MARIO BARBATTI

PERSONAL STRATEGIES FOR SCIENTIFIC COMMUNICATION

THE CHALLENGE OF WRITING

Must write

- Papers
- Projects
- Reports
- Thesis

However

- non intuitive

Man has an instinctive tendency to speak,
as we see in the babble of our young children,
but no child has an instinctive tendency
to **bake**, **brew, or write**.

Charles Darwin,
The Descent of Man

However

- nonintuitive
- not an English native speaker

Read, read & read

Science popularization	Philosophy of science	Fiction
• C Sagan • R Dawkins • J Diamond • S Pinker	• I Prigogine • G Bachelard • T Kuhn • S M Carroll	• F Kafka • P Roth • D Adams • T Chiang

+ essays (aeon.co, nautil.us)
+ papers

Frozen Gaussians: A very simple semiclassical approximation

J. Chem. Phys. **75**, 2923 (1981); https://doi.org/10.1063/1.442382

Eric J. Heller

ABSTRACT

A new and convenient semiclassical method is proposed. It relies only upon classical trajectories and Gaussian integrals. It seems to work very well for the model molecular vibrational spectra investigated here. It should be applicable to a wide variety of processes and can be variationally improved if necessary.

NEW YORK TIMES BESTSELLER

THE *Sense* OF *Style*

the THINKING PERSON'S GUIDE
to WRITING in the 21st CENTURY

STEVEN PINKER

author of THE BETTER ANGELS OF OUR NATURE
and THE LANGUAGE INSTINCT

ABOUT FORM

Make it beautiful

- WYSWYG as a philosophy
- Positive psychological impact

Master your tools

My choice:

- MS Word
- MathType
- Grammarly
- Endnote

Use templates and styles

The puzzling excited-state dynamics of 2-(2'-hydroxyphenyl) benzothiazole (HBT) in cyclohexane

Moumita Kar,[1*] Kakali Sen,[2] Saikat Mukherjee,[1] Giovanni Granucci,[3] Mario Barbatti[1,4*]

[1] *Aix Marseille University, CNRS, ICR, Marseille, France*
[2] *STFC Scientific Computing, Daresbury Laboratory, Keckwick Lane, Daresbury, Warrington WA4 4AD, United Kingdom*
[3] *Department of Chemistry and Industrial Chemistry, University of Pisa, v. G. Moruzzi 13, Pisa, Italy*
[4] *Institut Universitaire de France, 75231, Paris, France*

Corresponding authors: *MK: moumita.kar@univ-amu.fr*
MB: mario.barbatti@univ.amu.fr; www.barbatti.org

Abstract. This work aims to present an unsolved puzzle in photophysics, the excited-state dynamics of 2-(2'-hydroxyphenyl) benzothiazole (HBT) in cyclohexane. It has been experimentally shown that while the HBT excited-state lifetime is about 2.6 ns when this molecule is solvated in cyclohexane, its

Writing aid

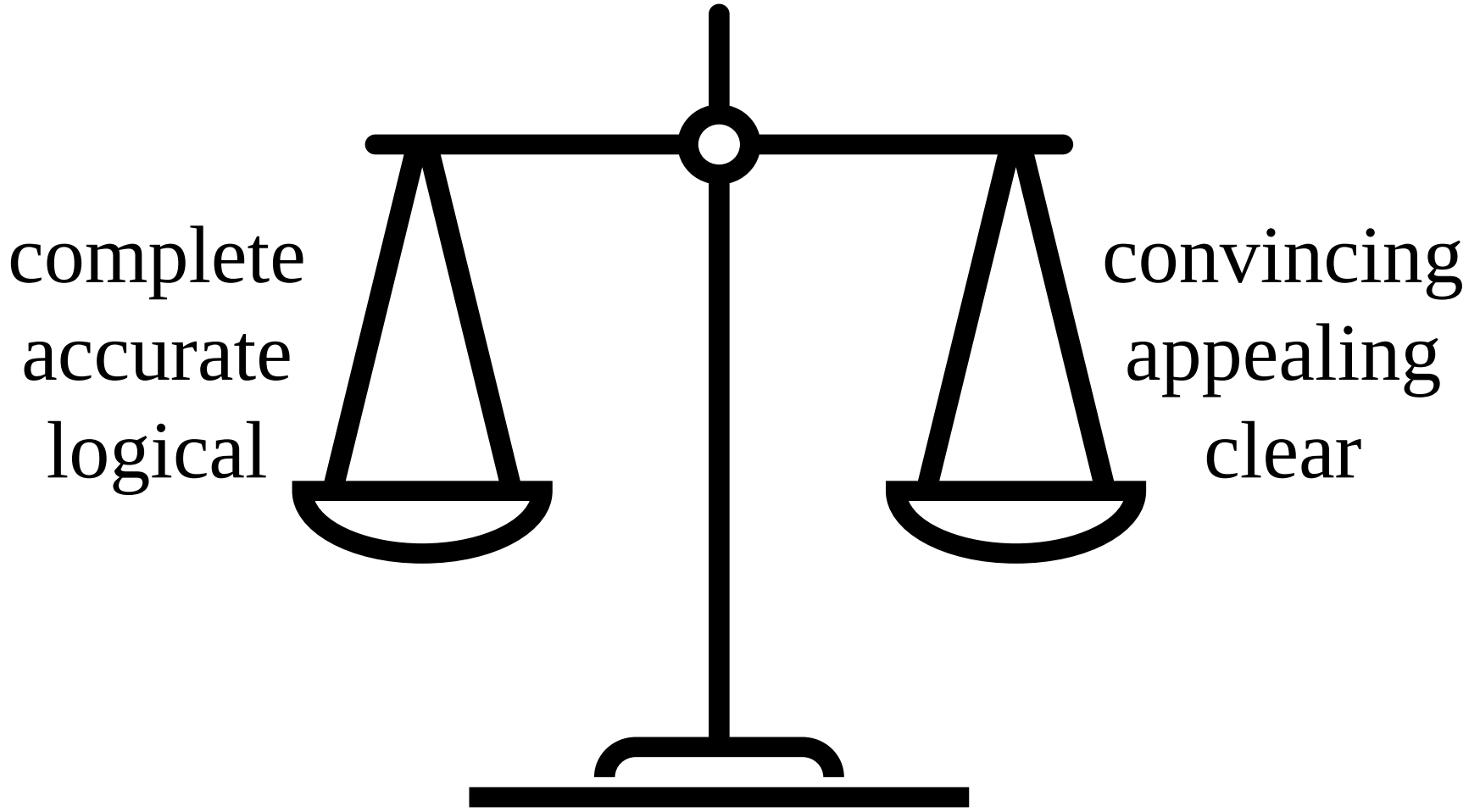
- Always use an advanced writing aid like Grammarly
- Always use a reference manager (Endnote, Mendeley, Zotero)
- Use ChatGPT and AI tools, but be extremely careful!
- For final revisions, use “Read aloud”

Why not LaTeX?

- Low productivity
- Prone to mistakes
- Bad for co-authoring
  (most of my colleagues don’t use it)
- Low-level WYSWYG

ABOUT CONTENT

Formal & Readable



Think of your reader

- Distracted
- In a hurry
- Different background

Story telling approach

- Think about your story
- Talk to your imaginary reader
- Let the story evolve

Beware the curse of knowledge

In the case of thymine dinucleotide, the excited-state lifetime revealed an Arrhenius-type dependence on the temperature, dropping from 2.0 to 0.8 ps when the system was heated from 100 to 300 K.

In the case of thymine dinucleotide, the excited-state lifetime revealed an Arrhenius-type dependence on the temperature $[\ln(\tau) \propto T^{-1}]$, dropping from 2.0 to 0.8 ps when the system was heated from 100 to 300 K.

Be clear

Fortunately, as **I will show later**, we can get an approximated solution for the number of microstates by supposing the ensemble of vibrational frequencies ...

Fortunately, as **I will show later (Section 2.5.3**), we can get an approximated solution for the number of microstates by supposing the ensemble of vibrational frequencies ...

1 paragraph = 1 idea

The first assumption implies that we will not describe anharmonic modes, like intramolecular hydrogen bonds or internal rotations (like those methyl groups are prone to). (...)

The second assumption implies that we will also not discuss temperature associated with the energy allocated in the translational and rotational modes. (...)

Speak to your reader

In the following sections, **we will discuss** the solution to the degenerated problem in the Boltzmann and Gibbs formulations. Although the solution in the Boltzmann formulation is well known,[23] **I am unaware of any demonstration using Gibbs**.

Show confidence

The better performance of the arithmetic over the harmonic mean is fortunate. **It suggests** that low frequencies **may not be** more relevant than high frequencies for temperature determination.

The better performance of the arithmetic over the harmonic mean is fortunate. **It implies** that low frequencies **are not** more relevant than high frequencies for temperature determination.

Some times, boring is better

The heating of a chromophore due to **internal conversion** is crucial to characterize photoprocesses. In this work, we simulated the dynamics of cytosine to determine its **nonradiative decay** time.

The heating of a chromophore due to **internal conversion** is crucial to characterize photoprocesses. In this work, we simulated the dynamics of cytosine to determine its **internal conversion** time.

Revise, revise, and revise

The time dependence of the following quantities is required by the model: (i) the population of the excited state and (ii) the potential energy of the molecule.

The model requires the excited-state population and the molecule’s potential energy, both as a function of time.

OVERCOMING WRITER'S BLOCK

Build a nest before laying eggs

- Work on your story
- Prepare a concept paper
- Make figures & tables
- Read the literature
- Find your inspiring author

Introduction

Methods

Results & Discussion

Conclusion

Introduction

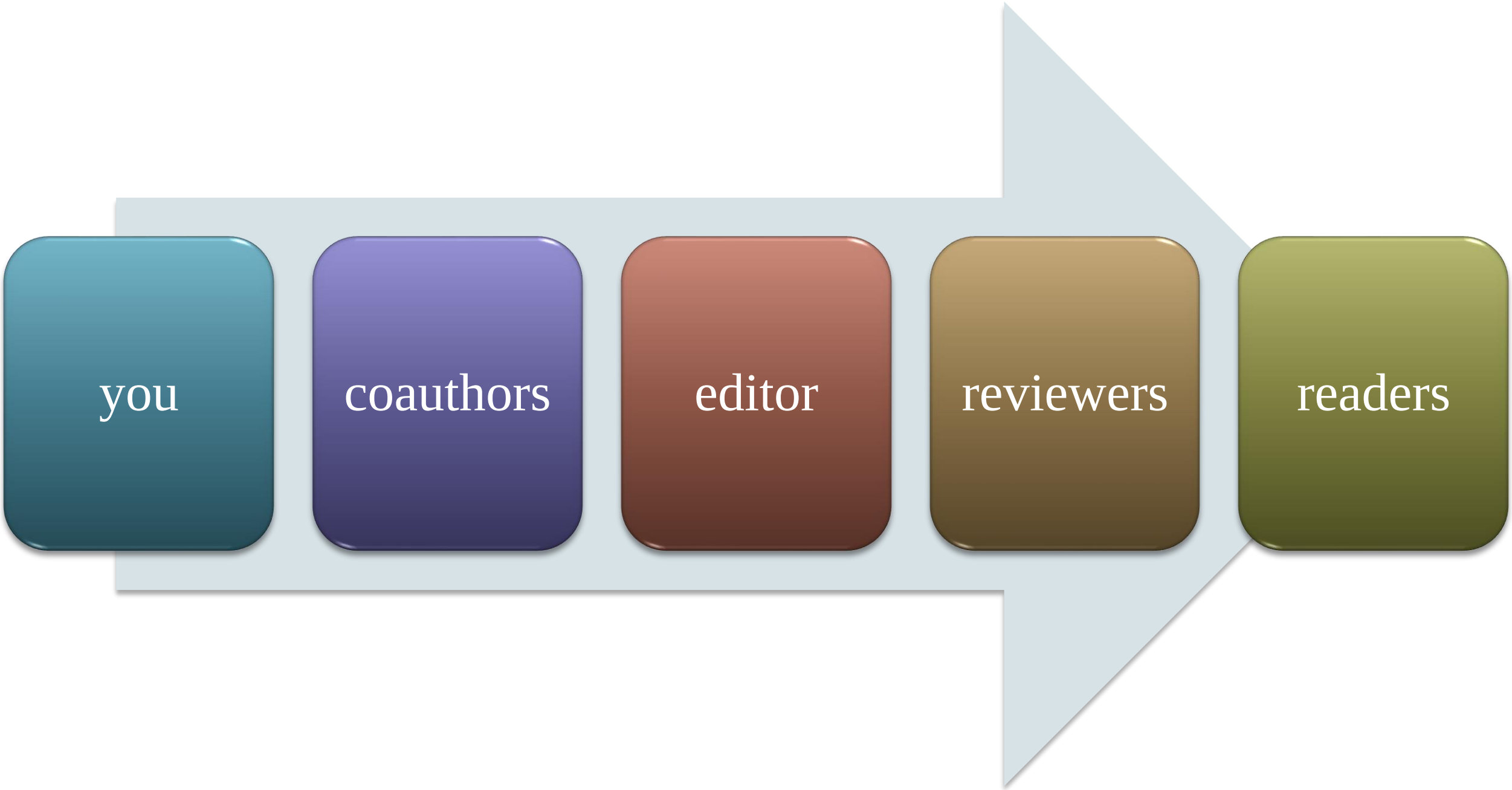
Methods

Results

Discussion

Conclusion

SCIENTIFIC WRITING IS COLLECTIVE


you
coauthors
editor
reviewers
readers

SLIDES AND PRESENTATIONS

Master your tools

My choice:

