Microphysics and chemistry modelling with KROME

Tommaso Grassi
tgrassi@nbi.dk

University of Copenhagen
STARPLAN - Centre for Star and Planet Formation

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Collaborators

STARPLAN

T. Haugbølle, Å. Nordlund, T. Frostholm, M. Küffmeier, S. Friemann, S. Dib, J. Ramsey, . . .

Others involved in KROME

- **D.R.G.Schleicher, S.Bovino, M.Latif** (Göttingen University, ENZO)
- **J.Prieto** (Conception University, RAMSES)
- **D.Seifried** (Köln University, FLASH)
- **E.Simoncini** (INAF Arcetri, planetary atmospheres, biomarkers)
- **D.Galli** (INAF Arcetri, chemical networks)
- **E.Tognelli** (Pisa University, thermonuclear networks in stars)
- **M.Satta** (CNR, University of Rome, theoretical chemistry)
- **F.A.Gianturco, F.Carelli** (University of Innsbruck, theoretical chemistry)
- **S.Danielache** (Tokyo Inst. of Technology, primordial Earth chemistry)
- **K.Omukai** (Tohoku University, Early Universe)

Why chemistry?

"Chemistry has been termed by the physicist
as the messy part of physics"
(Frederick Soddy)

ISM chemistry

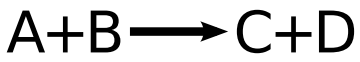
Why chemistry/microphysics? (in numerical simulations)

- 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 (see next slides)
- comparison with observations

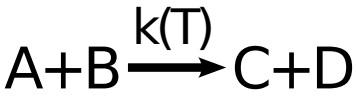
Why chemistry/microphysics is troublesome (in numerical simulations)

- very CPU demanding (solving stiff ODEs)
- has a non-linear/complex behaviour (e.g. MC)
- connected with (and influenced by) many physical processes (next slides)
- needs accurate rates for reaction rates
- network completeness (include all the necessary species)

Chemistry, the full story (1/24)

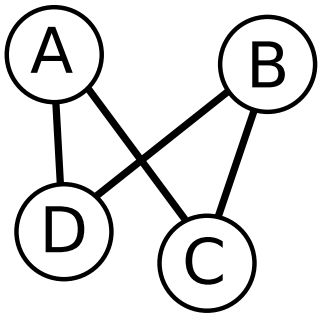


Chemistry, the full story (2/24)

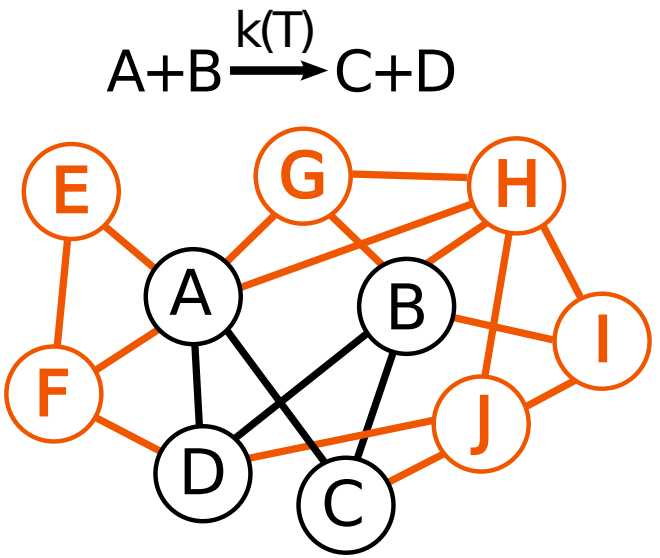


Chemistry, the full story (3/24)

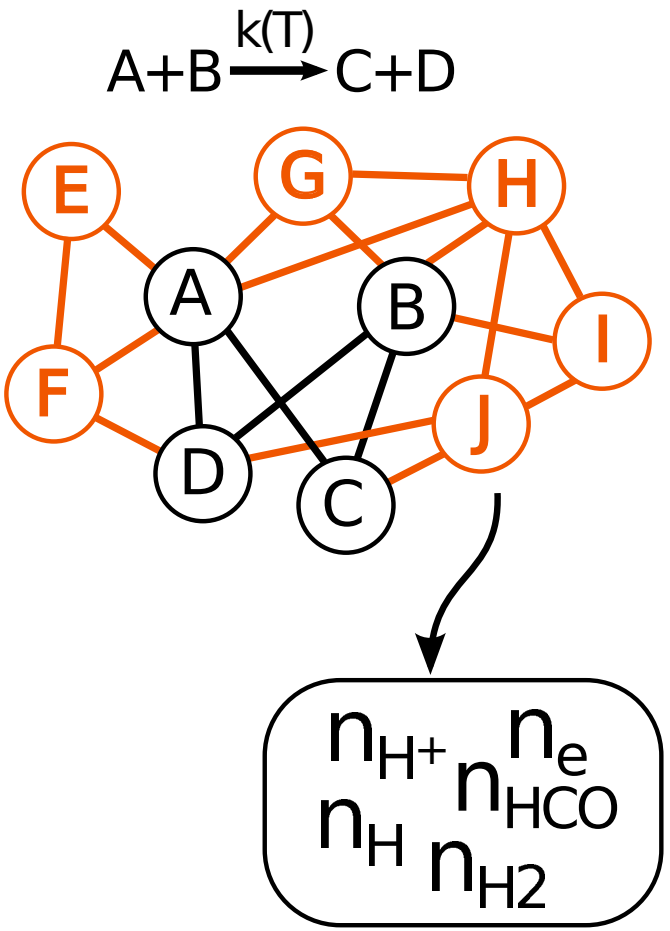
$$A + B \xrightarrow{k(T)} C + D$$



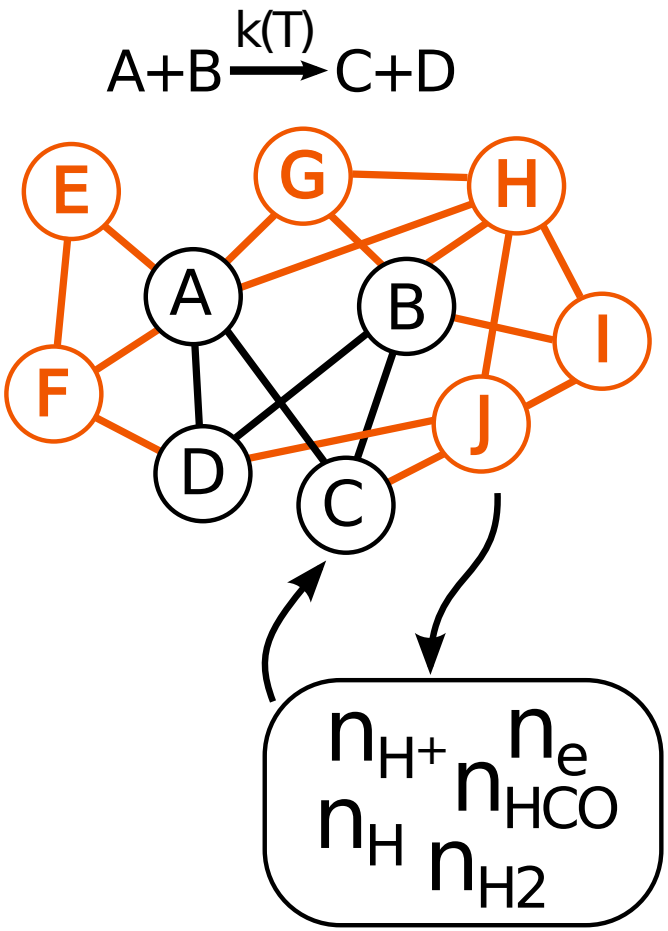
Chemistry, the full story (4/24)



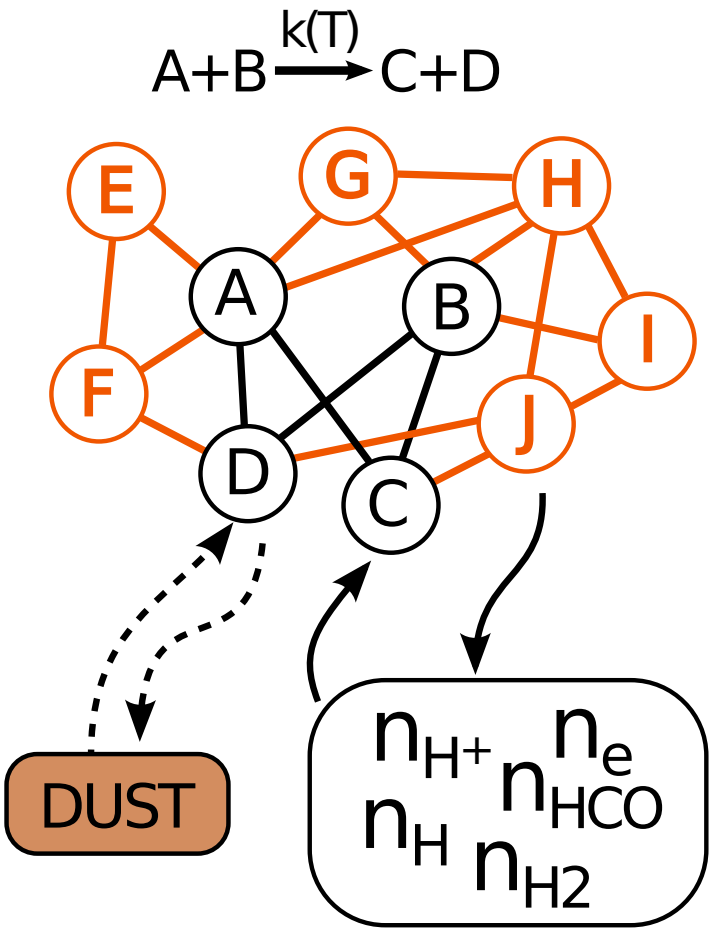
Chemistry, the full story (5/24)



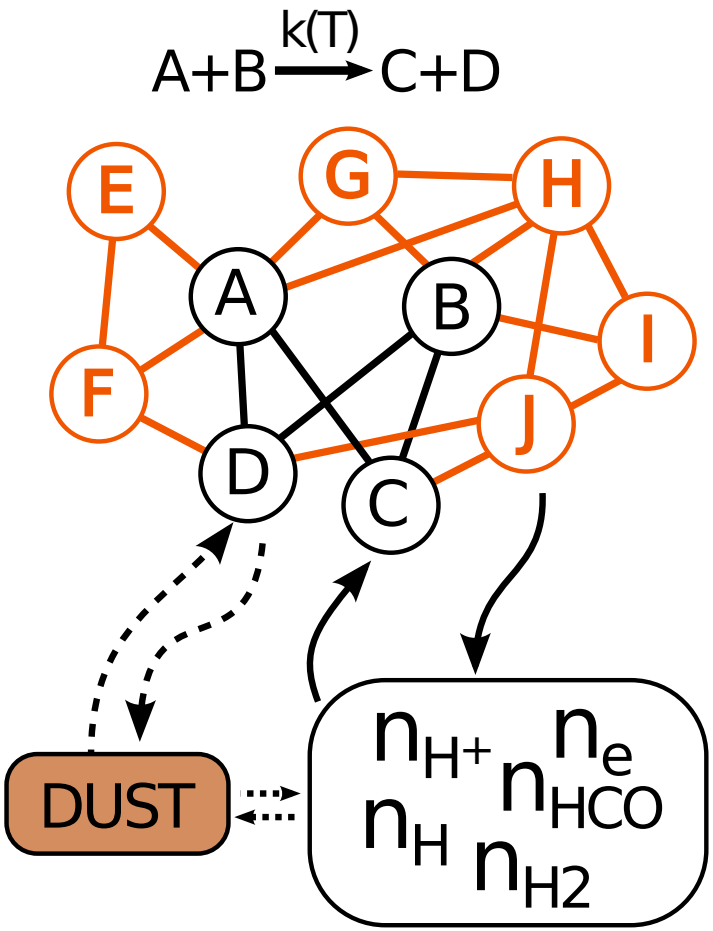
Chemistry, the full story (6/24)



