code
- note: KROME takes care of chemistry/microphysics
- fully-consistent non-equilibrium microphyiscs/chemistry
- KROME is flexible
- KROME successfully coupled with 3D simulations (but not only)

The eternal struggle (aka: cheap, fast, accurate. pick two)

$$\text{ACCURACY} \longleftrightarrow \text{EFFICIENCY}$$

Perspective

- go beyond compuational bottlenecks (solver: ~~GPU~~, vectorization, Xeon-Phi)
- improve dust model (see also above)
- release environment-tailored recipes (Bovino+2015, submitted)
- improve user interface and network format (coming soon)
- test! test! test!

Thank you for your attention!

"A git pull a day, keeps the doctor away."
(github.com/AntJanus)

T.Haugbølle (NBI), S.Bovino (UniHam), D.Schleicher (UniCon)
J.Ramsey (NBI), D.Seifried (UniKöln)
D.Galli (INAF), M.Satta (CNR), E.Simoncini (INAF)

`kromepackage.org/`
`kromepackage.org/bootcamp`
`bitbucket.org/tgrassi/krome`