- PowerPoint
- MathType
- Grammarly
- Endnote

Laws of slide composition

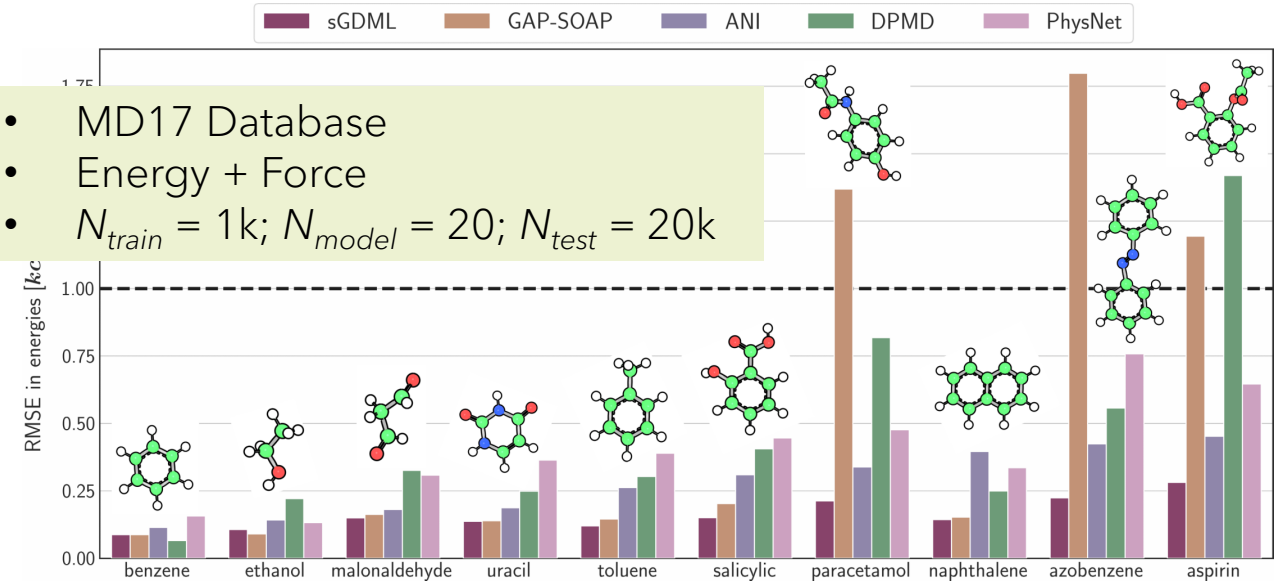
1. Background can have any color as long it’s white.

2. Font size in PTs must be at least half the age of the oldest person in the public.

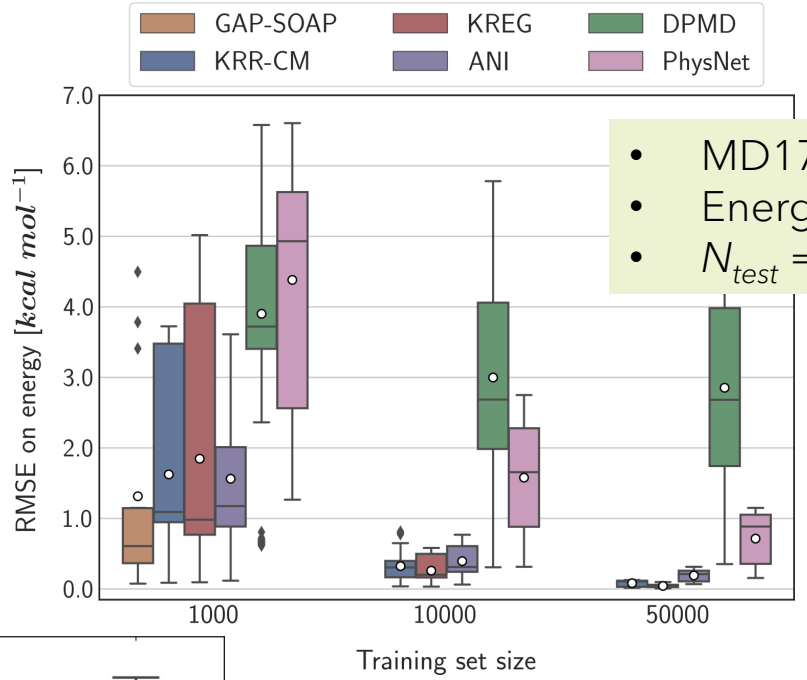
3. One slide fits one and only one piece of info. Slides are for free. Don’t save their number.

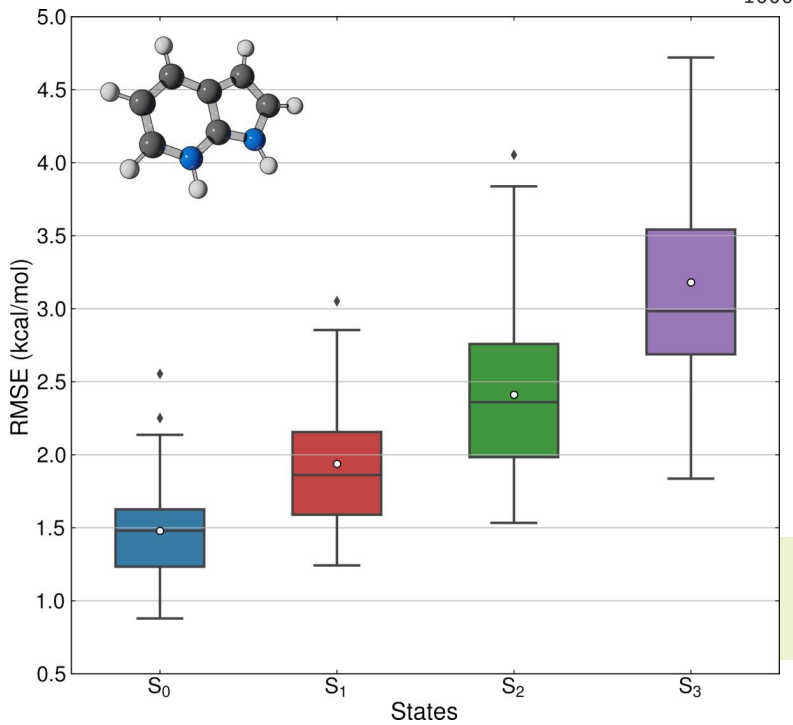
COULD HAVE DONE

- MD17 Database
- Energy + Force
- N_{train} = 1k; N_{model} = 20; N_{test} = 20k



- MD17 Database
- Energy only
- N_{test} = 20k

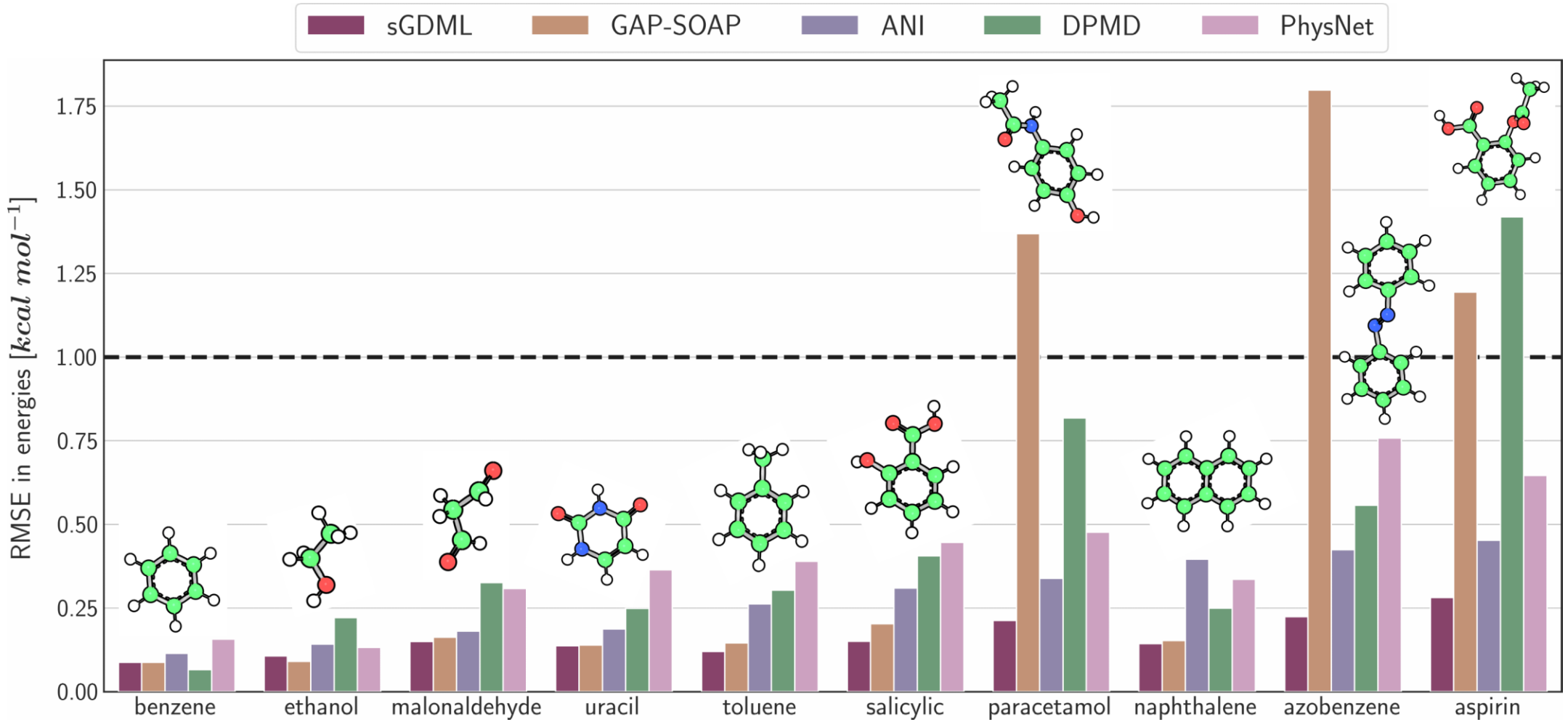




KREG x RI-ADC(2)/cc-pVDZ
DC-FSSH: 50 trajs; 0.5 fs; 300 ps

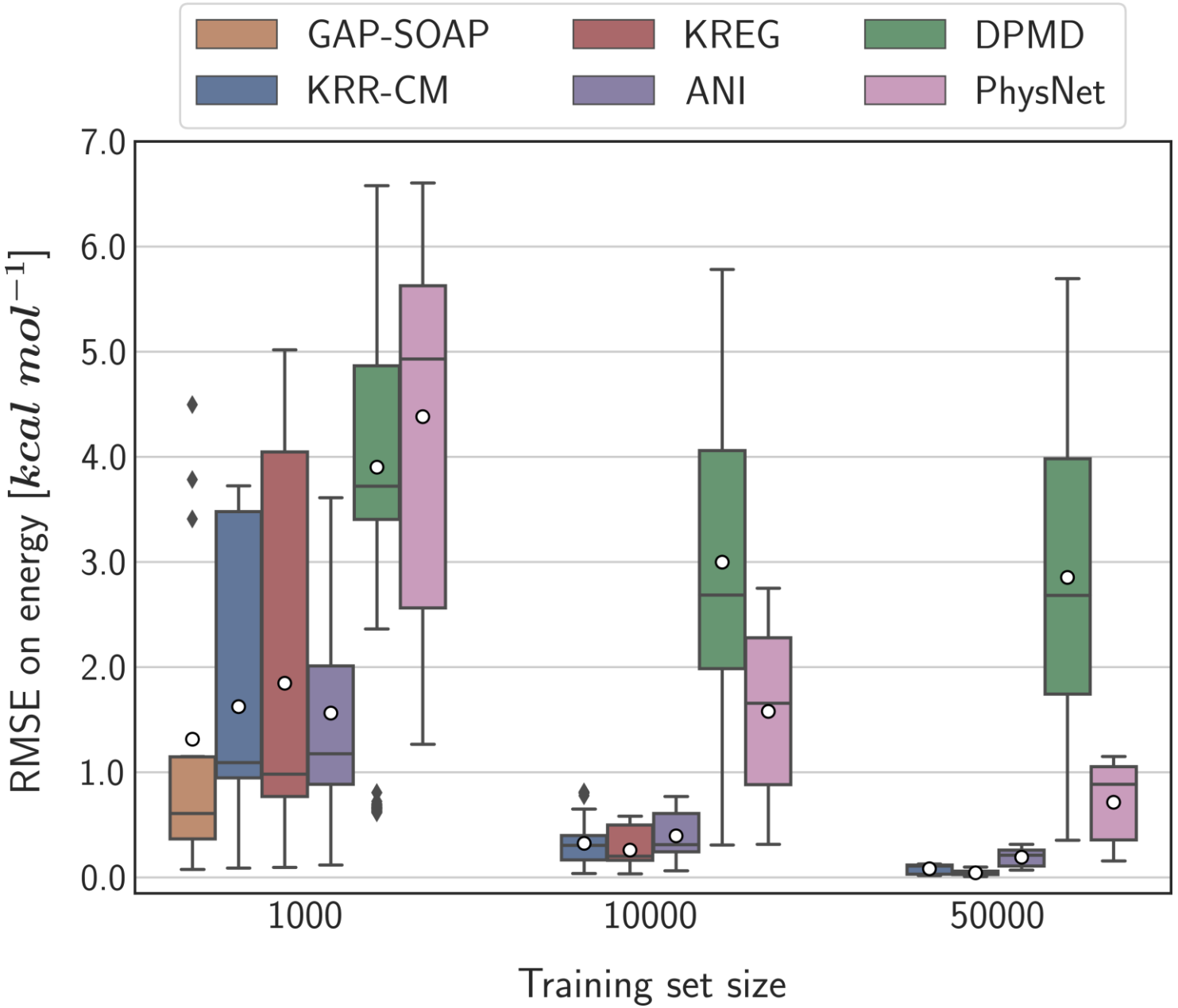
Pinheiro Jr, MB *et al*. *Chem Sci* **2021**, *12*, 14396; Mukherjee, MB *et al*. *Philos Trans R Soc A* **2022,** *80*, 20200382