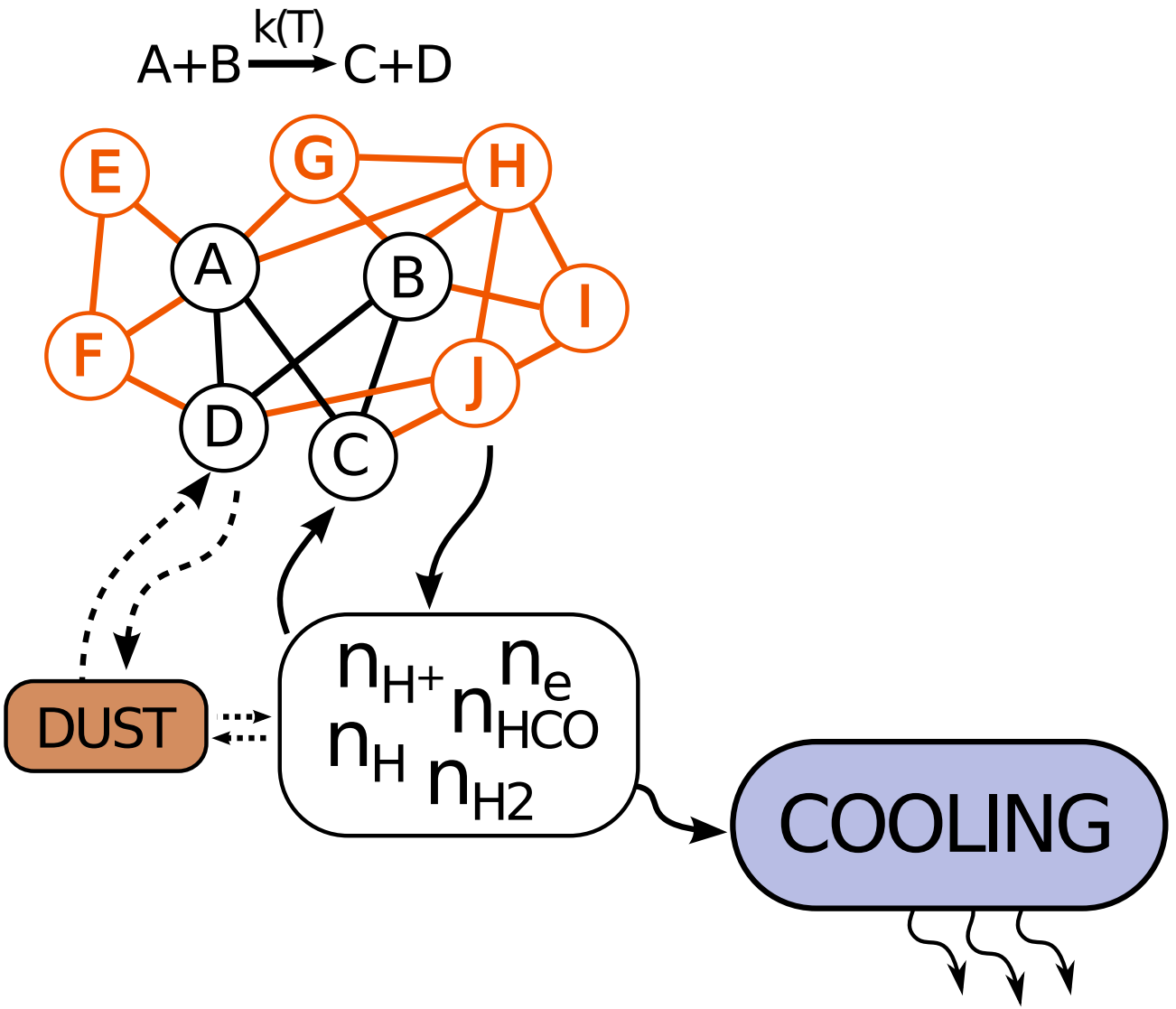
Chemistry, the full story (7/24)



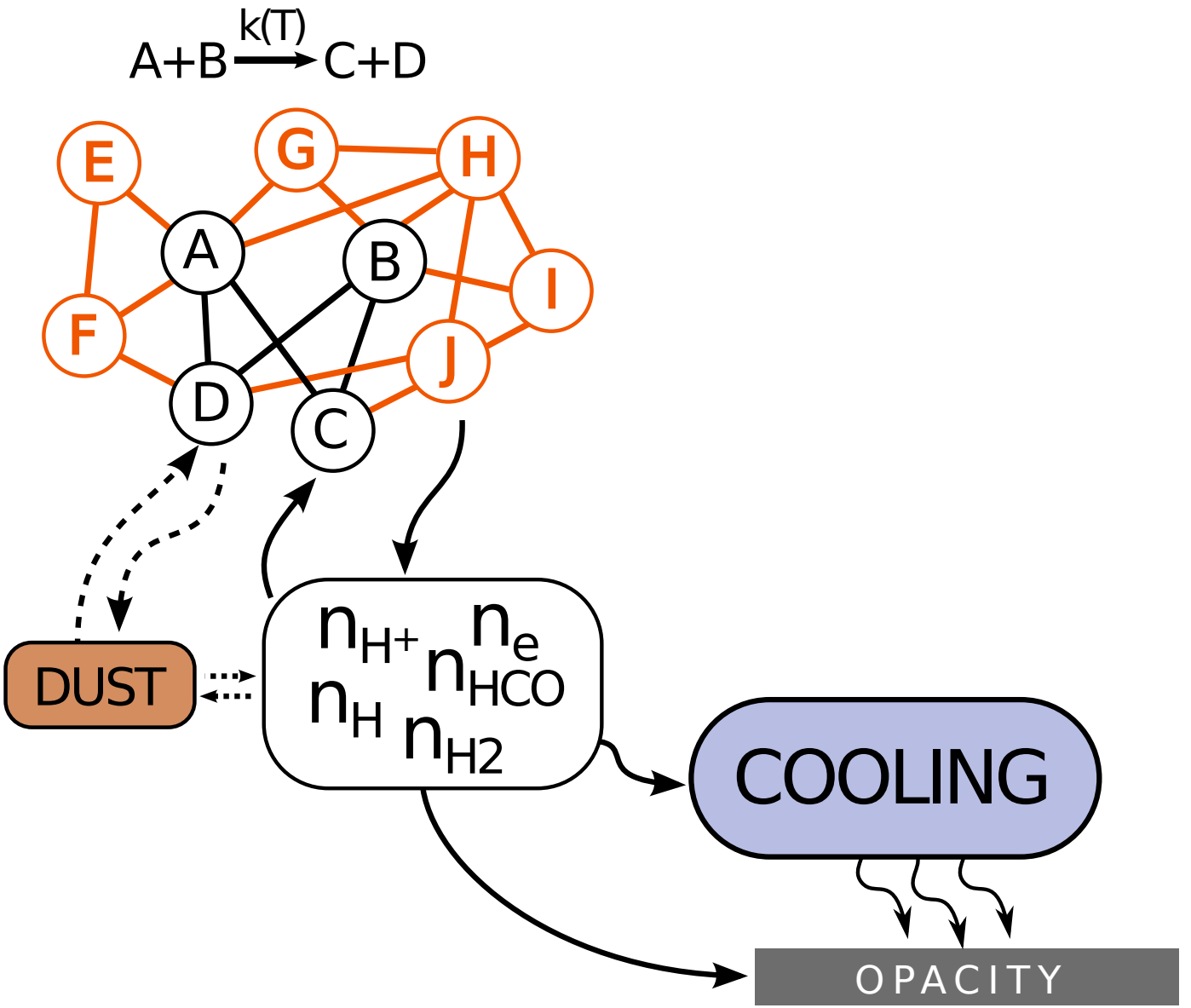
Chemistry, the full story (8/24)



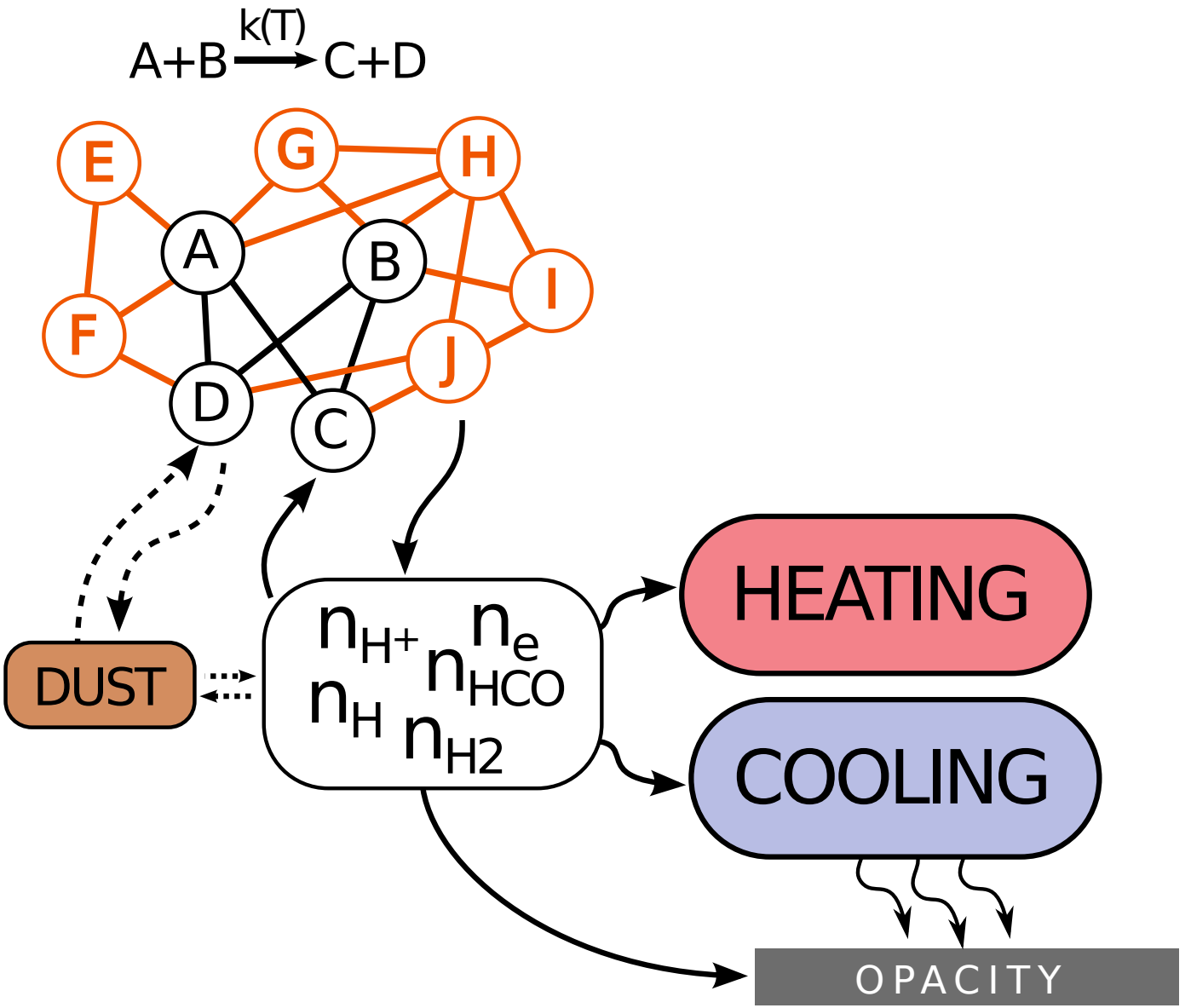
Chemistry, the full story (9/24)



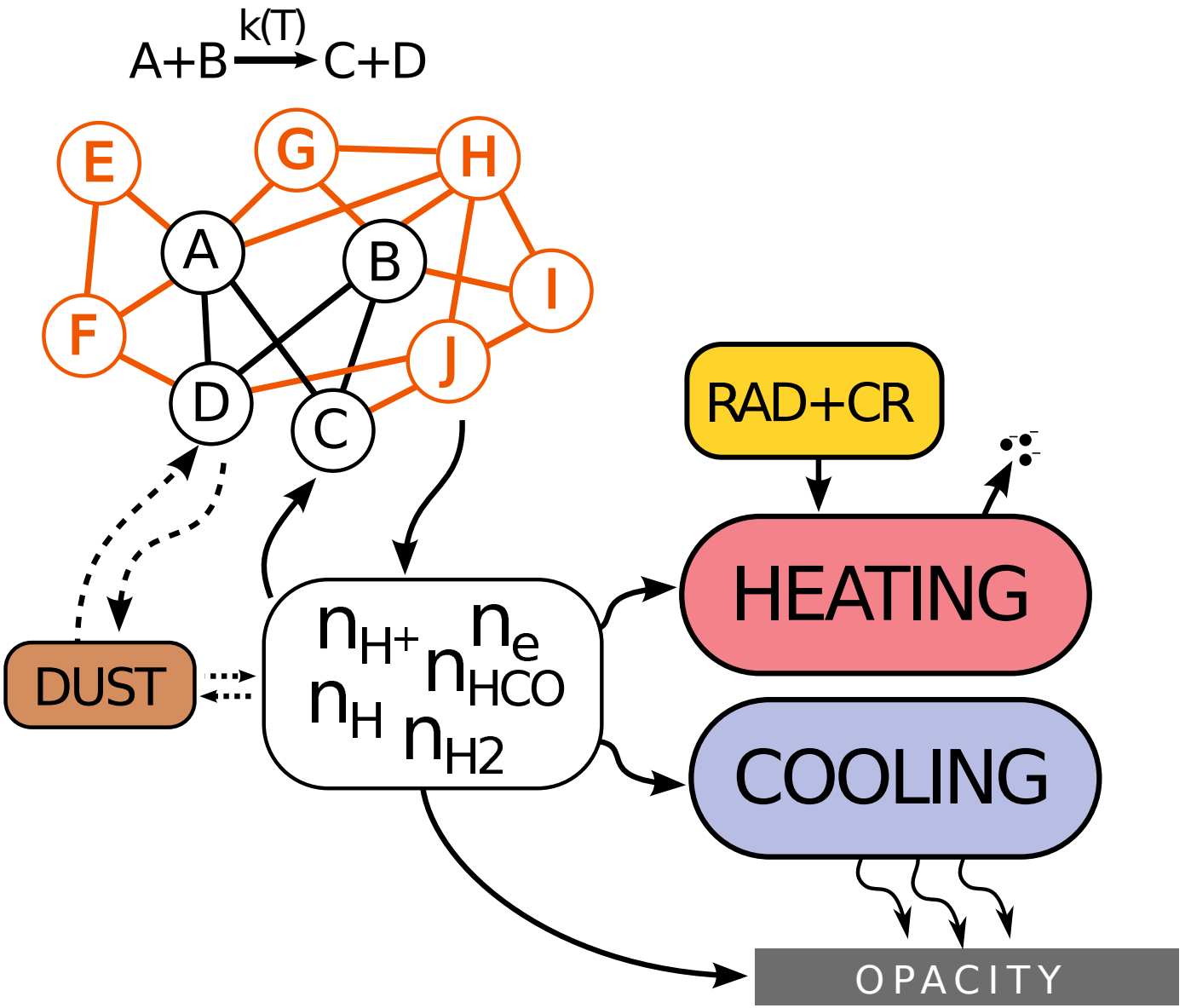
Chemistry, the full story (10/24)



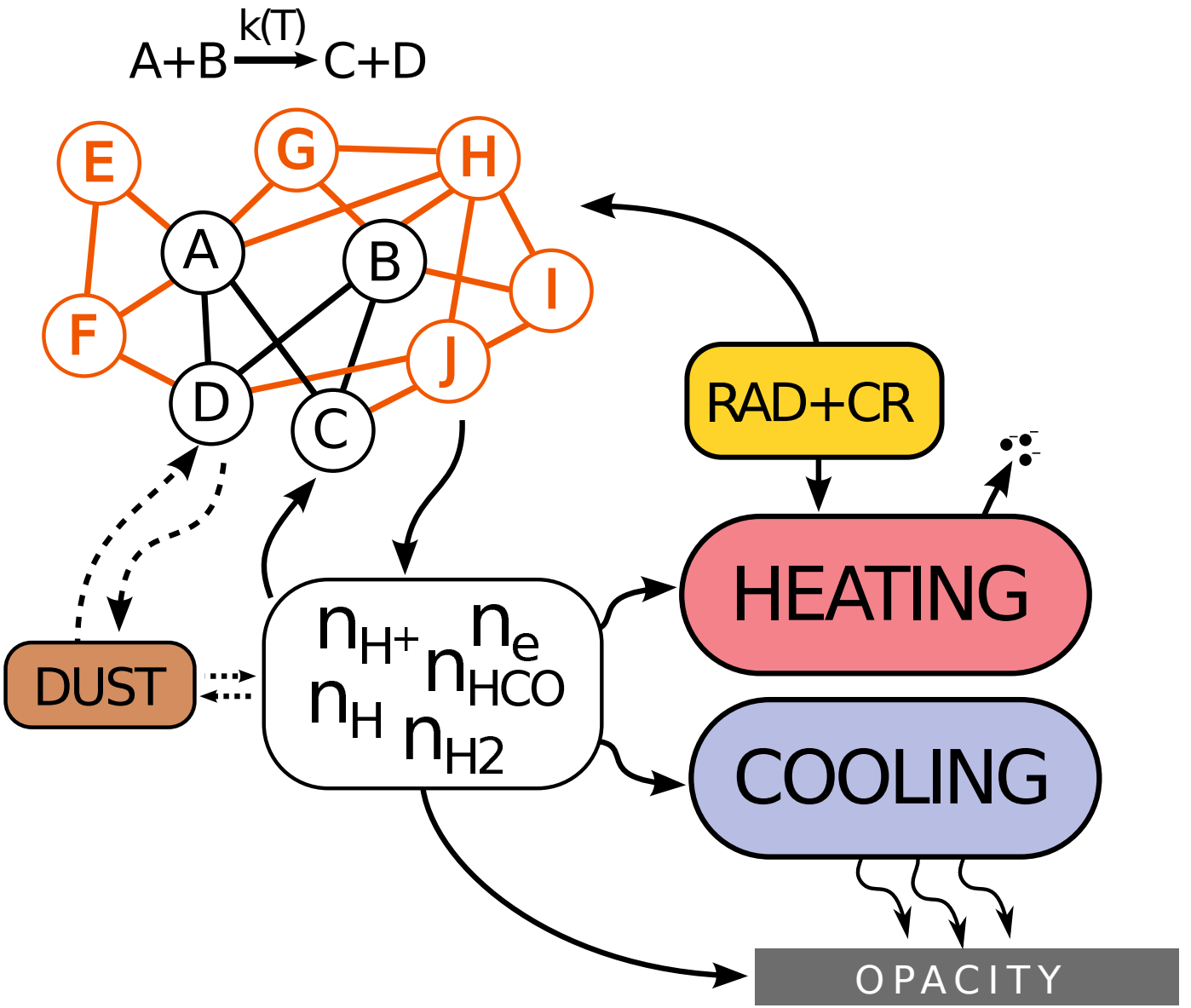
Chemistry, the full story (11/24)



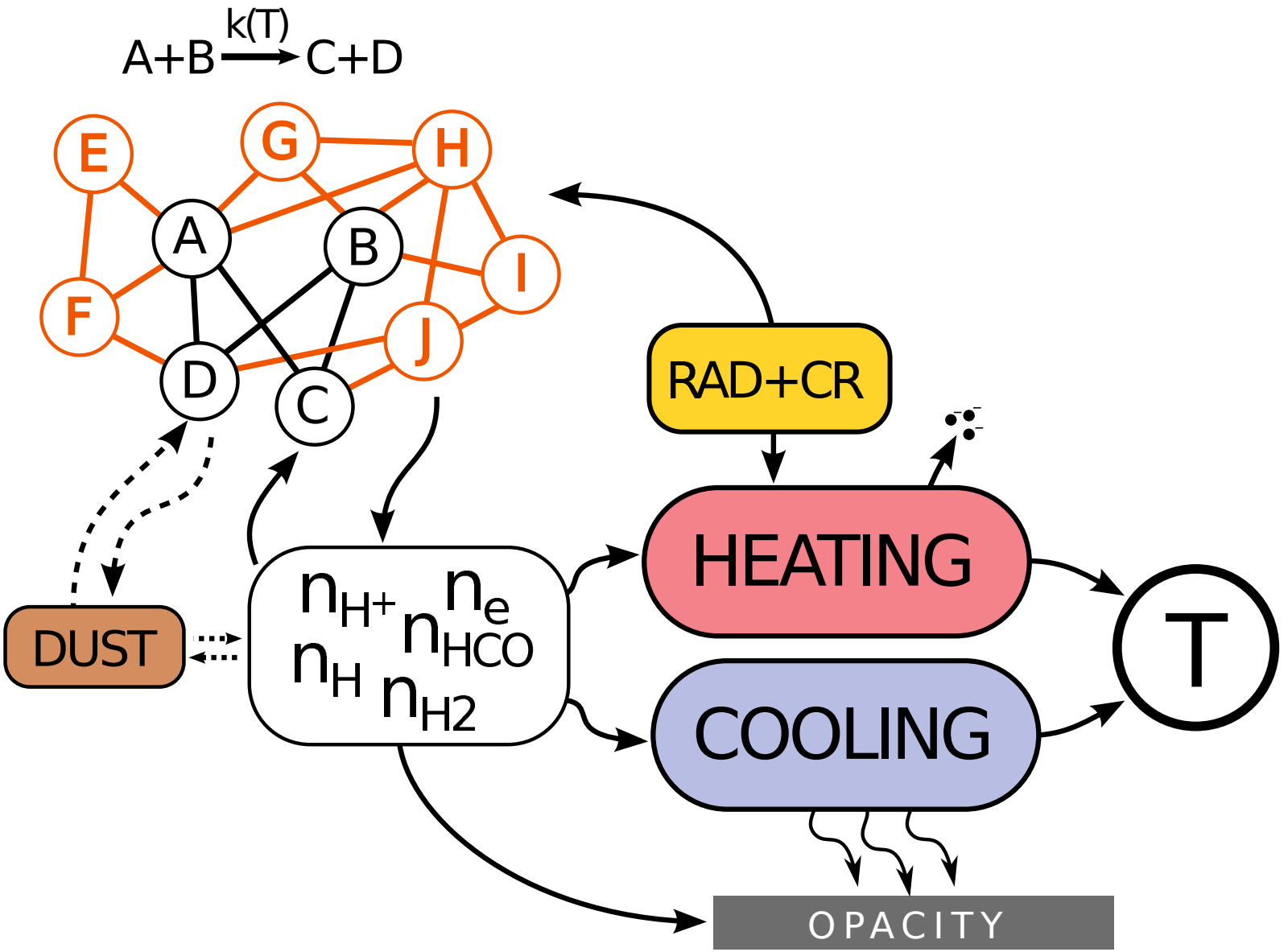
Chemistry, the full story (12/24)



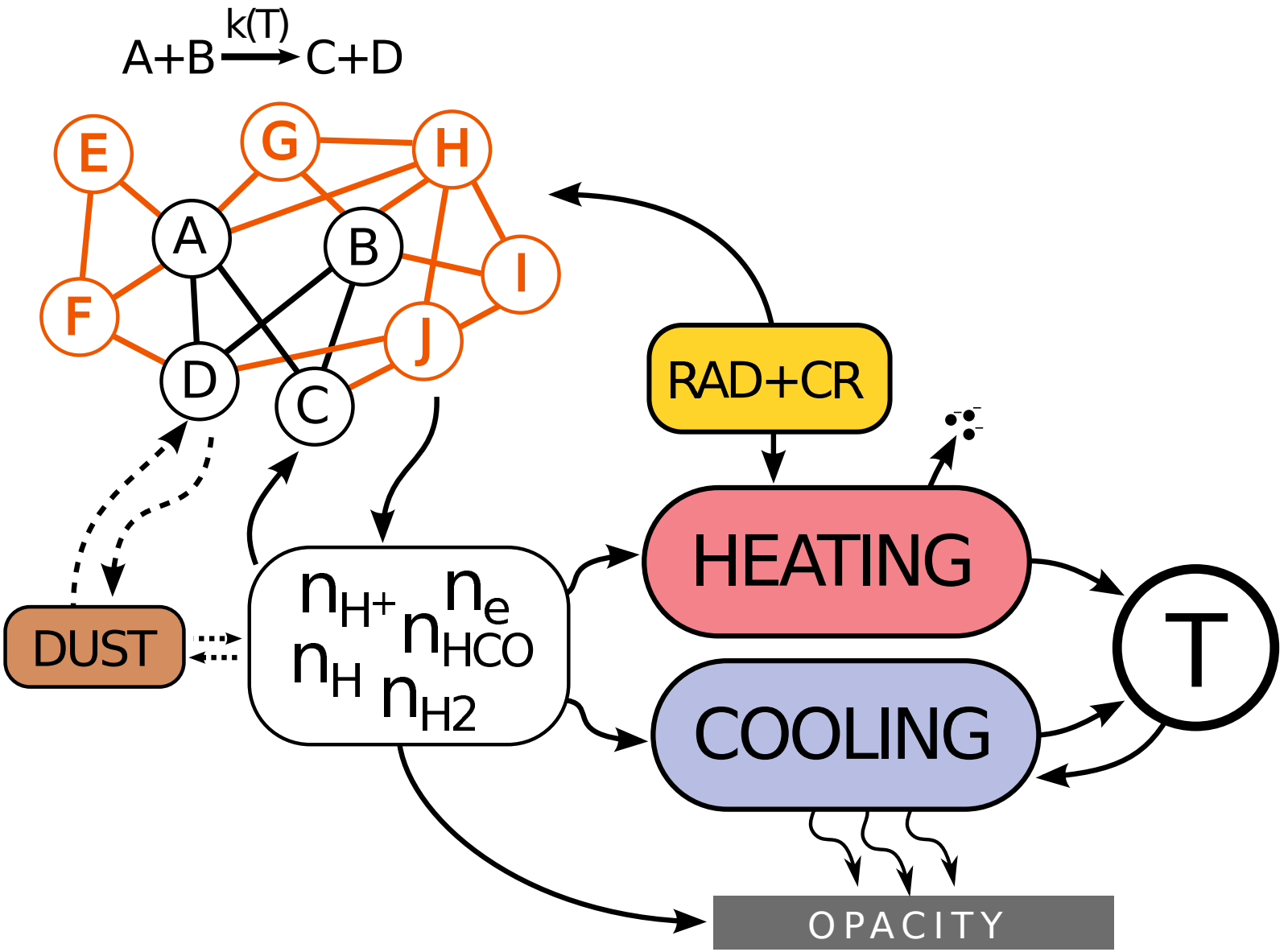
Chemistry, the full story (13/24)