BETTER



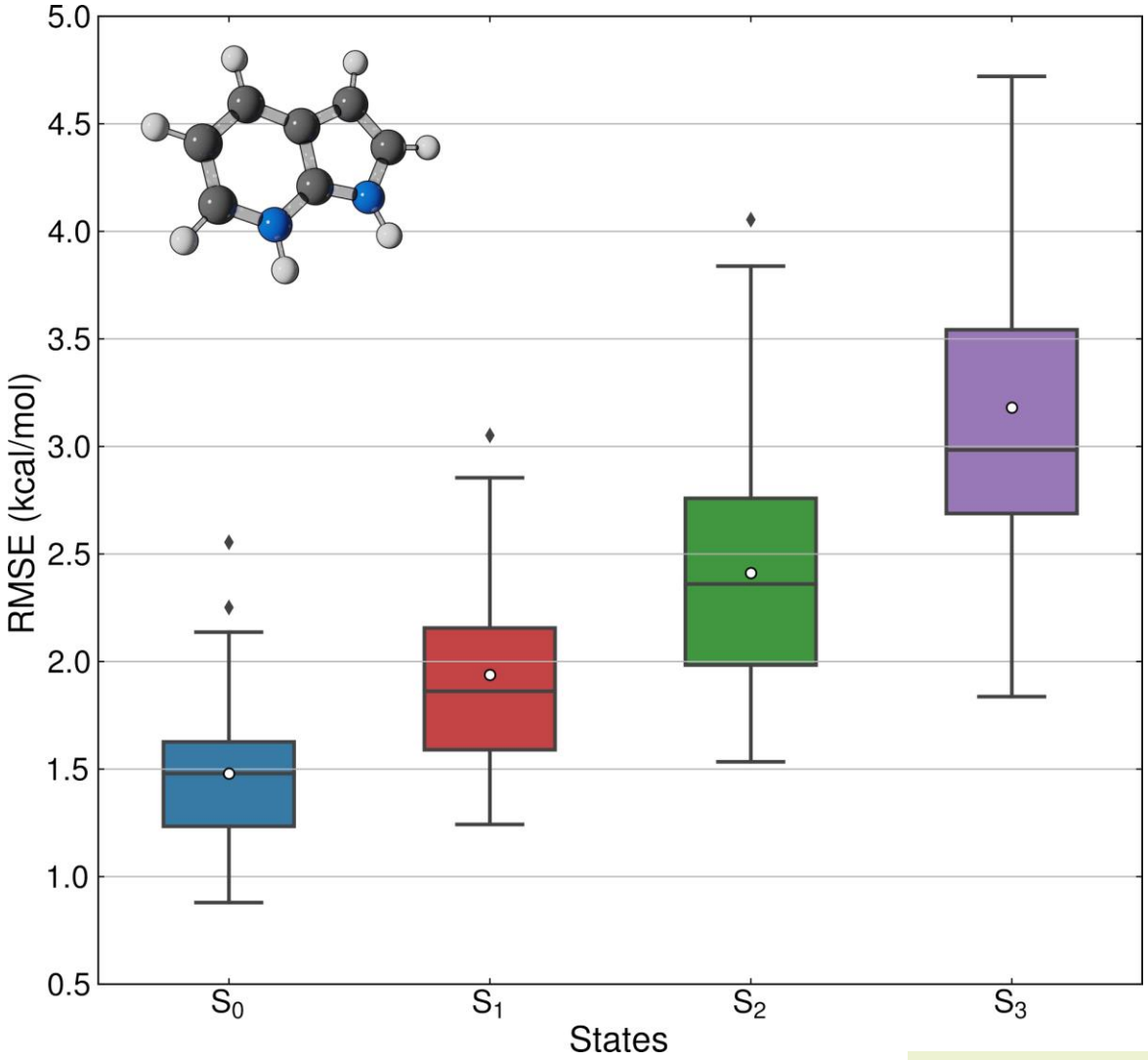
- MD17 Database
- Energy + Force
- N_{train} = 1k; N_{model} = 20; N_{test} = 20k

Pinheiro Jr, Barbatti *et al*. *Chem Sci* **2021**, *12*, 14396



- MD17 Database
- Energy only
- N_{test} = 20k

Pinheiro Jr, Barbatti *et al*. *Chem Sci* **2021**, *12*, 14396



- KREG x RI-ADC(2)/cc-pVDZ
- DC-FSSH: 50 trajs; 0.5 fs; 300 ps

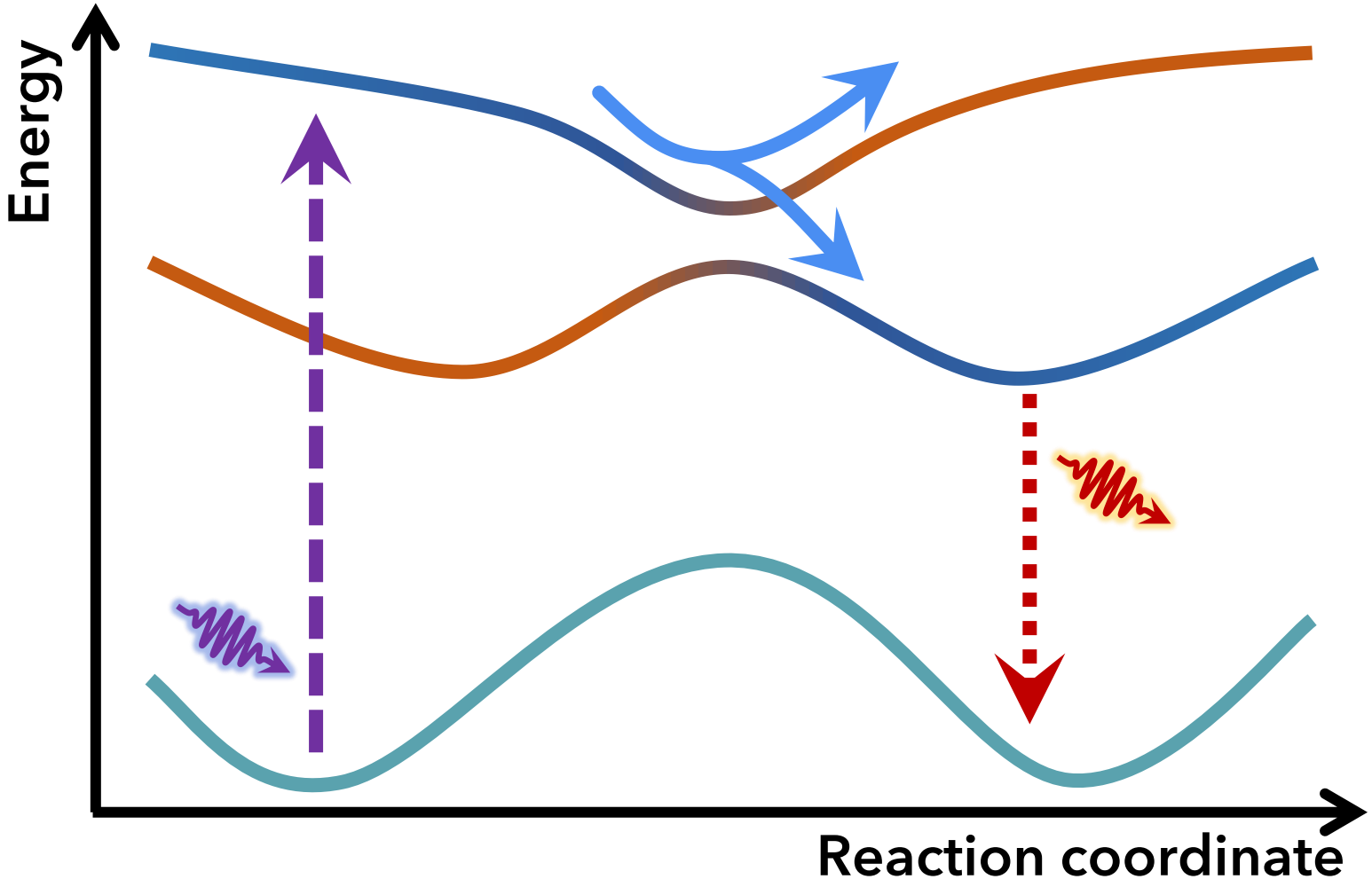
Mukherjee, Barbatti *et al*. *Philos Trans R Soc A* **2022,** *80*, 20200382

Master animations

Use animations to tell the public where to focus.

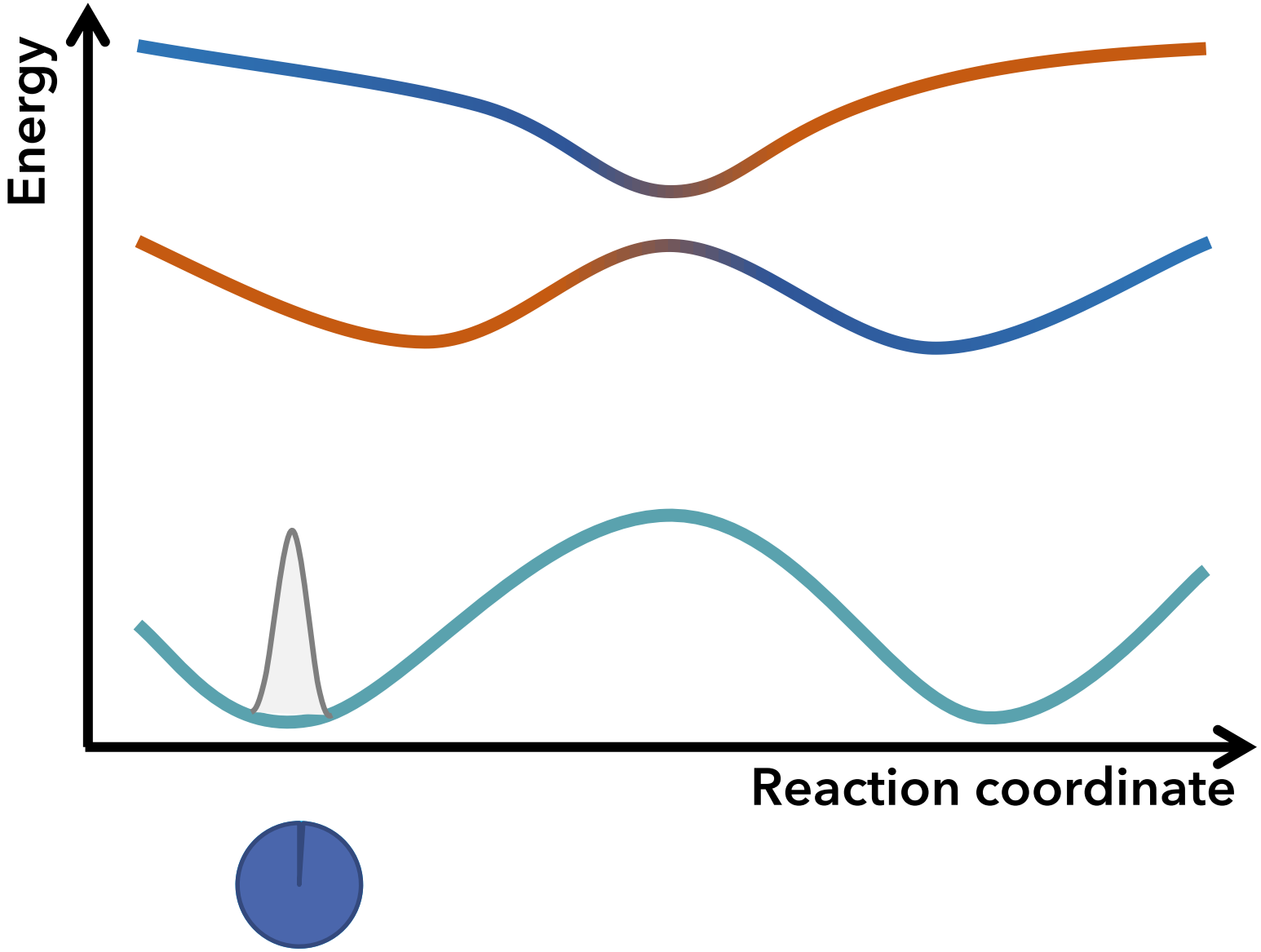
COULD HAVE DONE

Nonadiabatic dynamics

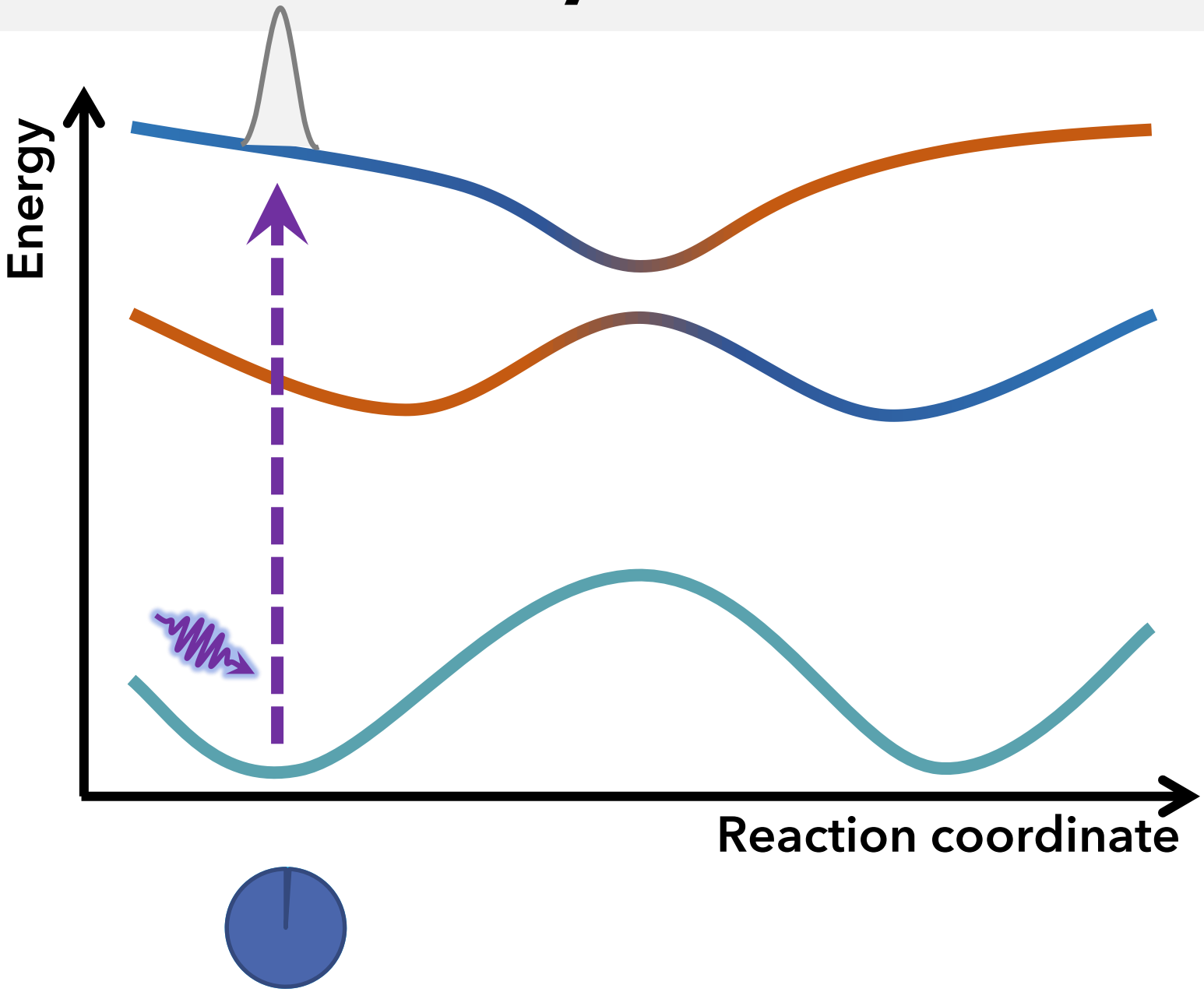


BETTER

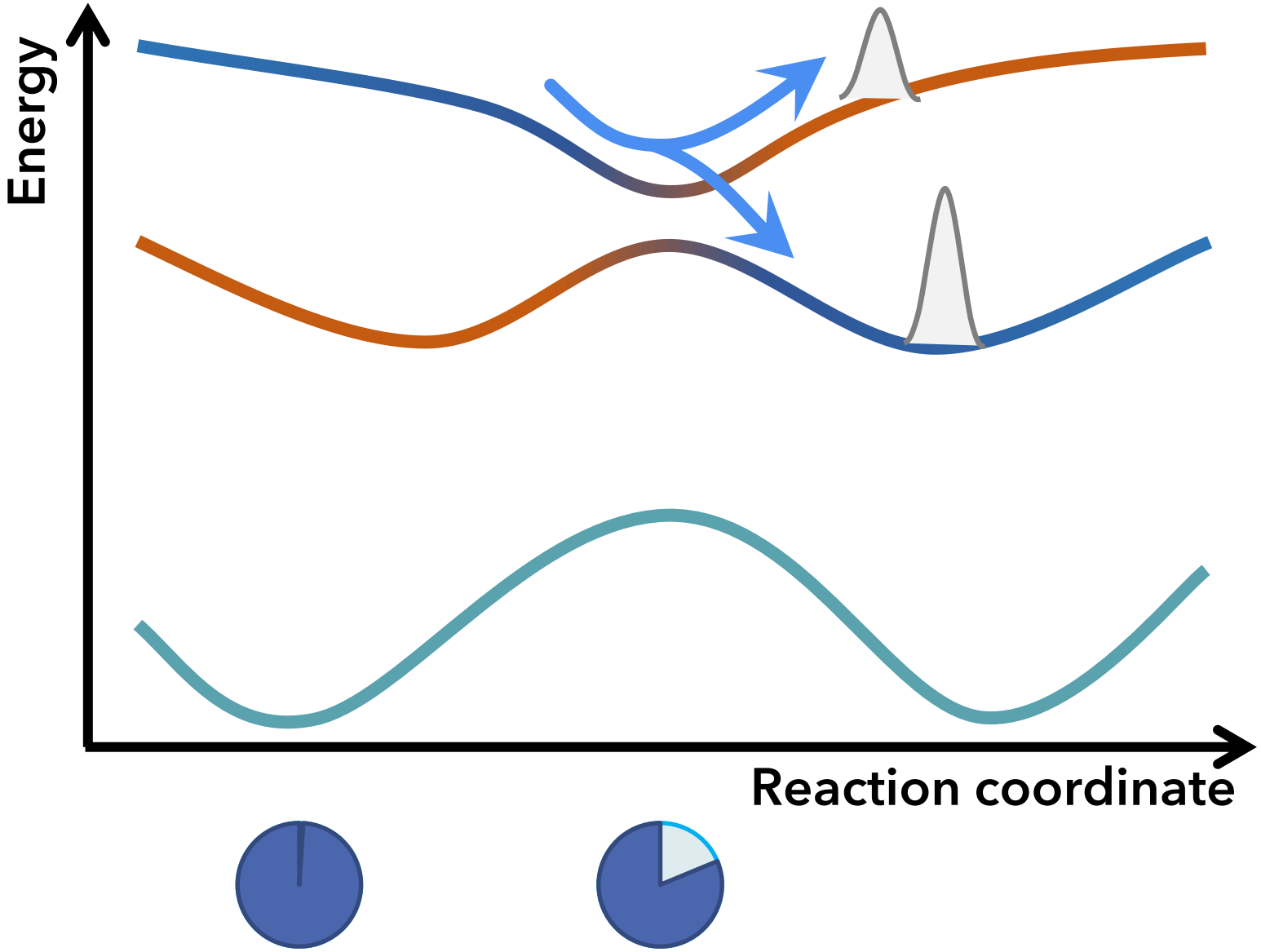
Nonadiabatic dynamics



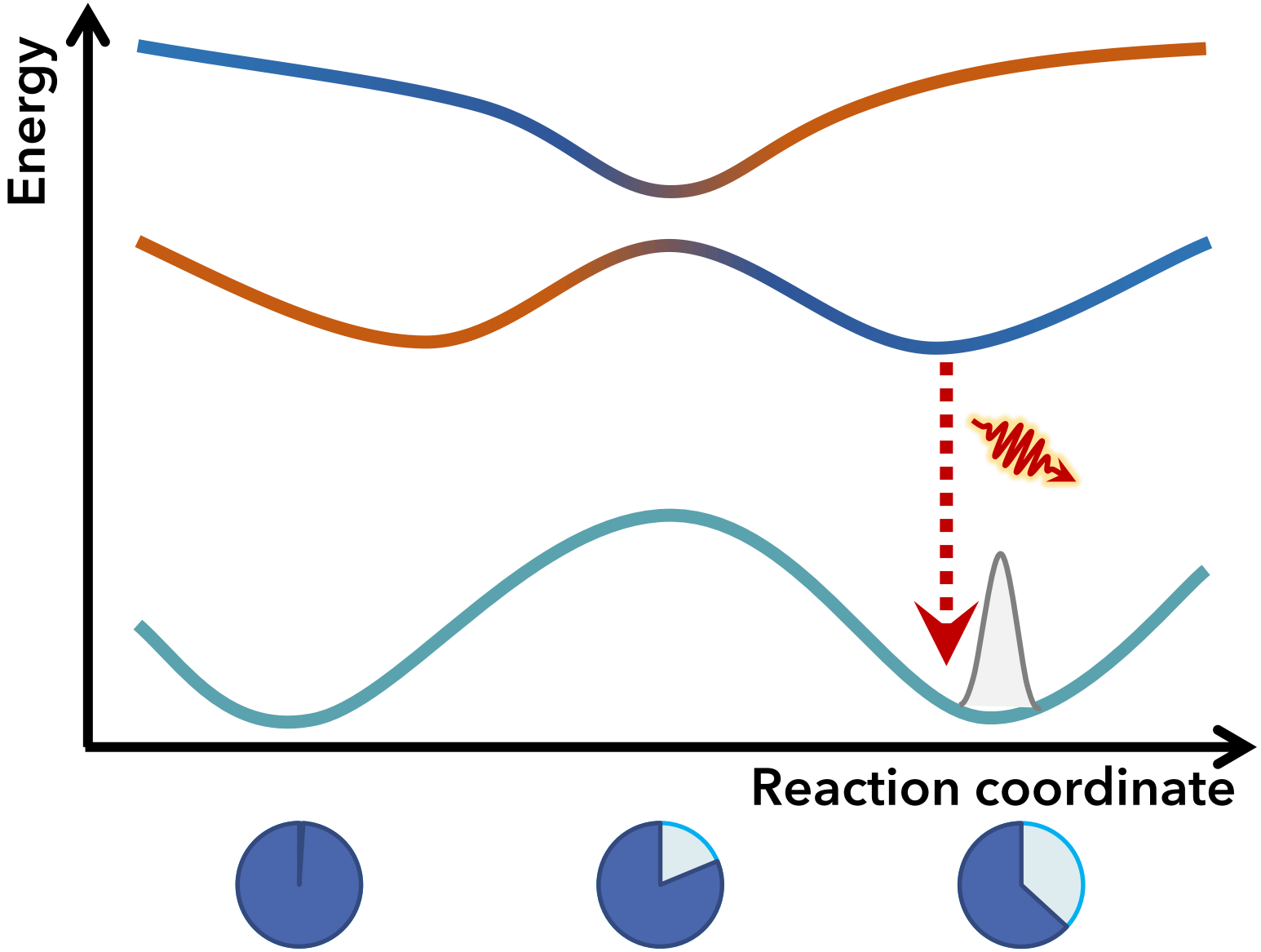
Nonadiabatic dynamics



Nonadiabatic dynamics

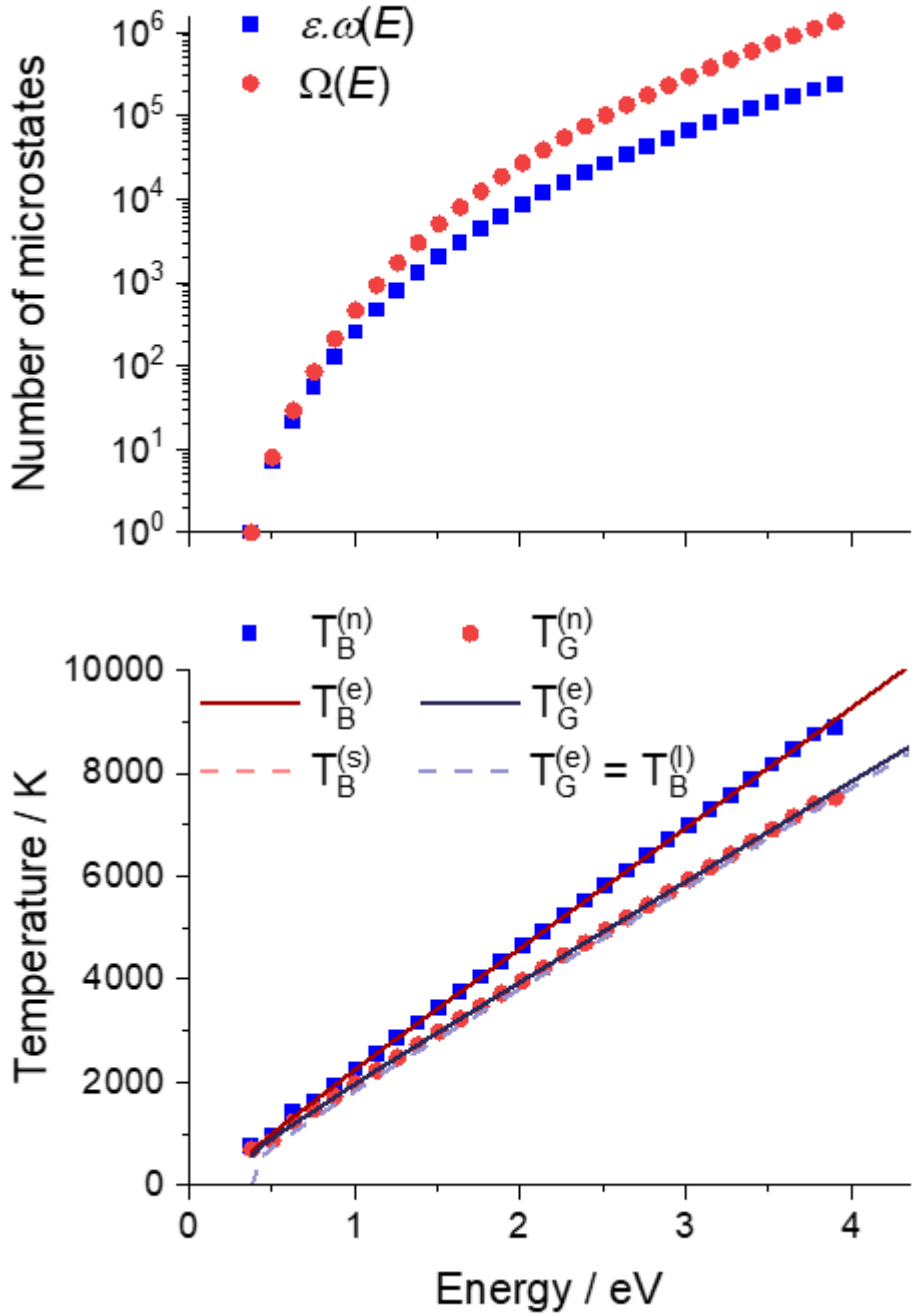


Nonadiabatic dynamics



DIFFERENT MEDIA, DIFFERENT APPROACHES

The figure as appearing in the paper



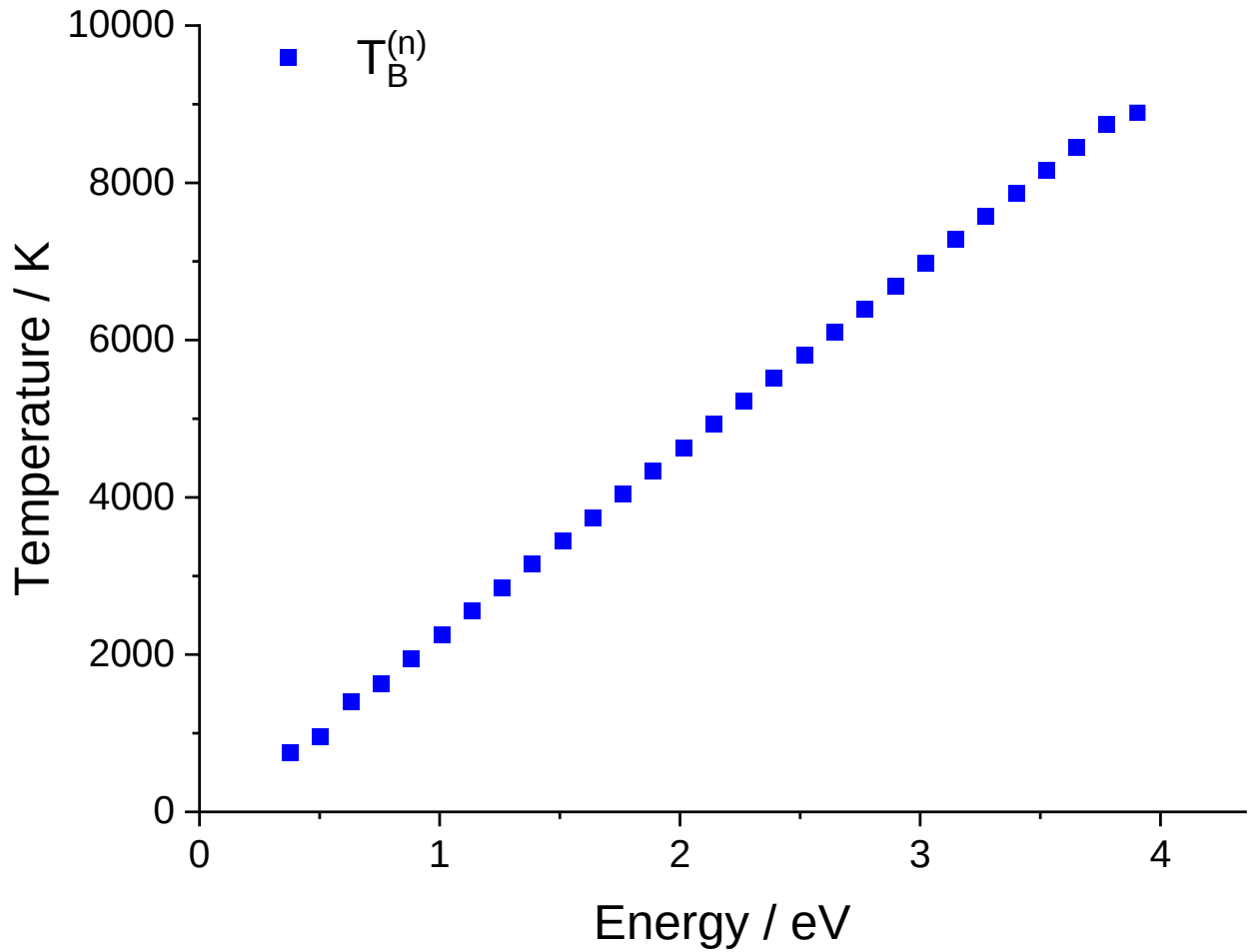
Boltzmann

$$\varepsilon\omega\left(E_M\right)=\left(\!\!\binom{N}{M}\!\!\right)=\binom{M+N-1}{M}$$

$$=\frac{\left(M+N-1\right)!}{\left(N-1\right)!M!}$$

$$S_B\left(E_M\right)=k_B\ln\left[\frac{\left(M+N-1\right)!}{\left(N-1\right)!M!}\right]$$

$$T_B^{(n)}=\left(\frac{\Delta S_B}{\Delta E}\right)^{-1}$$



Multiset: en.wikipedia.org/wiki/Multiset

LIGHT AND MOLECULES

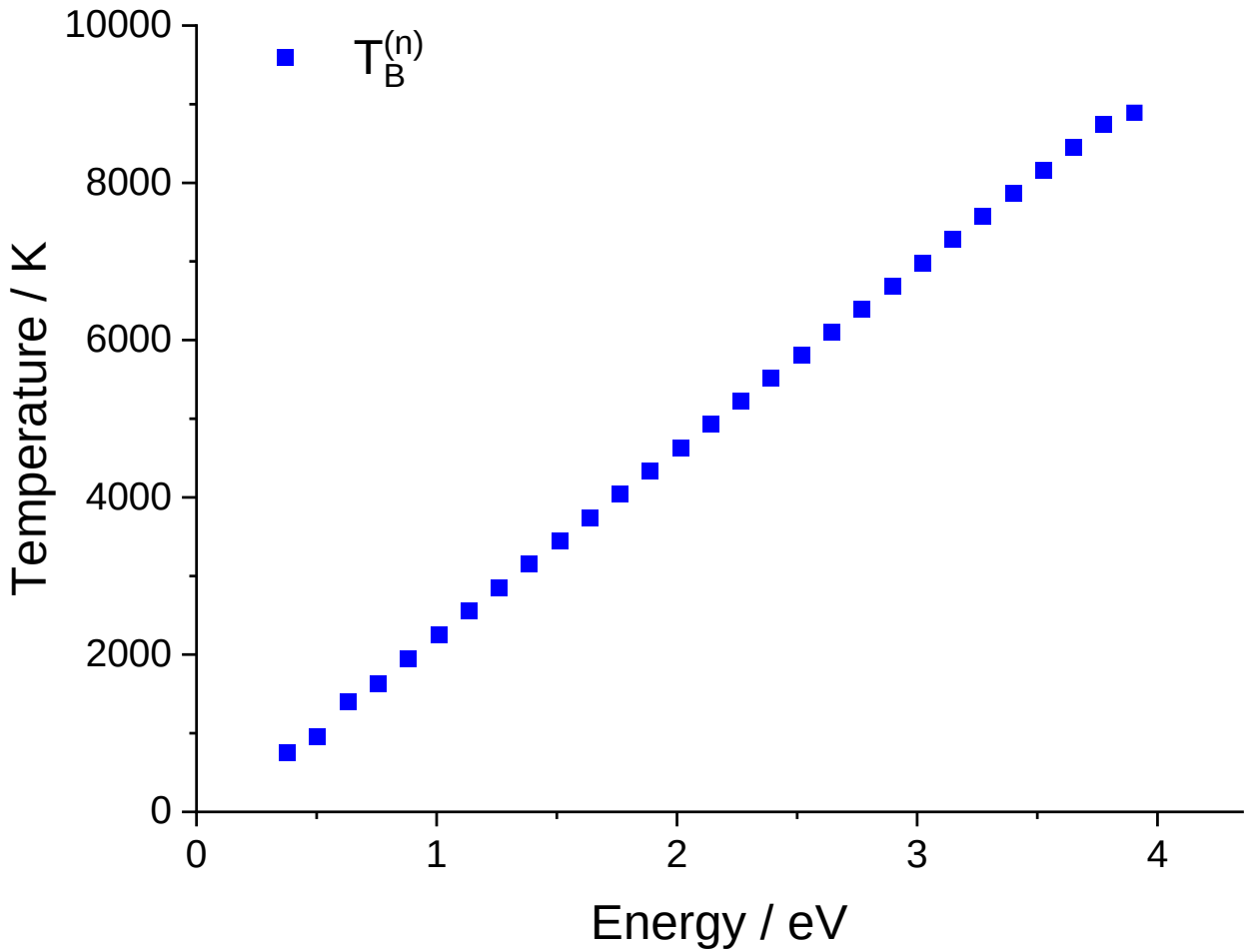
$$S_B\left(E_M\right) = k_B \ln\left[\frac{\left(M+N-1\right)!}{\left(N-1\right)!M!}\right]$$