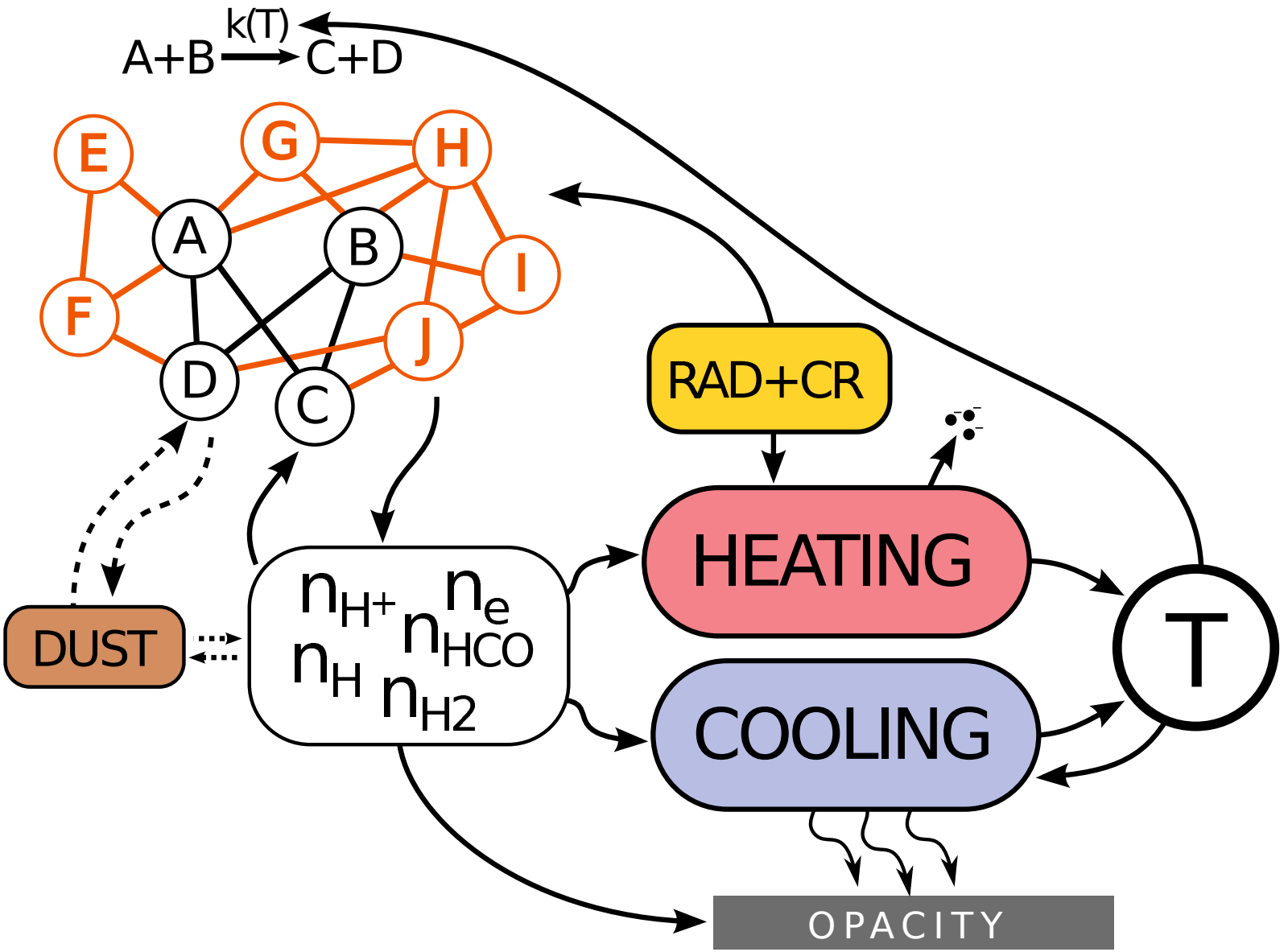
Chemistry, the full story (14/24)



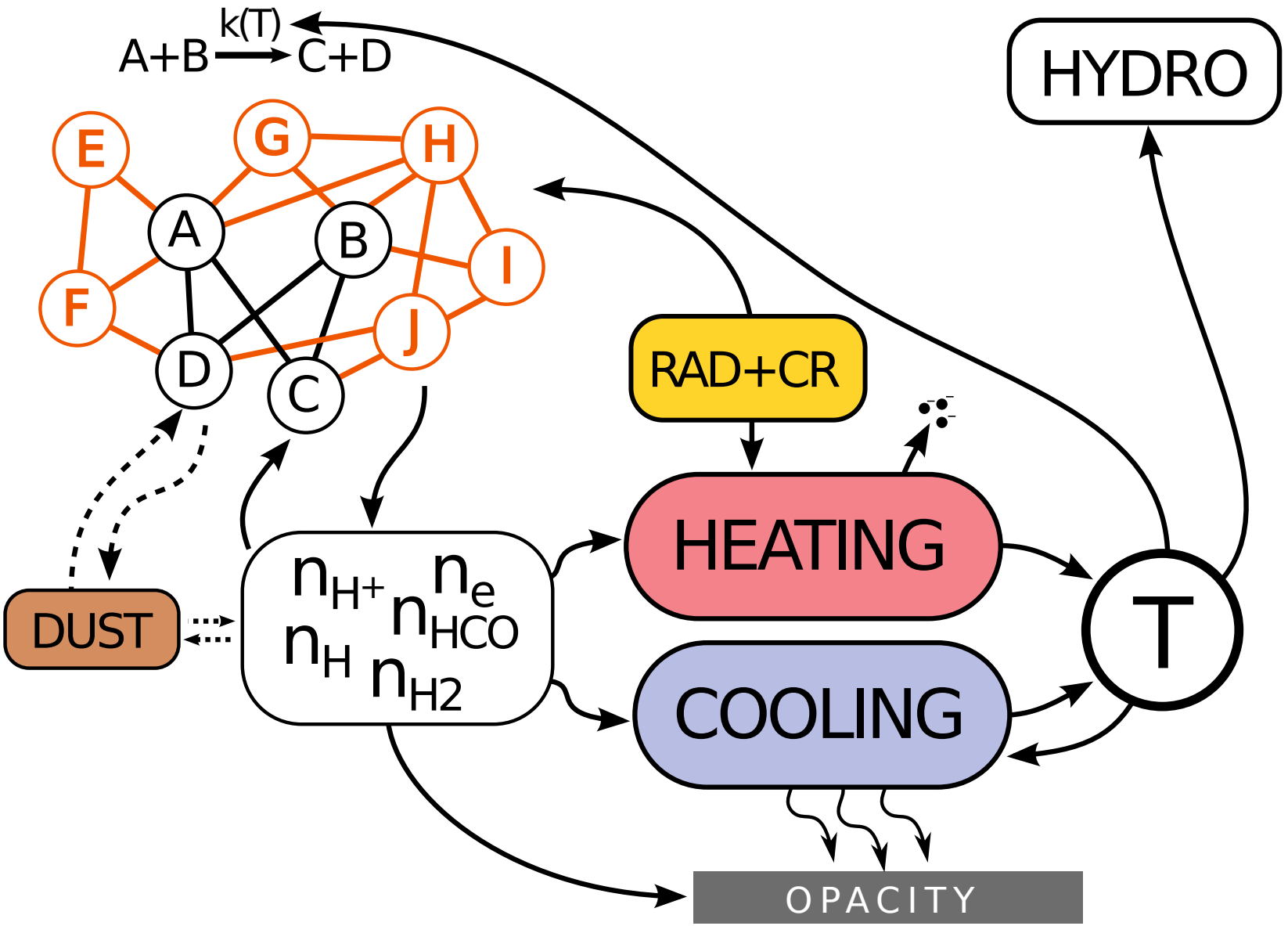
Chemistry, the full story (15/24)



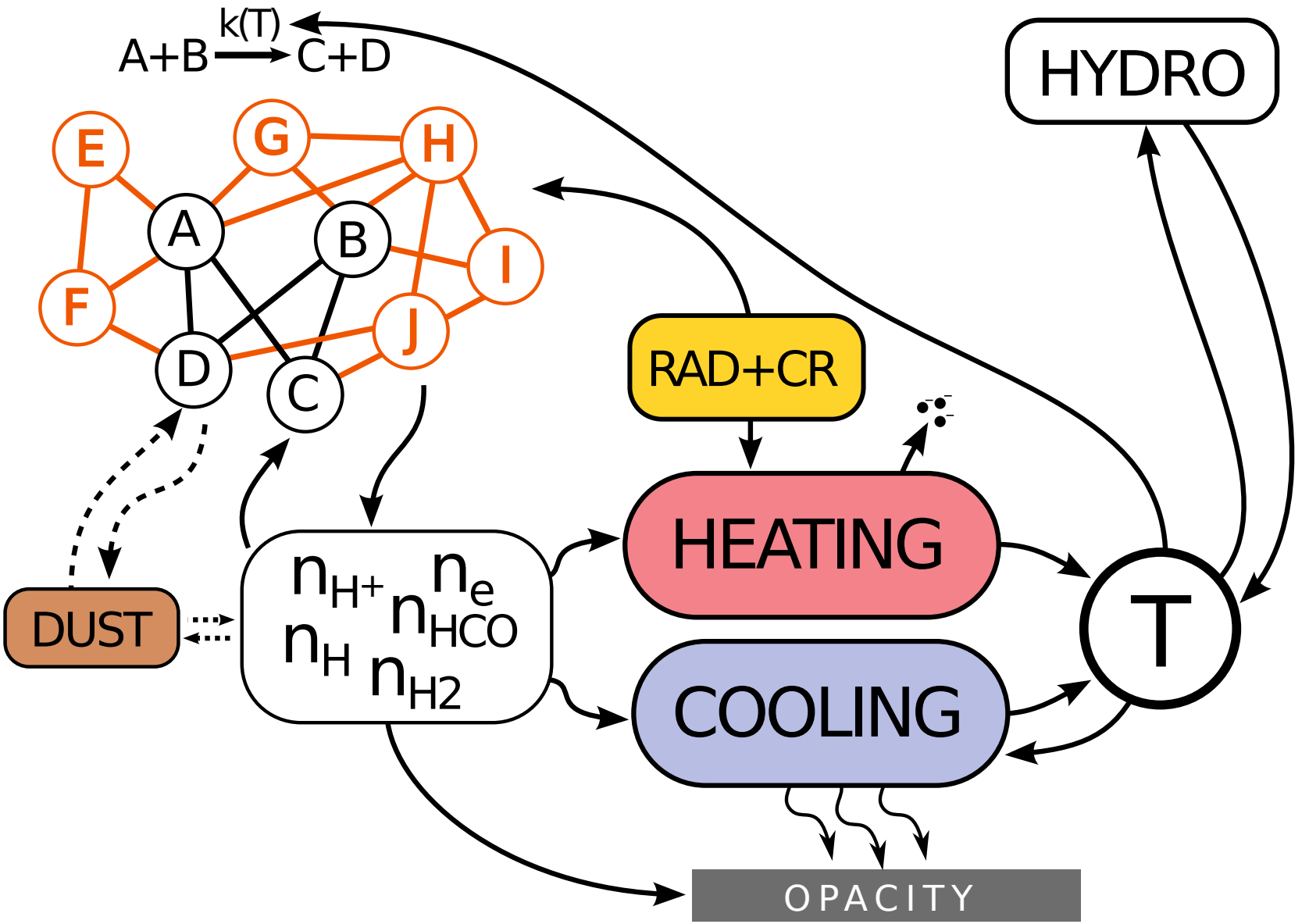
Chemistry, the full story (16/24)



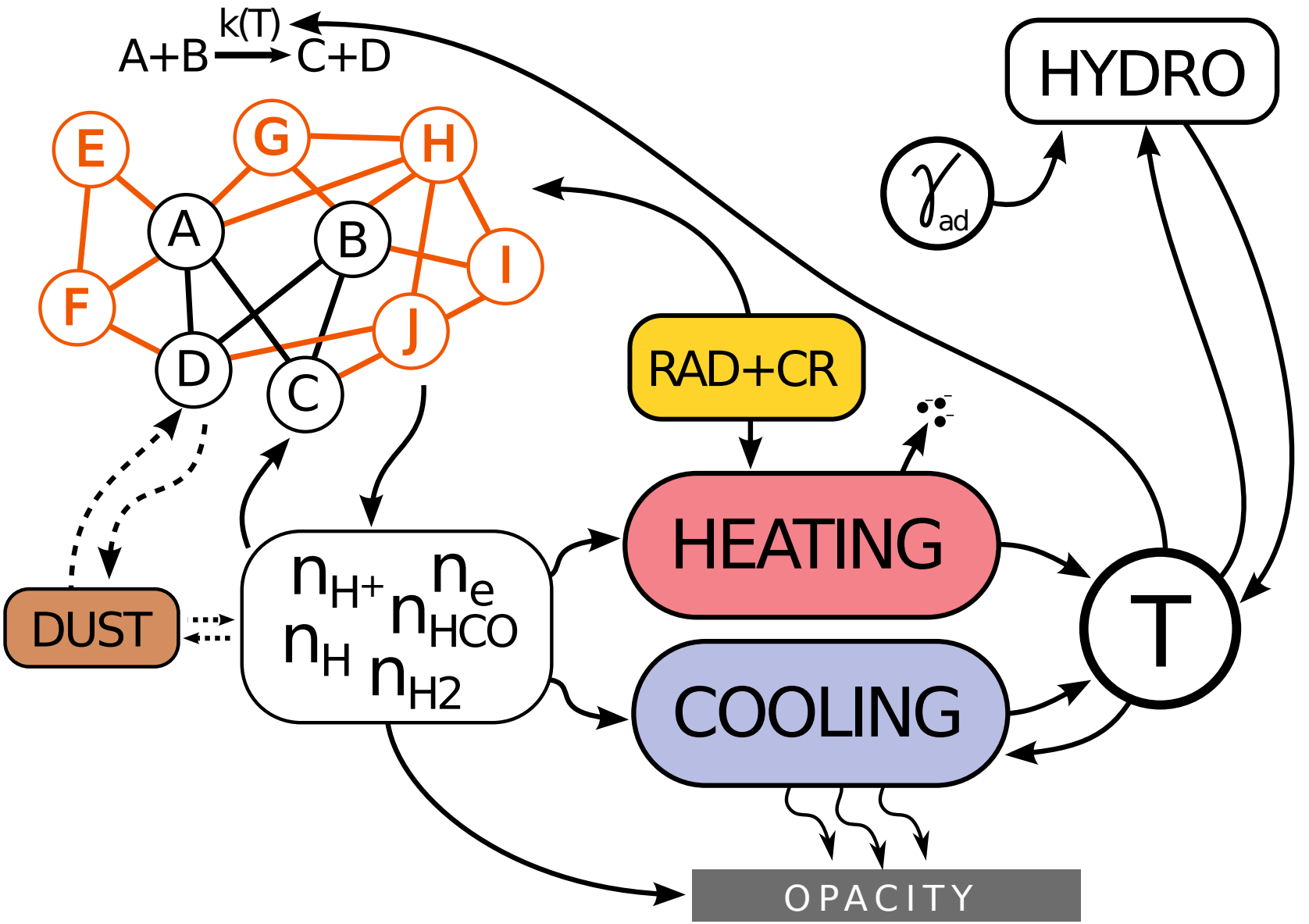
Chemistry, the full story (17/24)



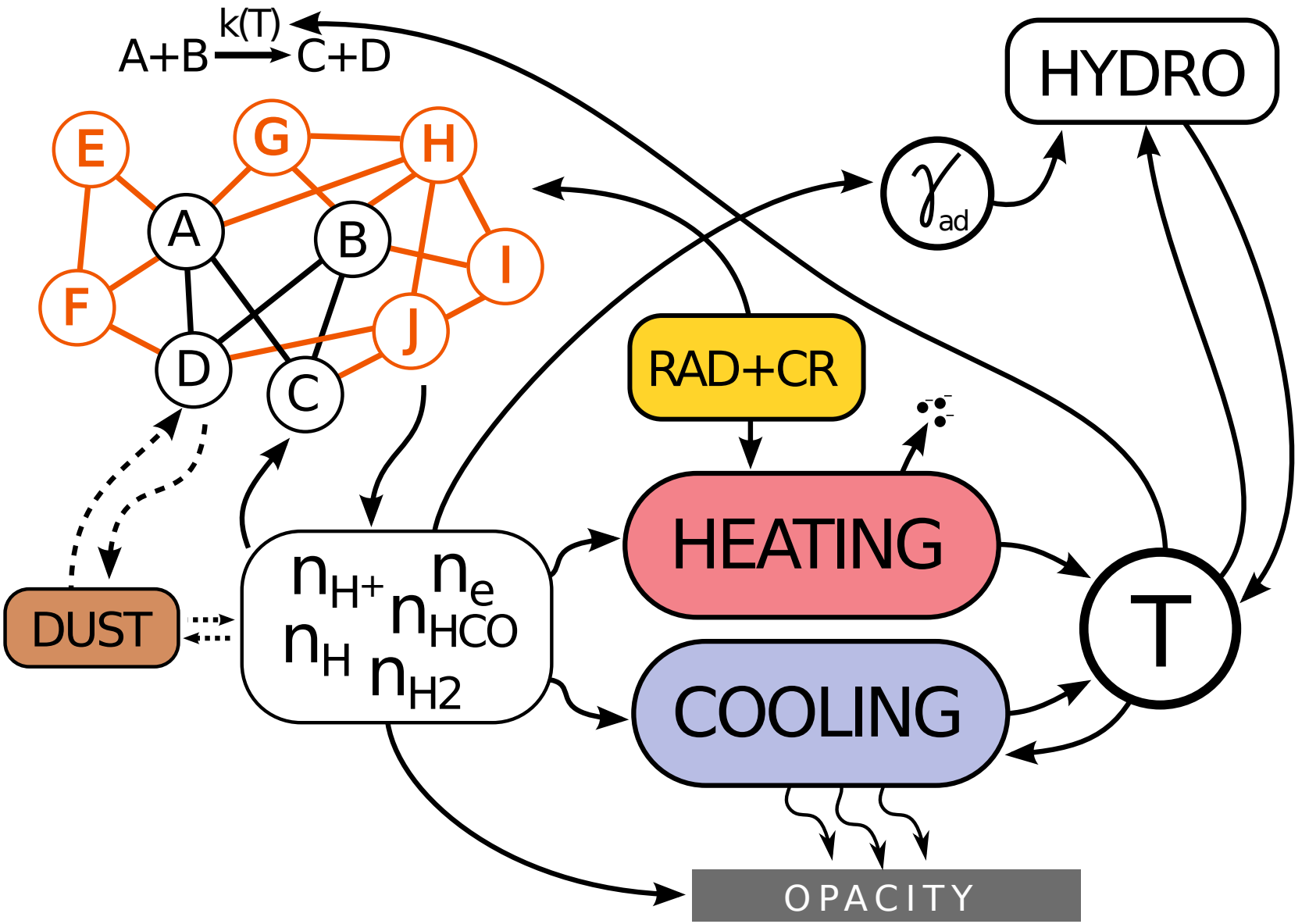
Chemistry, the full story (18/24)



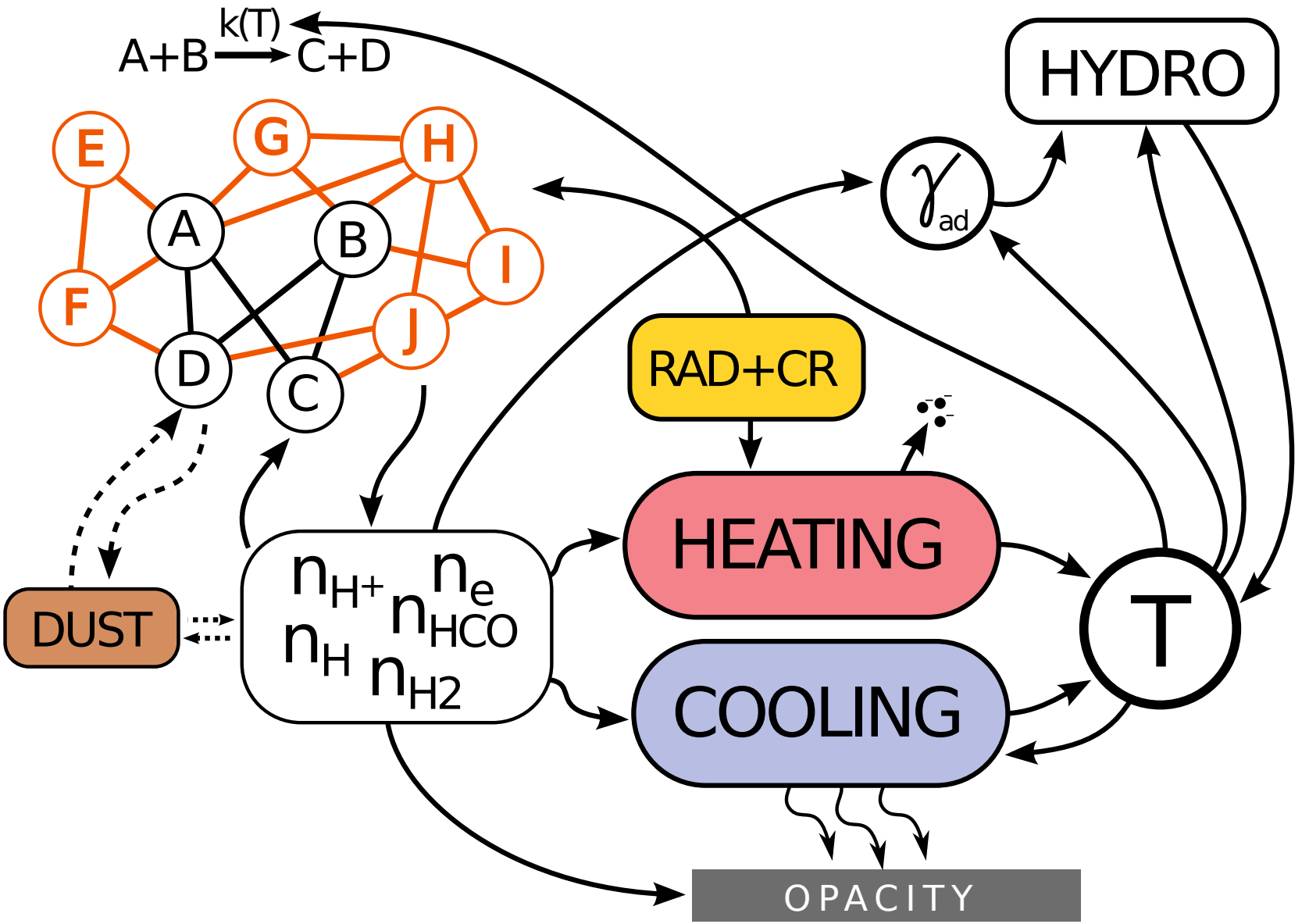
Chemistry, the full story (19/24)