Stirling's approximation

$$\ln\left(n!\right) \approx n\ln\left(n\right) - n$$

$$T_B^{(s)} = \left(\frac{\partial S_B}{\partial E}\right)^{-1}$$

$$= \left(\ln\left[\frac{\left(2E+\left(N-2\right)h\bar{\nu}\right)}{\left(2E-Nh\bar{\nu}\right)}\right]\right)^{-1} \frac{h\bar{\nu}}{k_B}$$



$$S_B\left(E_M\right) = k_B \ln\left[\frac{(M+N-1)!}{(N-1)!M!}\right]$$

Stirling's approximation

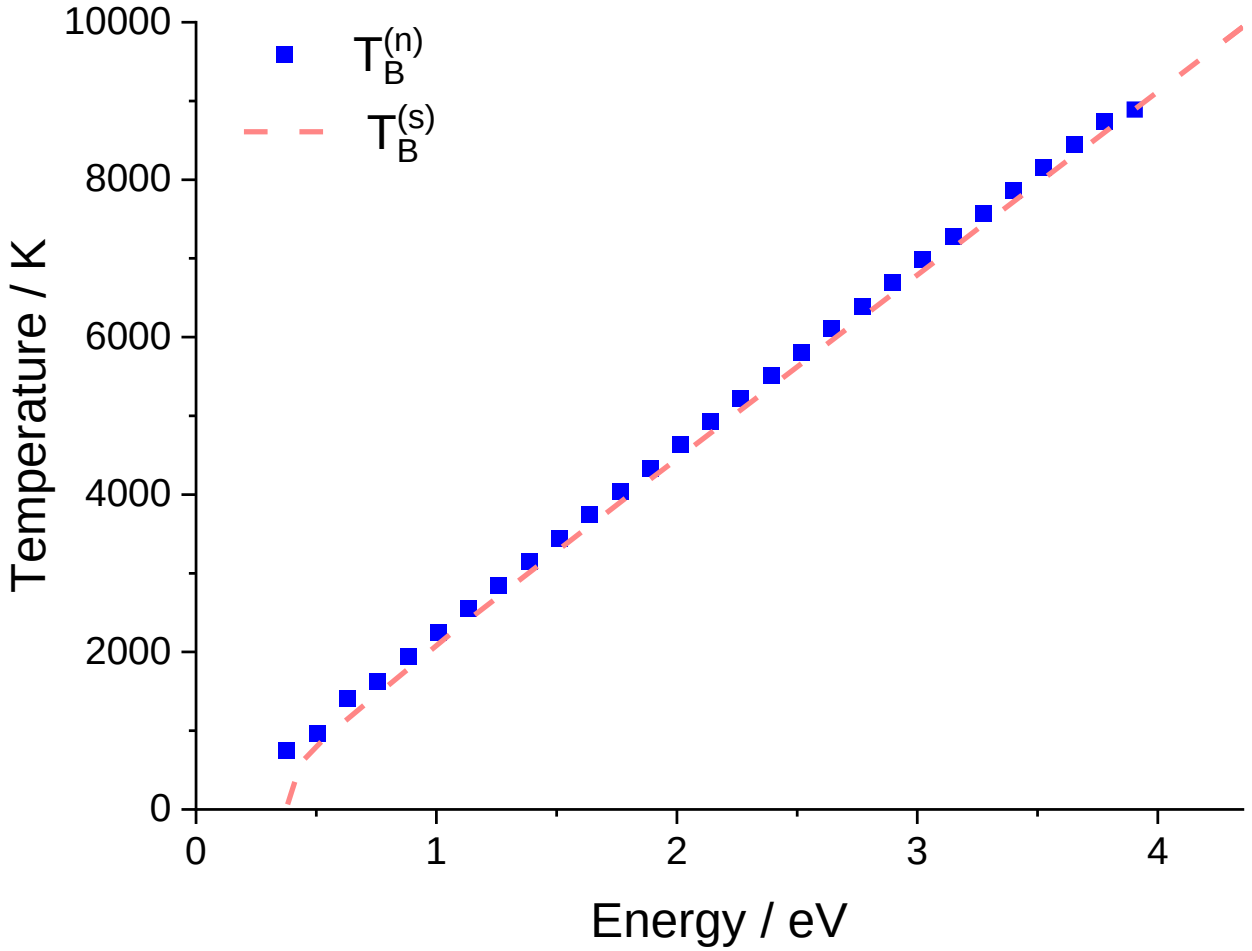
$$\ln(n!) \approx n\ln(n) - n$$

$$T_B^{(s)} = \left(\frac{\partial S_B}{\partial E}\right)^{-1}$$

$$= \left(\ln\left[\frac{\left(2E + (N-2)h\bar{\nu}\right)}{\left(2E - Nh\bar{\nu}\right)}\right]\right)^{-1} \frac{h\bar{\nu}}{k_B}$$

$N >> 2$ approximation

$$T_B^{(l)} = \left(\ln\left[\frac{2E + Nh\bar{\nu}}{2E - Nh\bar{\nu}}\right]\right)^{-1} \frac{h\bar{\nu}}{k_B}$$



$$S_B\left(E_M\right)=k_B\ln\left[\frac{\left(M+N-1\right)!}{\left(N-1\right)!M!}\right]$$