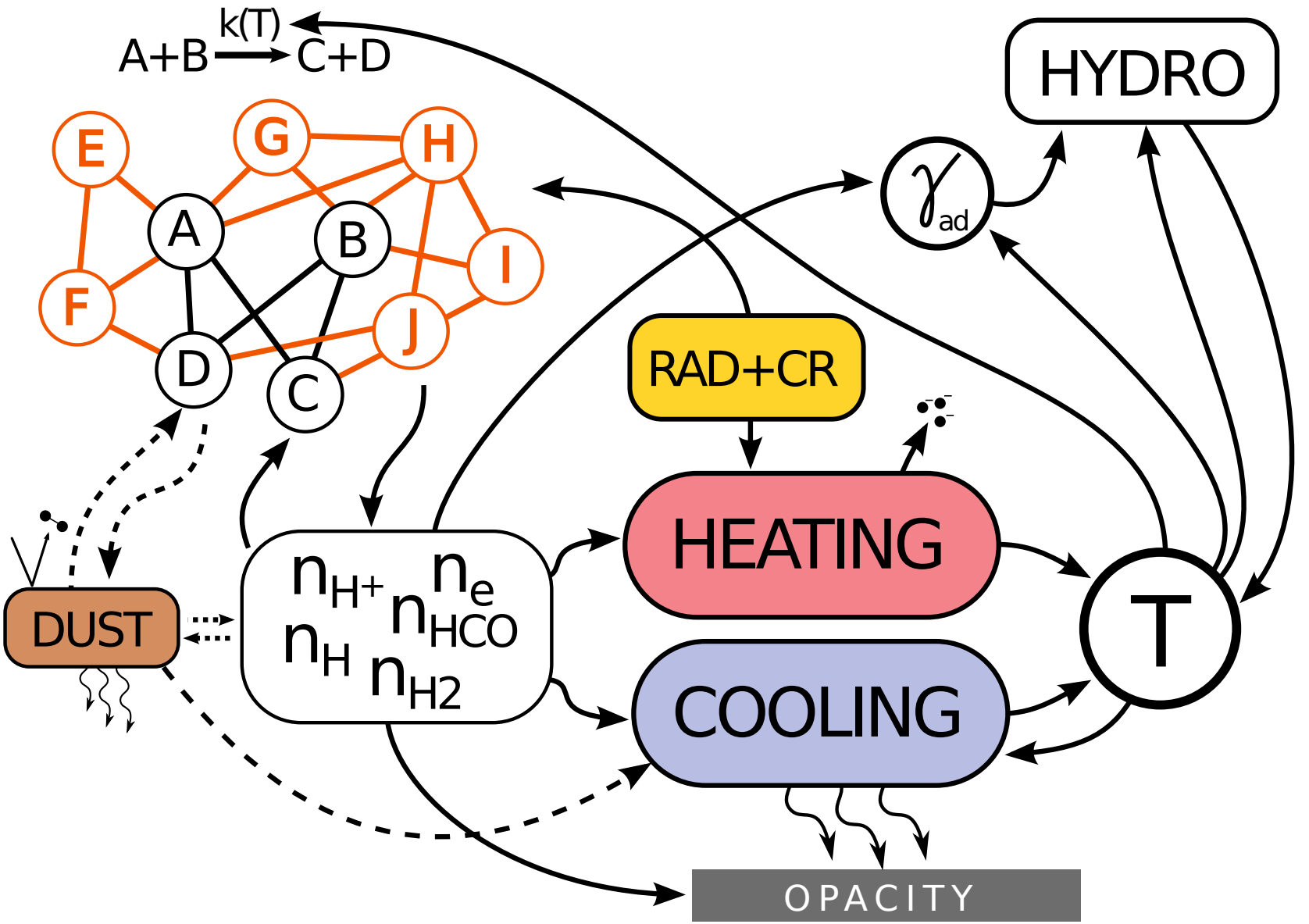
Chemistry, the full story (20/24)



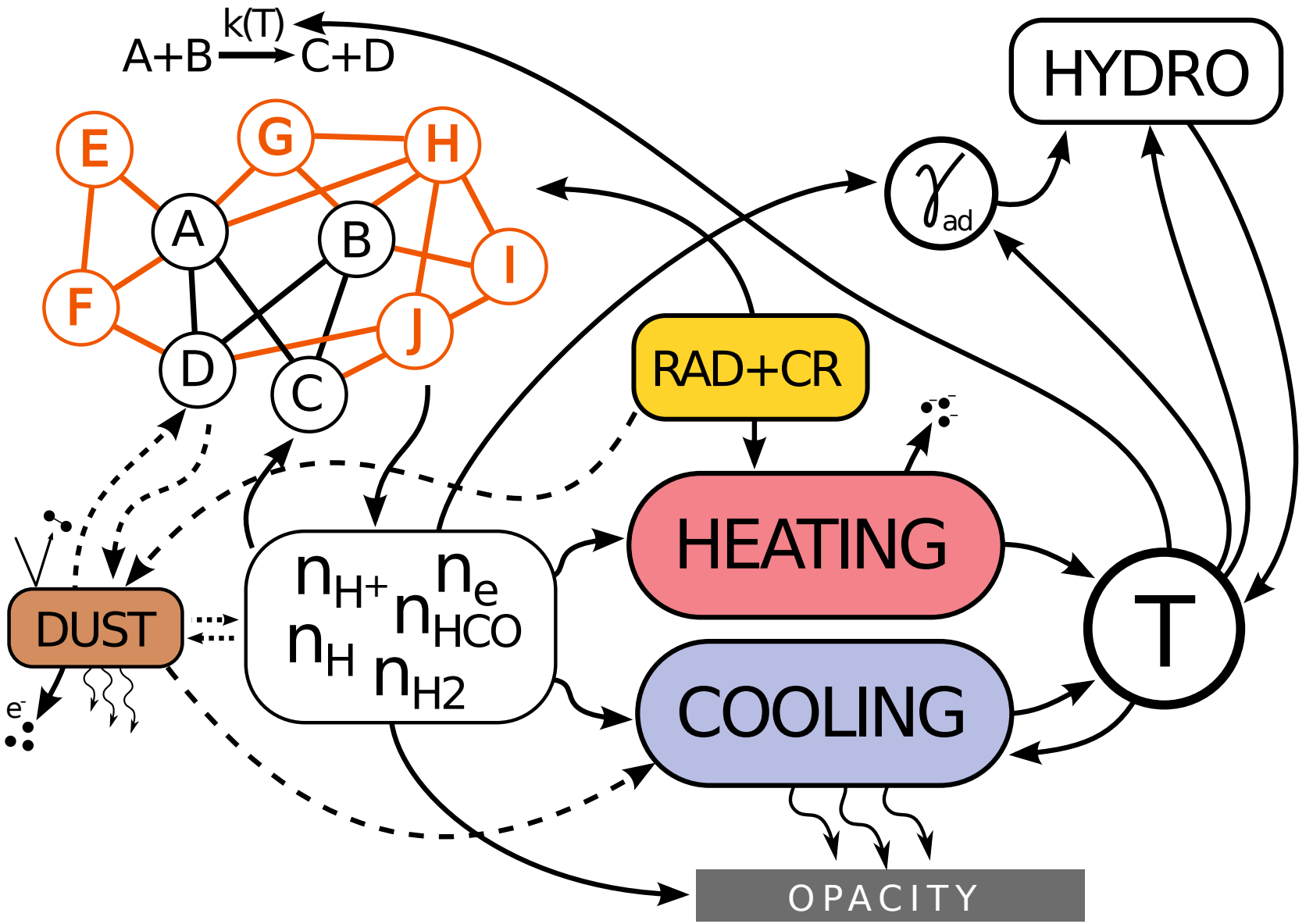
Chemistry, the full story (21/24)



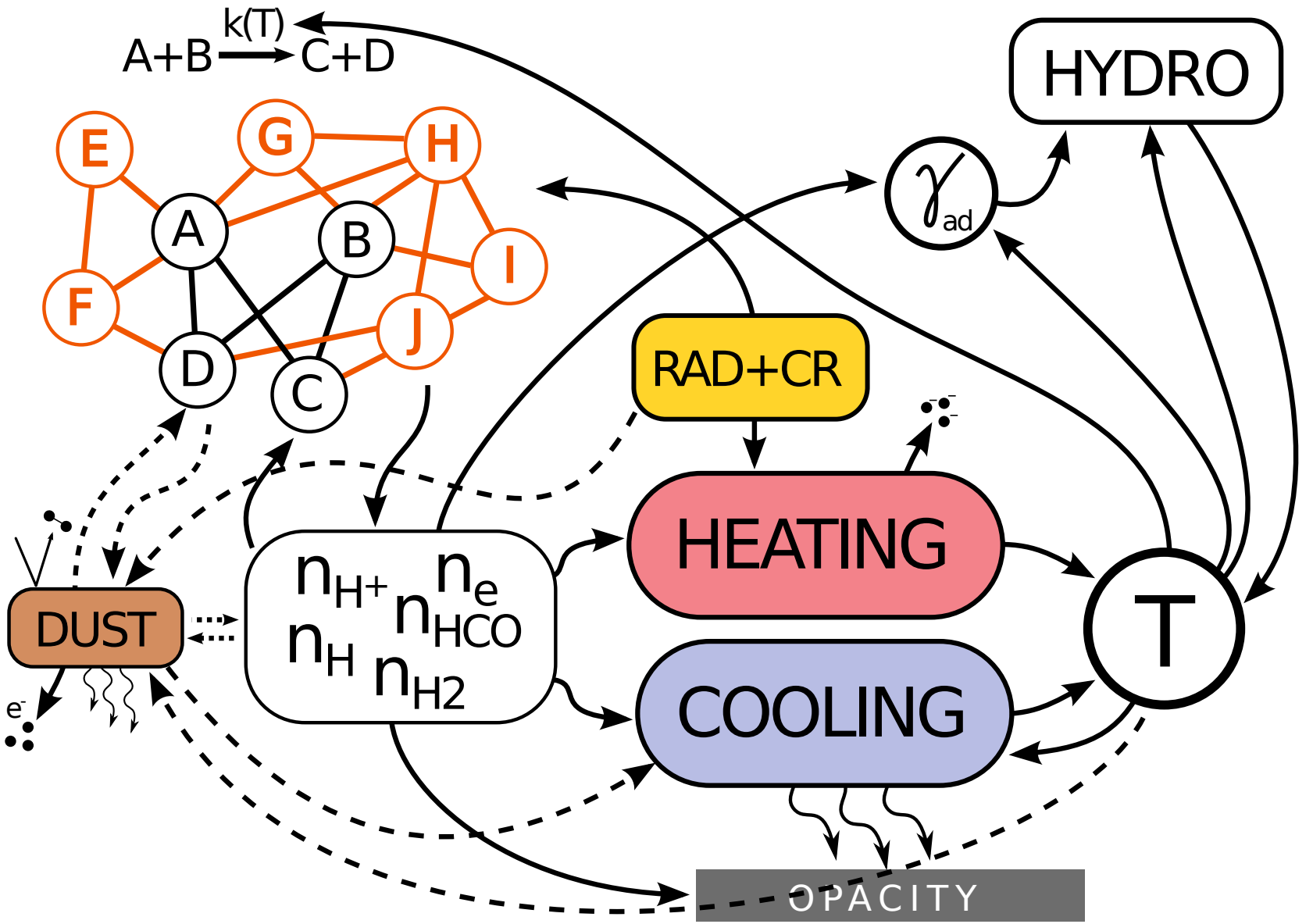
Chemistry, the full story (22/24)