Stirling's approximation

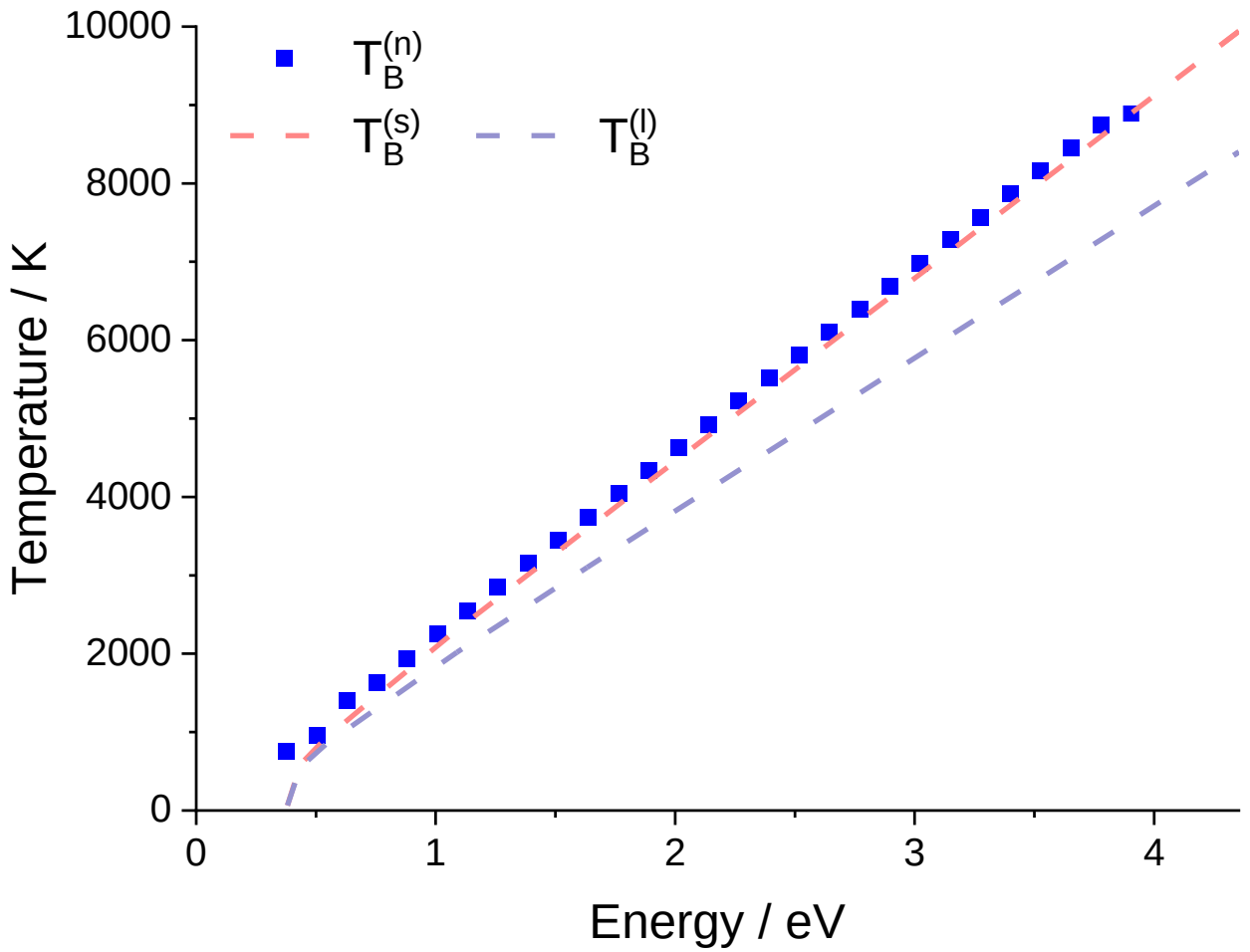
$$\ln\left(n!\right)\approx n\ln\left(n\right)-n$$

$$T_B^{(s)}=\left(\frac{\partial S_B}{\partial E}\right)^{-1}$$

$$=\left(\ln\left[\frac{\left(2E+\left(N-2\right)h\bar{\nu}\right)}{\left(2E-Nh\bar{\nu}\right)}\right]\right)^{-1}\frac{h\bar{\nu}}{k_B}$$

$N >> 2$ approximation

$$T_B^{(l)}=\left(\ln\left[\frac{2E+Nh\bar{\nu}}{2E-Nh\bar{\nu}}\right]\right)^{-1}\frac{h\bar{\nu}}{k_B}$$

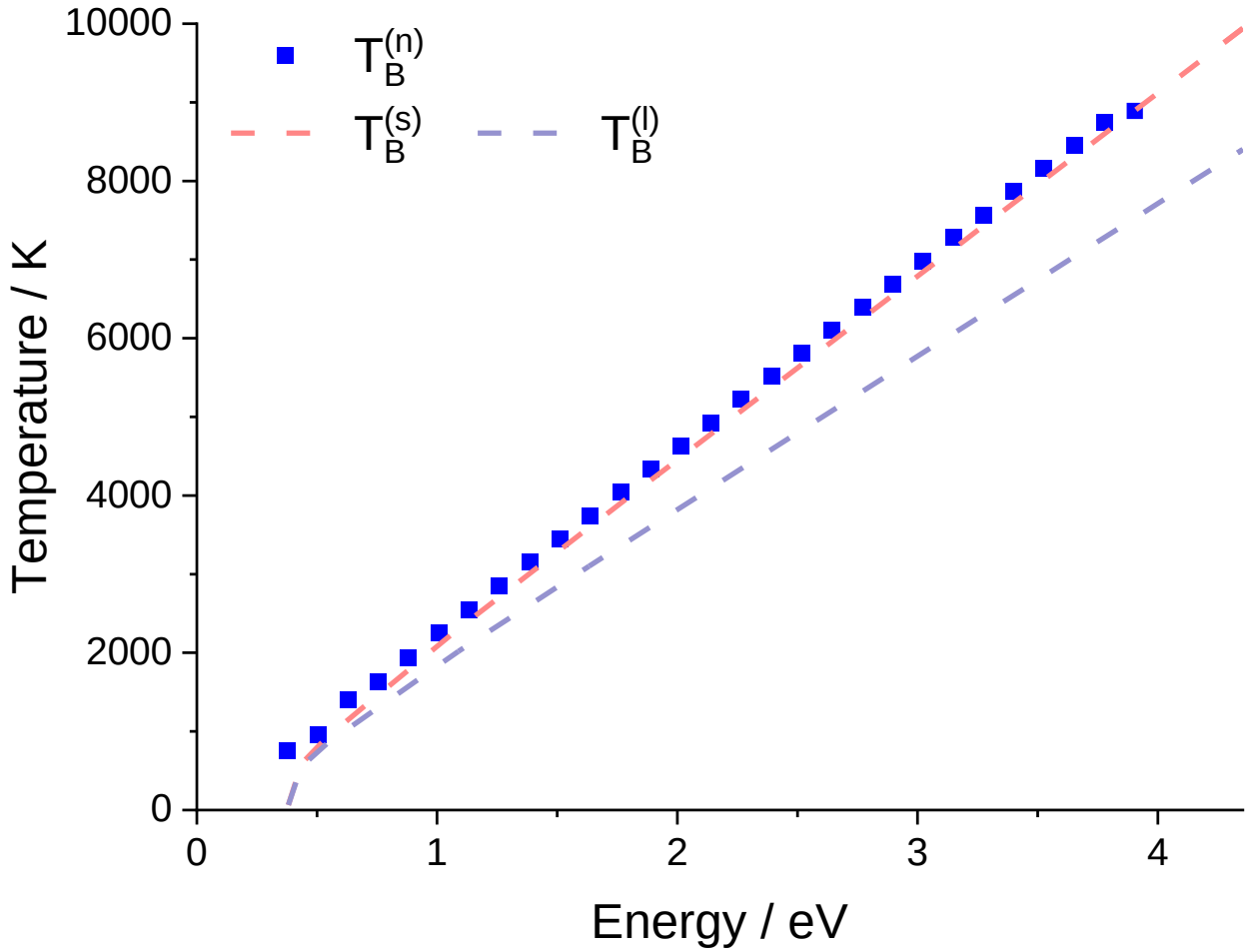


Gibbs volume

$$\Omega(E_M) = \sum_{K=0}^{M} \left(\!\binom{N}{K}\!\right) = \binom{M+N}{M} = \frac{(M+N)!}{N!M!}$$

Hockey-stick identity

$$\sum_{j=0}^{n-r} \binom{j+r}{r} = \binom{n+1}{n-r}$$



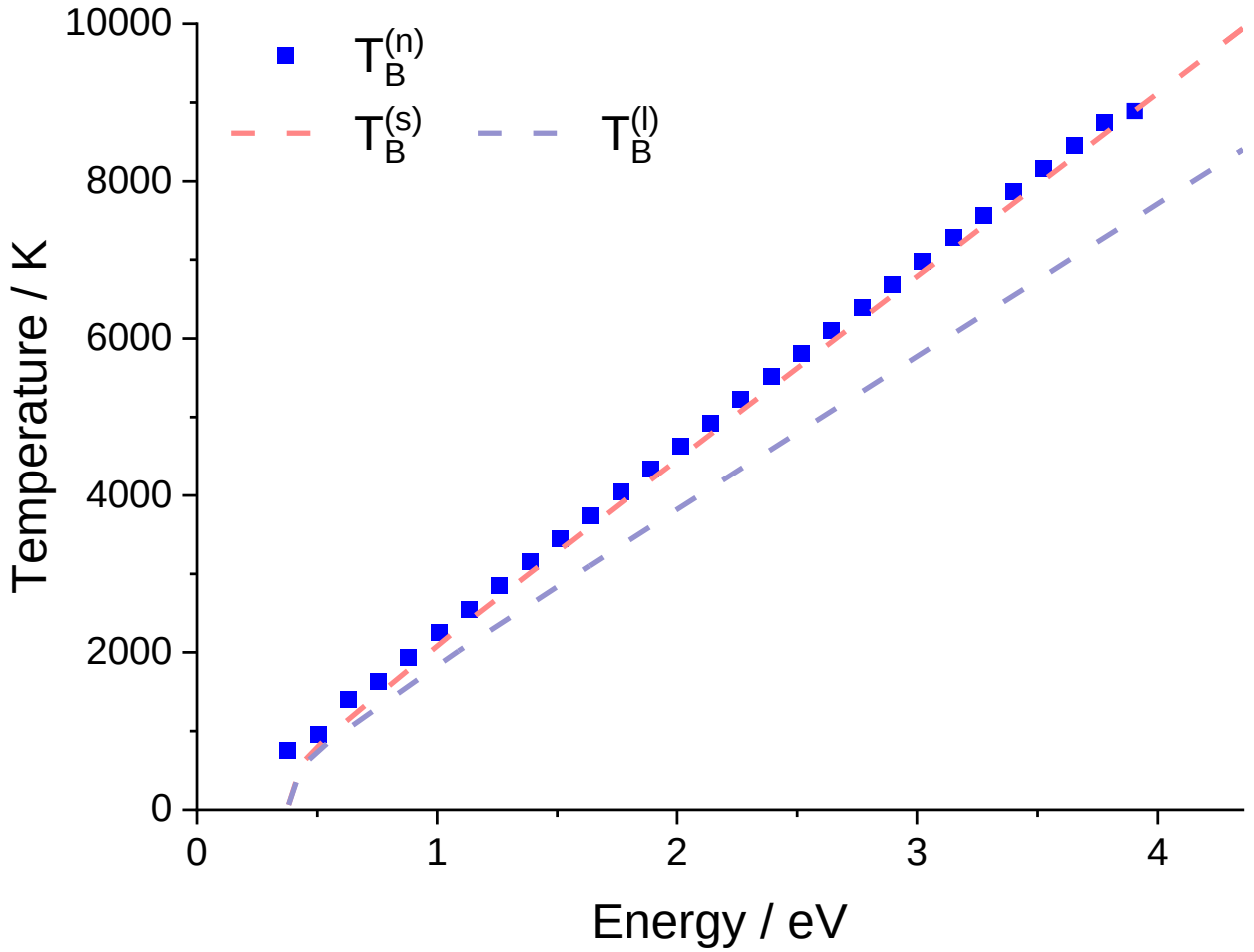
Hockey-stick identity: en.wikipedia.org/wiki/Hockey-stick_identity

Gibbs volume

$$\Omega(E_M) = \sum_{K=0}^{M} \left(\!\binom{N}{K}\!\right) = \binom{M+N}{M} = \frac{(M+N)!}{N!M!}$$

$$S_G(E_M) = k_B \ln\left[\frac{(M+N)!}{N!M!}\right]$$

$$T_G^{(n)} = \left(\frac{\Delta S_G}{\Delta E}\right)^{-1}$$



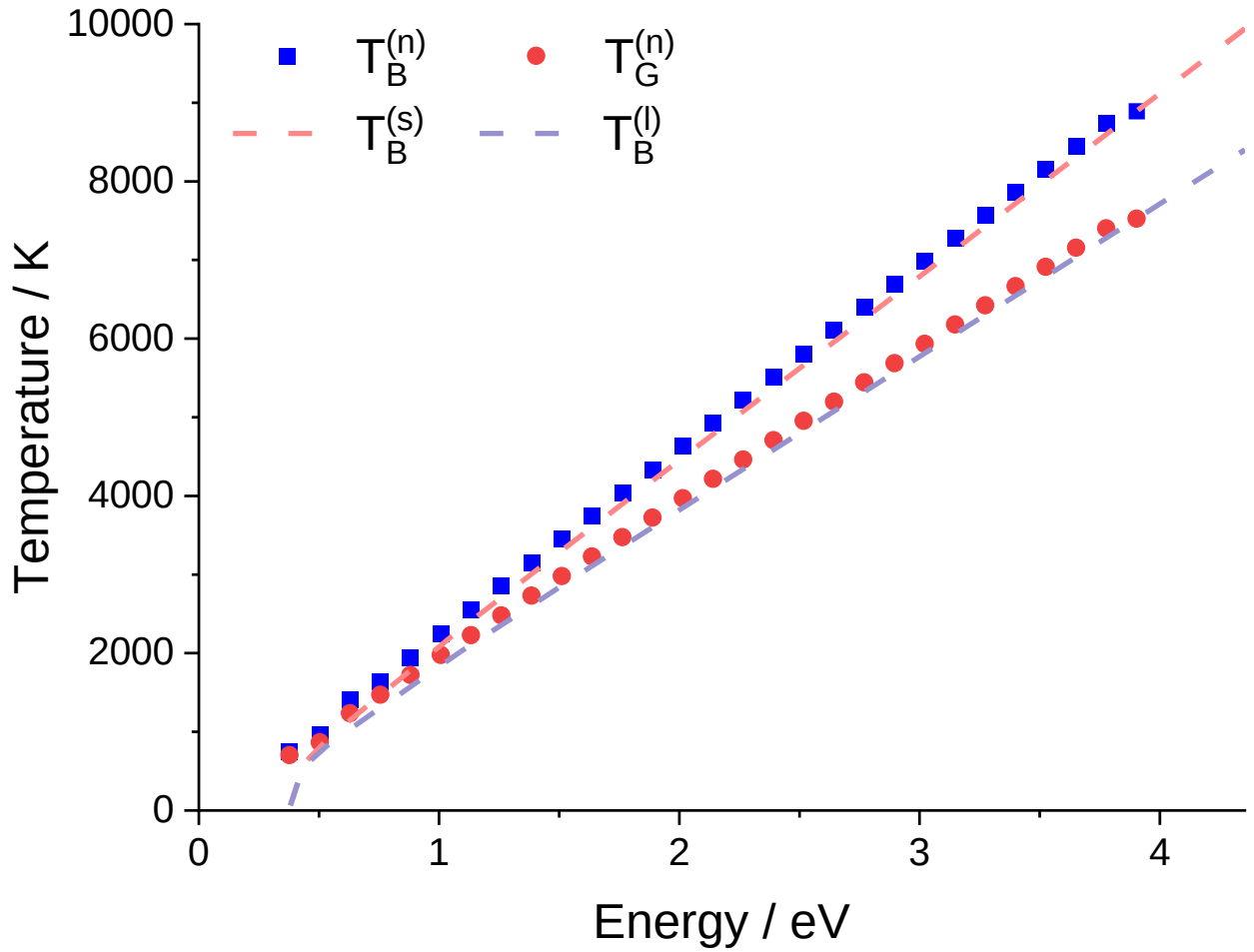
LIGHT AND MOLECULES

Gibbs volume

$$\Omega(E_M) = \sum_{K=0}^{M} \left(\!\binom{N}{K}\!\right) = \binom{M+N}{M} = \frac{(M+N)!}{N!M!}$$

$$S_G(E_M) = k_B \ln\left[\frac{(M+N)!}{N!M!}\right]$$

$$T_G^{(n)} = \left(\frac{\Delta S_G}{\Delta E}\right)^{-1}$$



LIGHT AND MOLECULES

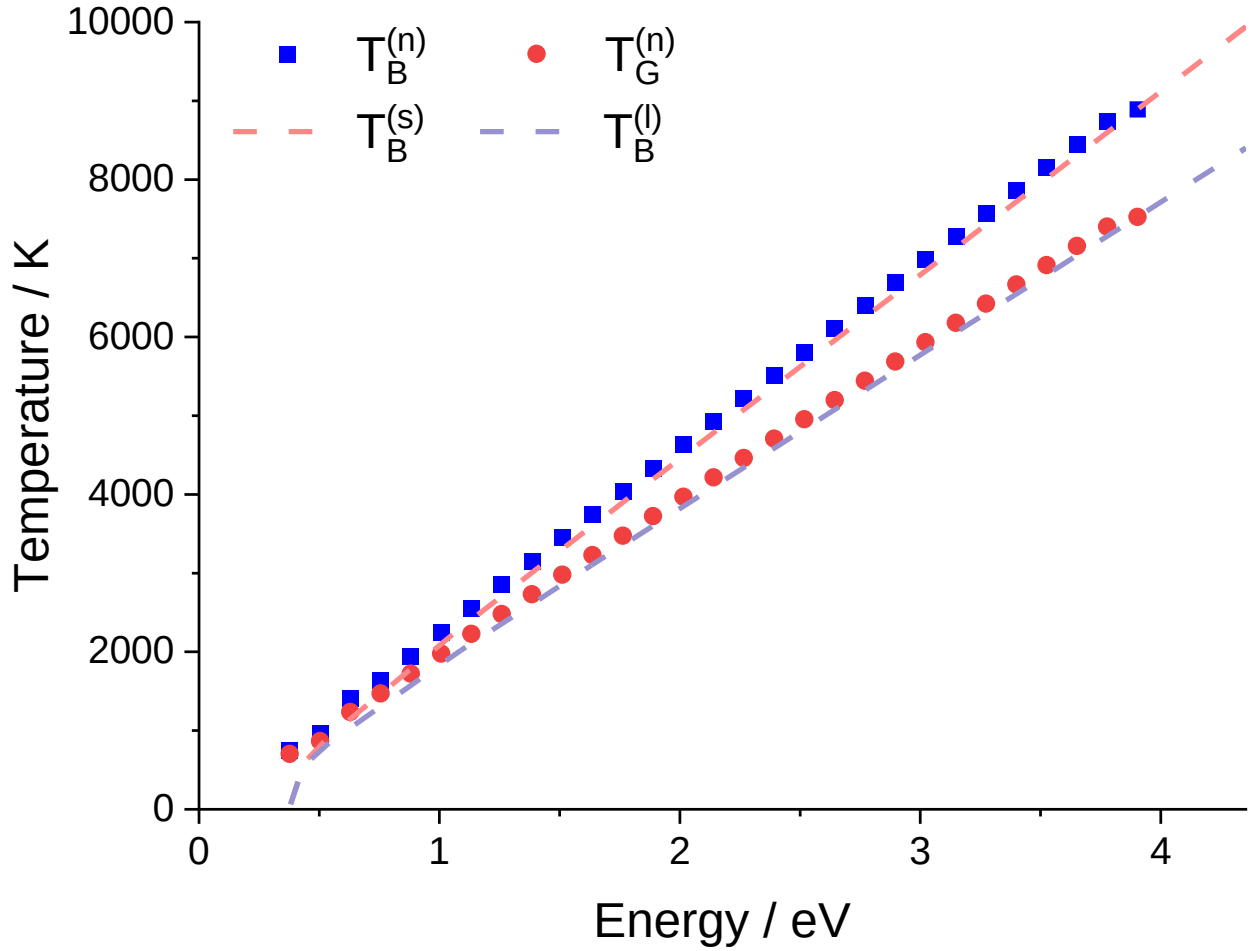
$$S_G\left(E_M\right) = k_B \ln\left[\frac{(M+N)!}{N!M!}\right]$$

$$T_G^{(n)} = \left(\frac{\Delta S_G}{\Delta E}\right)^{-1}$$

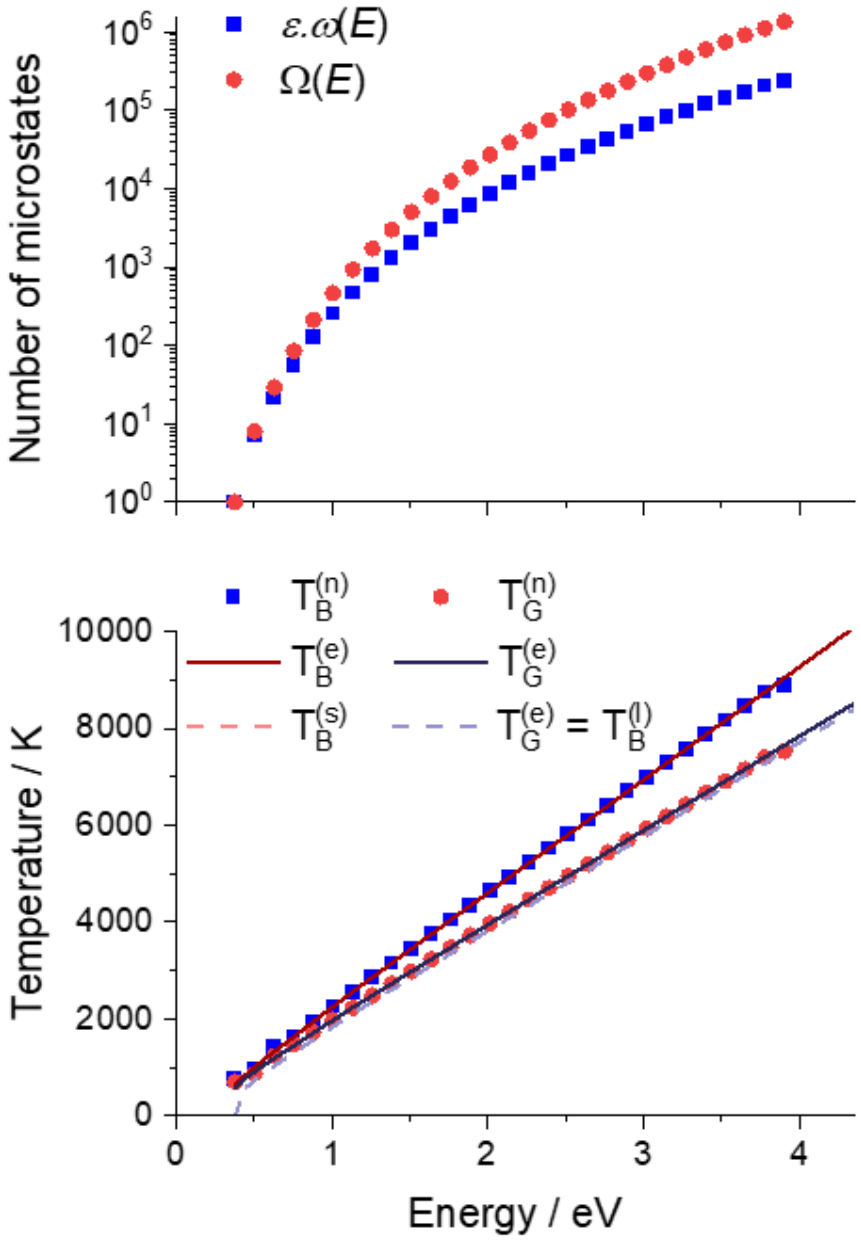
Stirling's approximation

$$T_G^{(s)} = \left(\frac{\partial S_G}{\partial E}\right)^{-1} = \left(\ln\left[\frac{2E + N\hbar\bar{\nu}}{2E - N\hbar\bar{\nu}}\right]\right)^{-1} \frac{\hbar\bar{\nu}}{k_B}$$

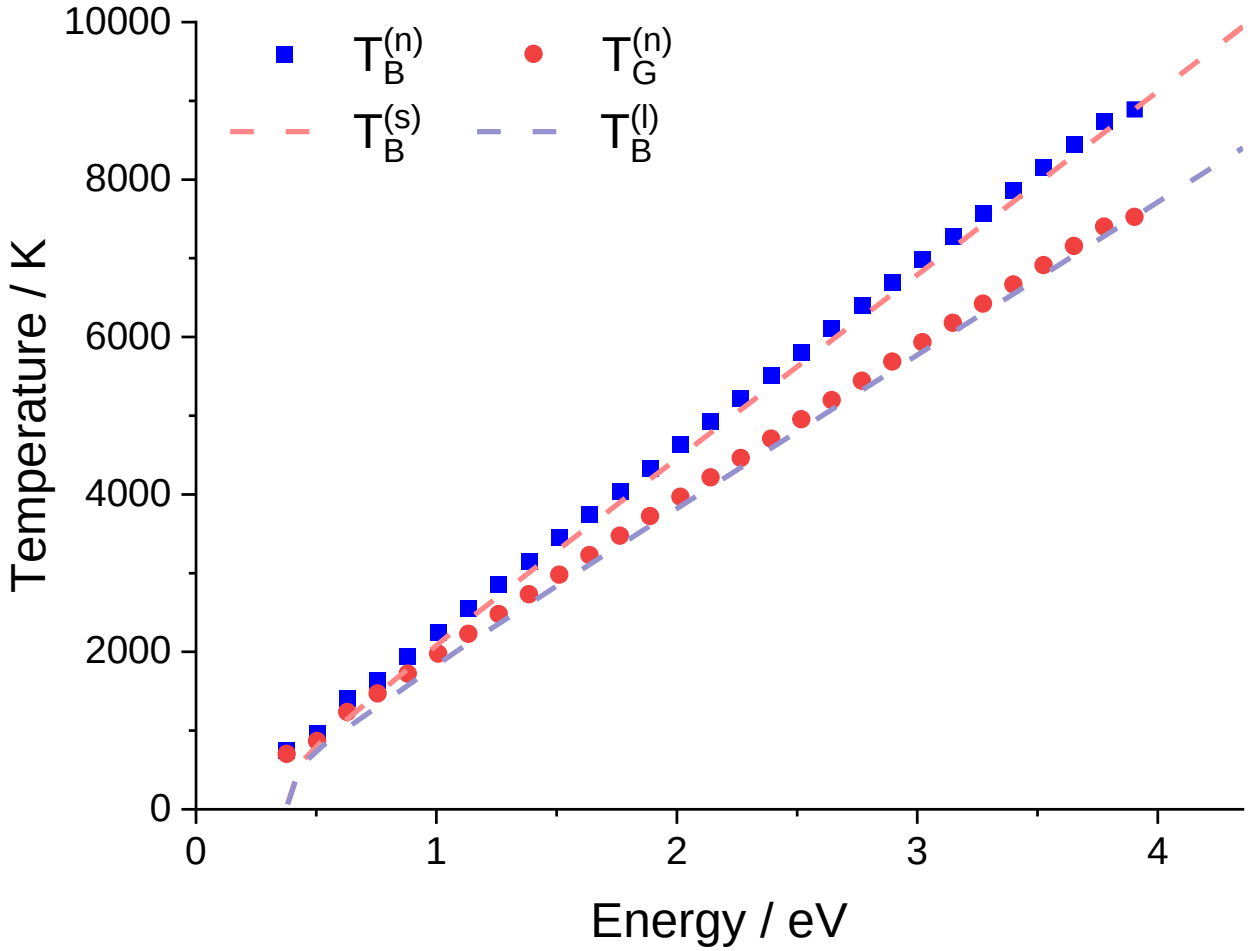
$$T_G^{(s)} = T_B^{(l)}$$



Good for a paper



Good for a seminar



BEYOND FORMAL WRITING

Social media

- Establish presence
  (Social net, ORCID, Google scholar, GitHub)
- Highlight your work
- Make yourself known
- Counteract Matthew effect