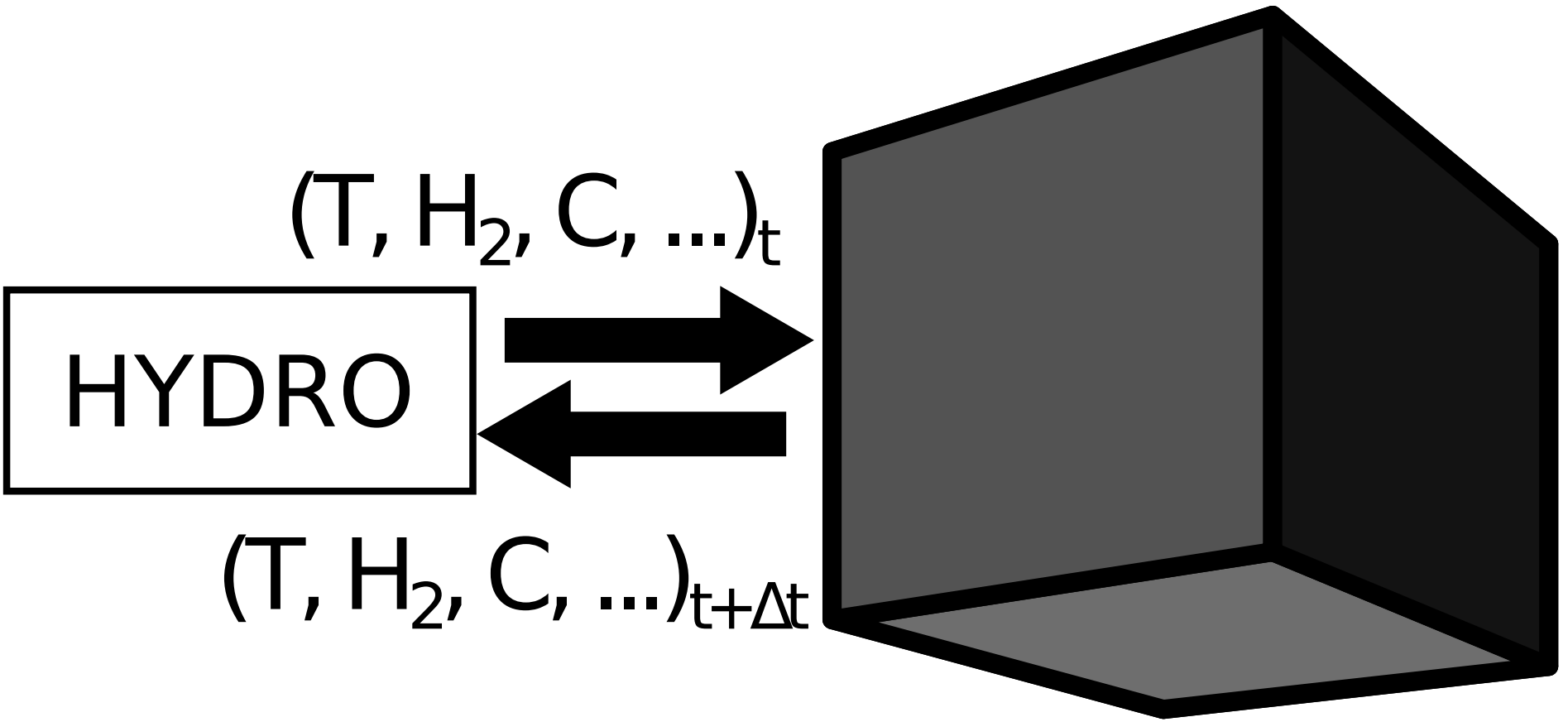
Chemistry, the full story (23/24)



Chemistry, the full story (24/24)



A useful blackbox




```
call krome(x(:), Tgas, dt_hydro)
```

a package for astrochemistry

"Any given program, when running, is obsolete"
(Anonymous)

KROME (overview)

KROME (http://kromepackage.org/)

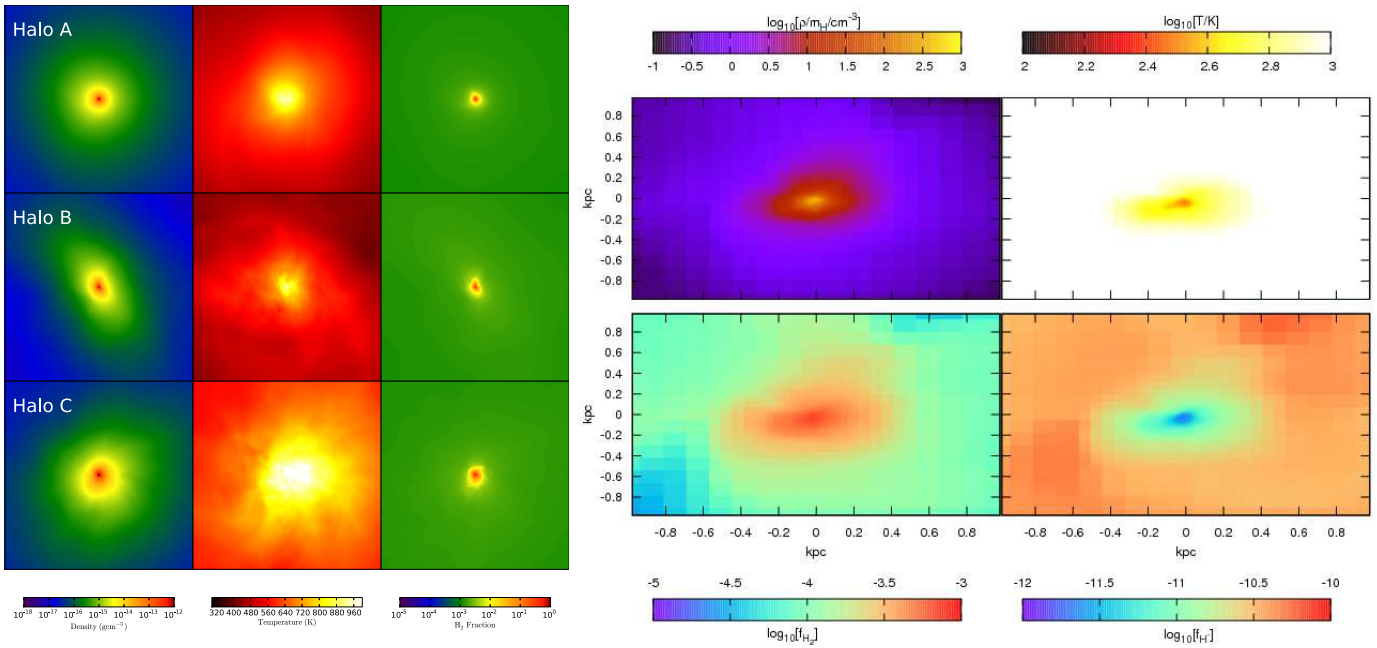
- Python Pre-processor provides Fortran routines
- Creates F90 modules from chemical network and option flags
- Dust evolution, Cooling, Heating, Photoionization, ...
- Open source, bitbucket community
- Highly optimized, fast solvers (DLSODES, DVODE F90)
- Test suite (MC, 1D SNe, planet, 3D and C/C++ wrappers, ...)
- Grassi et al. 2014 (arXiv:1311.1070), TG+2011 (arXiv:1012.1142)

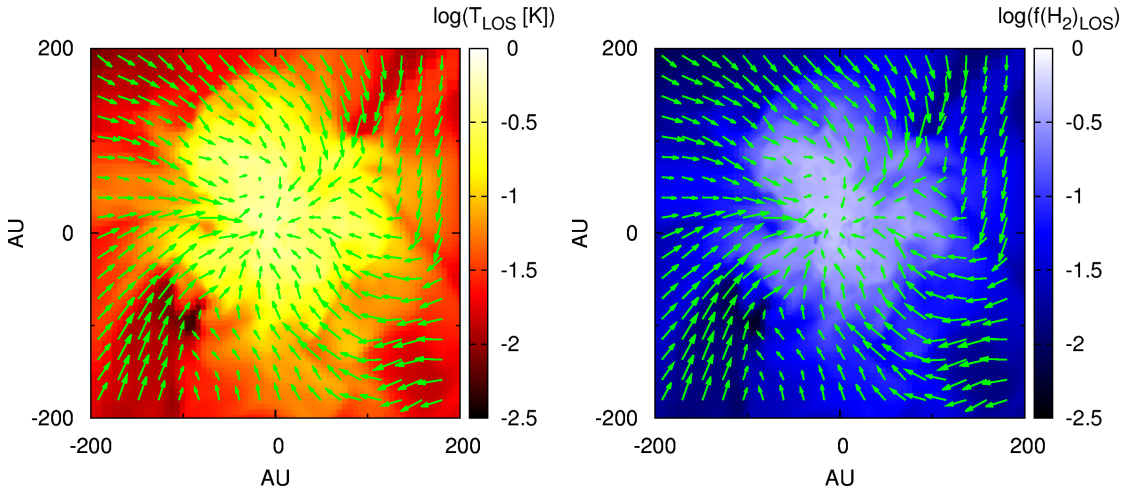
Processes overview

- Solving chemical network (ODEs+Jacobian+sparsity+tables)
- Several chemical networks provided (from primordial up to >5k reacts)
- Photodissociation and photoionisation (ν-dependent xsecs)
- Cosmic rays (rate approximation, $a\zeta_{\rm CR}$)
- Atomic cooling (H, H^+, He, He^+, He^{++}, as Cen1992)
- H_2^{rv} cooling (GP98+GA08), HD (Lipovka+2005)
- H_2^{cd} cooling (Martin+98, Glover+Jappsen2007)
- CIE cooling (Ripamonti+Abel2004)
- C, O, Si, Fe, and ions cooling (Maio+2007, HM79, at runtime)
- Continuum (Omukai2000, Lenzuni+91)
- Chemical heating, including H_2 on dust (Omukai2000, HM79)
- Photoheating (ν-dependent, GA08)
- bins in size for dust (graphite and Si-based, incl. optical prop, e.g. Grassi+2011)
- Dust growth by sticking (Dwek98, G+11), thermal sputtering (Nozawa2006)
- H_2 formation on dust (Cazaux+Spaans2009)
- More details in Grassi+2014 (arXiv:1311.1070, MNRAS in press)

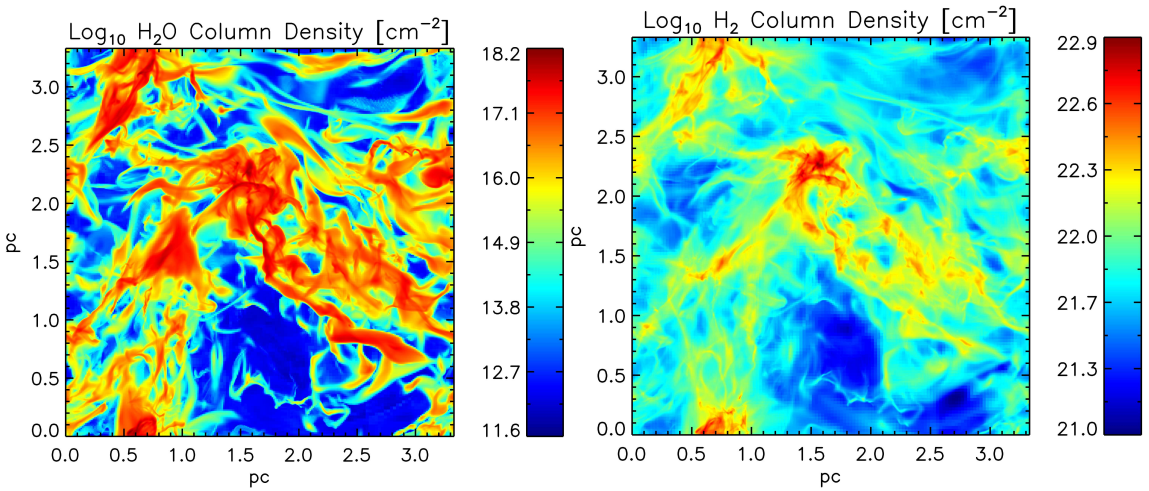
KROME in 3D codes (patches)

ENZO (S.Bovino, D.Schleicher) + RAMSES (J.Prieto) + FLASH (D.Seifried)

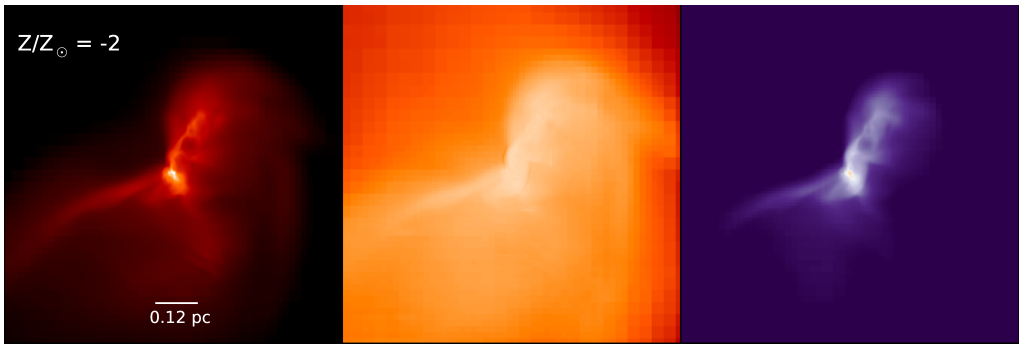




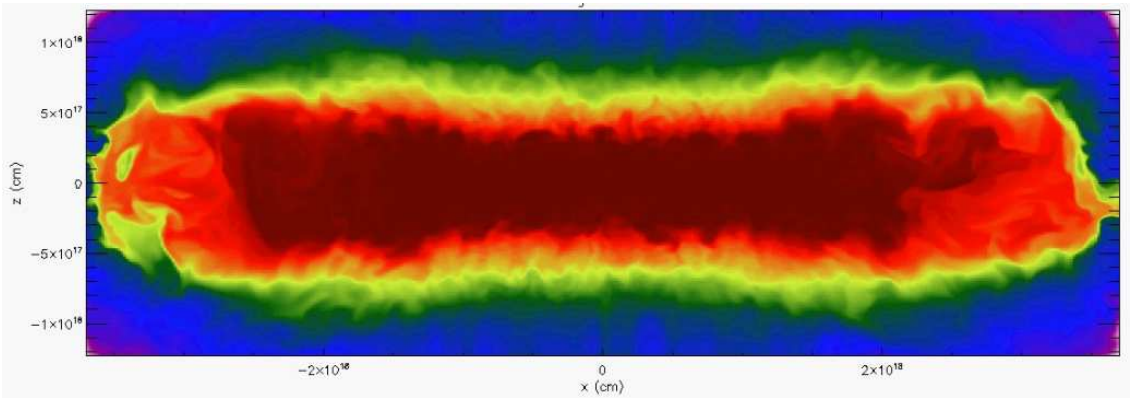
KROME in 3D codes/2



- T. Haugbølle
- RAMSES
- Turbulent MC (MHD)