Matthew effect: en.wikipedia.org/wiki/Matthew_effect

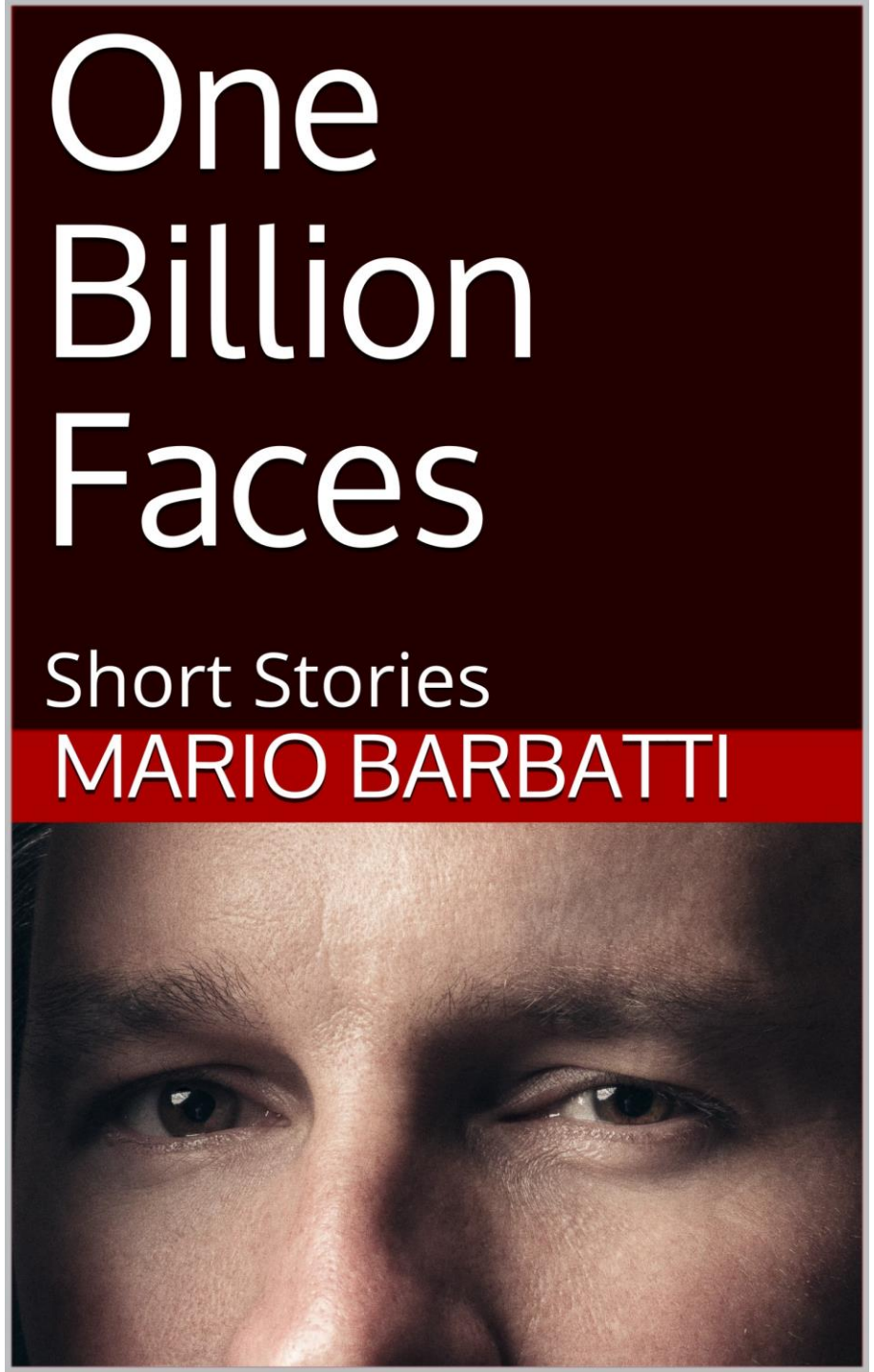
Blog

- Make yourself a reference
- Create a memory of your work
- Speak to a broader public

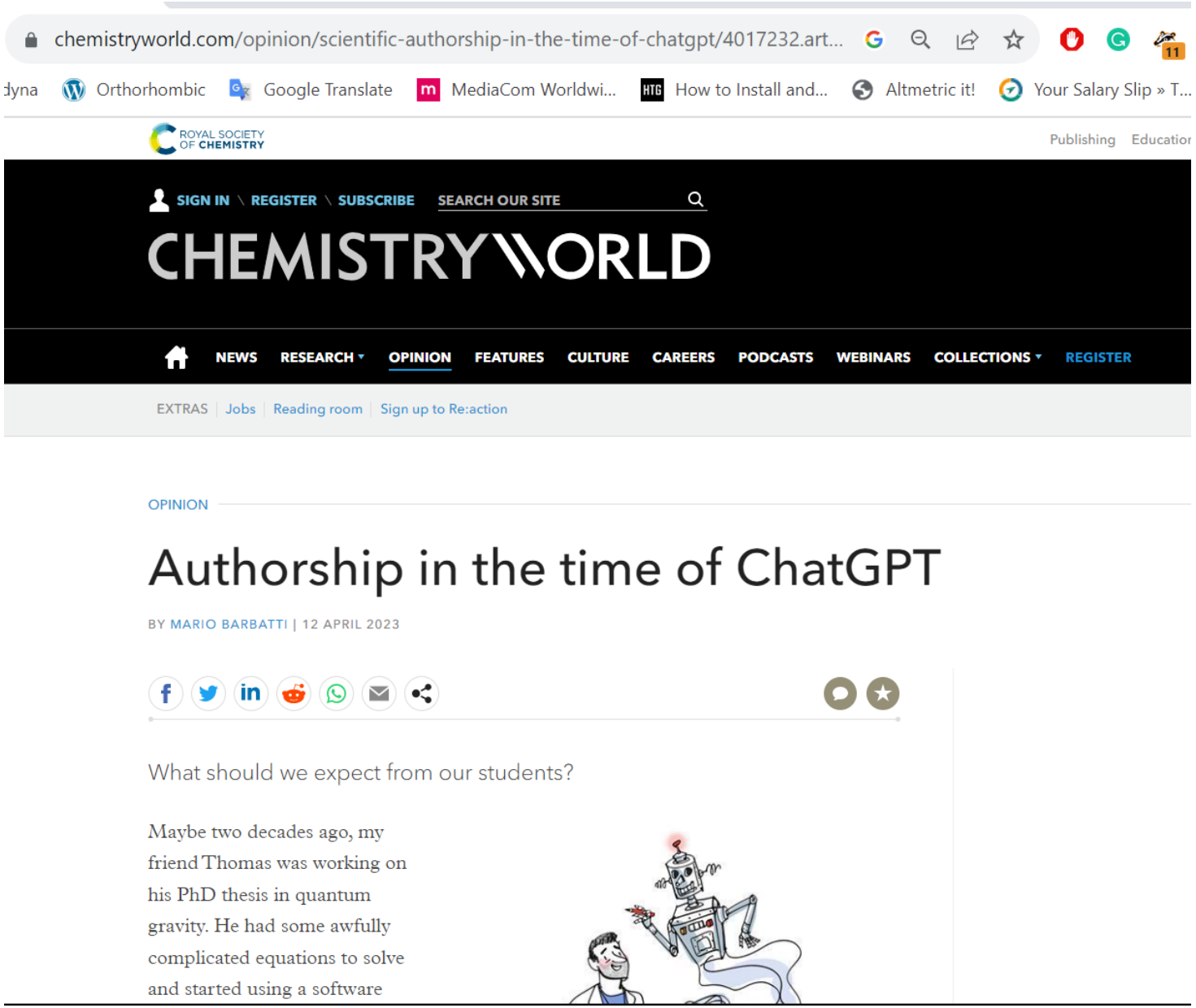
My own experience: www.barbatti.org

New adventures!

Available on Amazon
Kindle and paperback

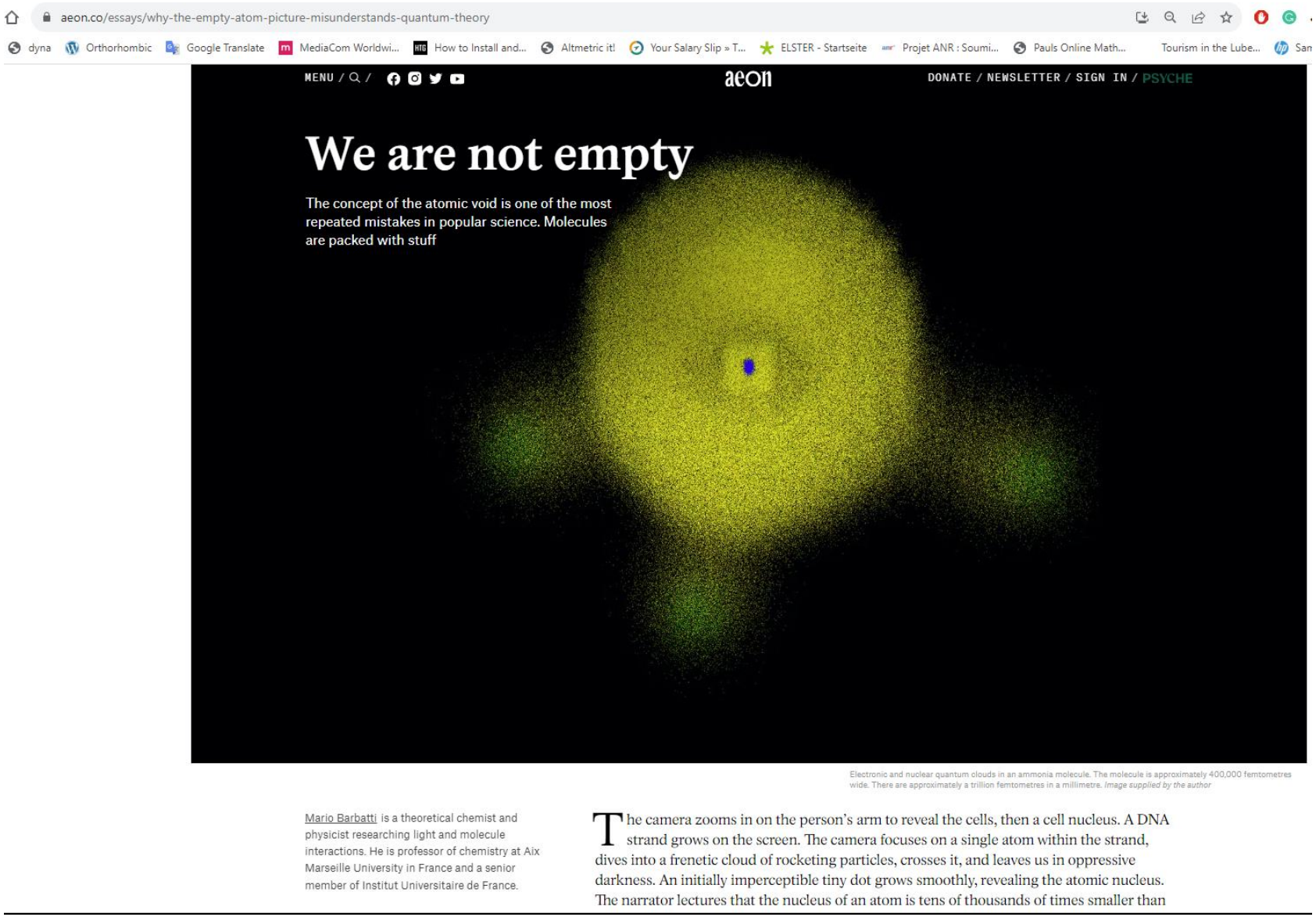


New adventures!



tinyurl.com/cwchatgpt

New adventures!



tinyurl.com/emptyatom

New adventures!

iai news

Home | Philosophy | Science | Politics | Arts | Issue Archive

The many answers to the quantum measurement problem

Has physics tamed the wavefunction?

21st June 2024

Mario Barbatti | Physicist, writer and Professor at Aix Marseille University. He is specialized in the development and application of quantum-classical dynamics and quantum chemistry.

2,022 words

Read time: approx. 10 mins

tinyurl.com/qmeasure

Thank you

www.barbatti.org

mario.barbatti@univ-amu.fr

@MarioBarbatti