- S. Bovino+D. Schleicher
- Enzo
- Metal-poor C-rich star



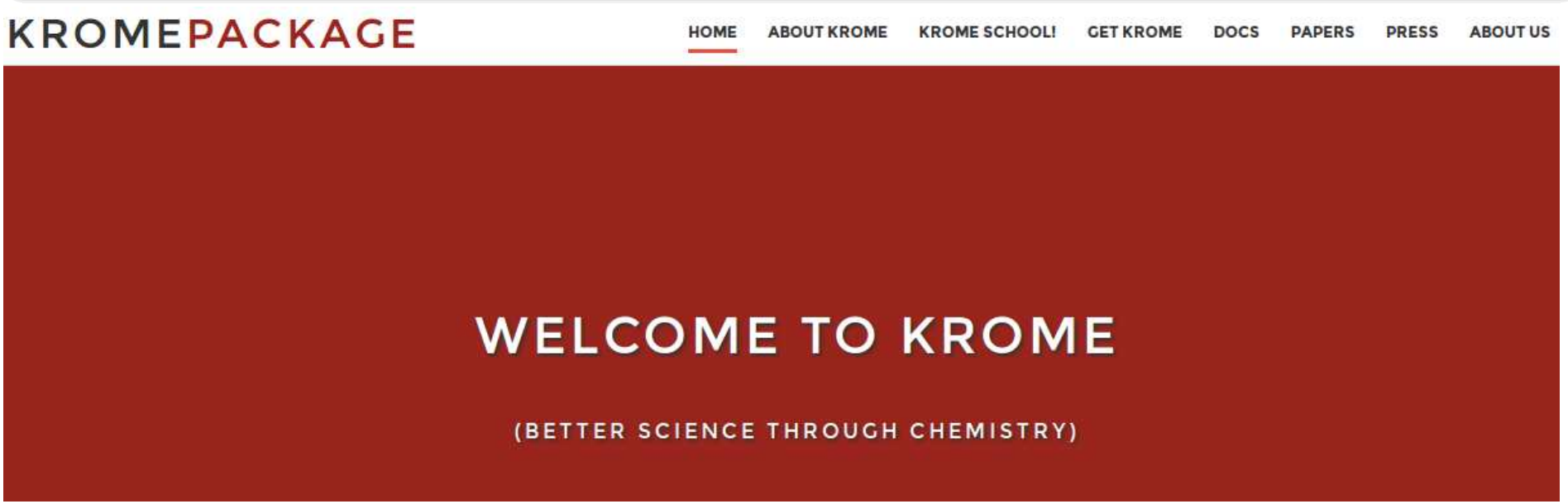
- D. Seifried
- FLASH
- “Filamentology”

Community

“Programming would be so much easier without all the users.”
(Anonymous)

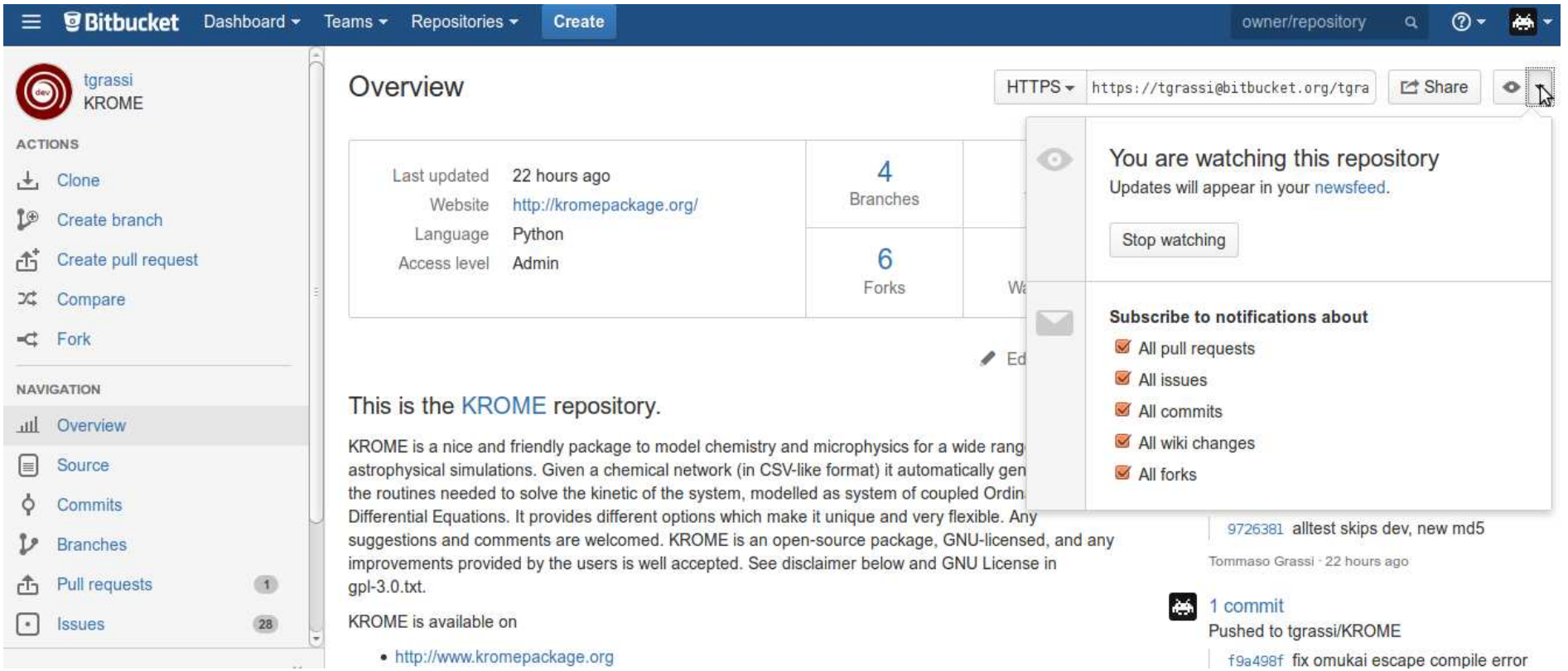
KROME (website)

kromepackage.org



KROME (bitbucket)

`bitbucket.org/tgrassi/krome/`

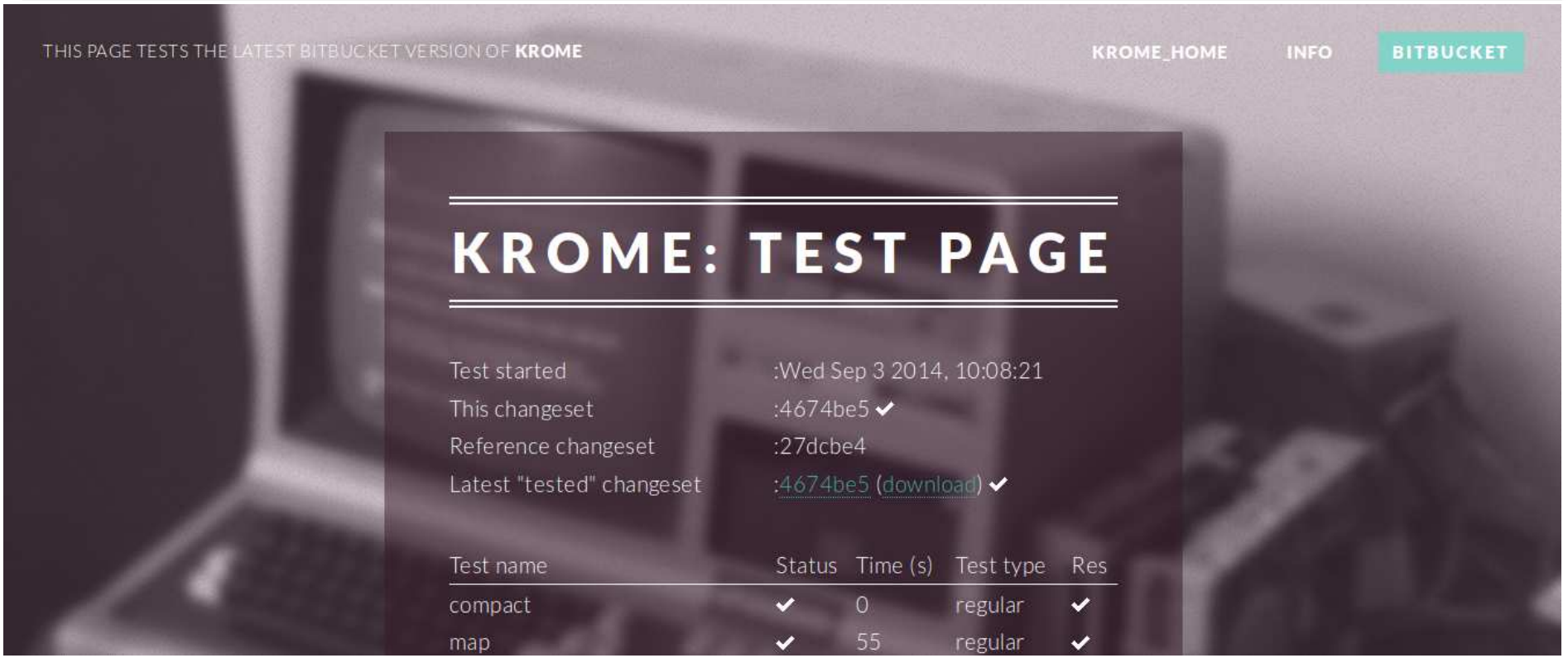


"Developers! Developers! Developers!" (Steve Ballmer)

KROME (test page)

- DEVELOPER
- ~~STABLE~~
- TESTED

`kromepackage.org/test`



KROME - bootcamp 2015

KROME **computational school** | 20-24 July 2015 | Copenhagen

`http://kromepackage.org/bootcamp`

School topics

- Solvers and chemical networks
- Thermal processes and dust
- Optimization and code tuning
- Interfacing KROME to your own code
- Chemistry & synthetic observations
- Exercises with participants
- ★ GRANTS AVAILABLE!

Speakers (preliminary)

S. Bovino (IfA, Goe), **D. Galli** (INAF Arcetri), **T. Grassi** (STARPLAN/NBI, Cph), **T. Haugbølle** (STARPLAN/NBI, Cph), **J. Jørgensen** (STARPLAN, Cph), **K. Omukai** (Tohoku Uni), **D. Schleicher** (IfA, Goe), **D. Seifried** (Hamburg Observatory).

KROME - final remarks

Next steps

- complete dust module (e.g. charge)
- complete surface reactions (adsorption, evaporation, 2body, CR, photo)
- improve Jacobian
- ...

The eternal struggle

EFFICIENCY $\longleftrightarrow$ ACCURACY

Some questions (out of thousands)

- Has your code the right microphysics and/or chemistry?
- What happens to hydrodynamics with fully consistent microphysics (e.g. $\gamma_{\rm ad}$)?
- What is the smallest set of microphysical processes?
- What is the best realistic/efficient model for each astrophysical environment?
- What is the influence of the rate accuracy on the global model?
- Are chemical networks complete?

Thank you for your attention!

"All models are wrong, but some are useful"
(George Box)

`http://kromepackage.org/`
`http://kromepackage.org/bootcamp`
Grassi et al. 2014 (arXiv:1311.1070)