



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

- C Sagan
- R Dawkins
- J Diamond
- S Pinker

Philosophy of science

- I Prigogine
- G Bachelard
- T Kuhn
- S M Carroll

Science fiction

- I Asimov
- A C Clarke
- D Adams
- T Chiang

Fiction

- F Kafka
- G G Marques
- M de Assis
- P Roth

+ 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



Kar *et al.* Excited state dynamics of HBT in cyclohexane. Preprint, 2023.

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

Styles

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- Affiliation
- Authors
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- Caption
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- Heading 1 no Number
- 1.1 Heading 2
- 1.1.1 Heading 3
- 1.1.1.1 Heading 4
- Normal
- Table text
- Title
- Emphasis
- Footer

Show Preview
 Disable Linked Styles

Options...

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

+ 1 Introduction

+ 2 Computational details

+ 3 Results

+ 3.1 QM models

+ 3.1.1 FOMO-CASCI Results

+ 3.1.2 TDDFT Results

+ 3.2 QM/MM models

+ 3.2.1 Thermalization Results

+ 3.2.2 Simulated Spectra and Excited state Dynamics

+ 3.2.3 Comparison with other force field

+ Conclusions

+ Acknowledgments

+ Conflicts of interest

+ Author contributions

Styles

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- Abstract
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- 1.1.1.1 Heading 4
- Normal
- Table text
- Title
- Emphasis
- Footer

Show Preview Disable Linked Styles

A+ A- A Options...

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

complete
accurate
logical



convincing
appealing
clear

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

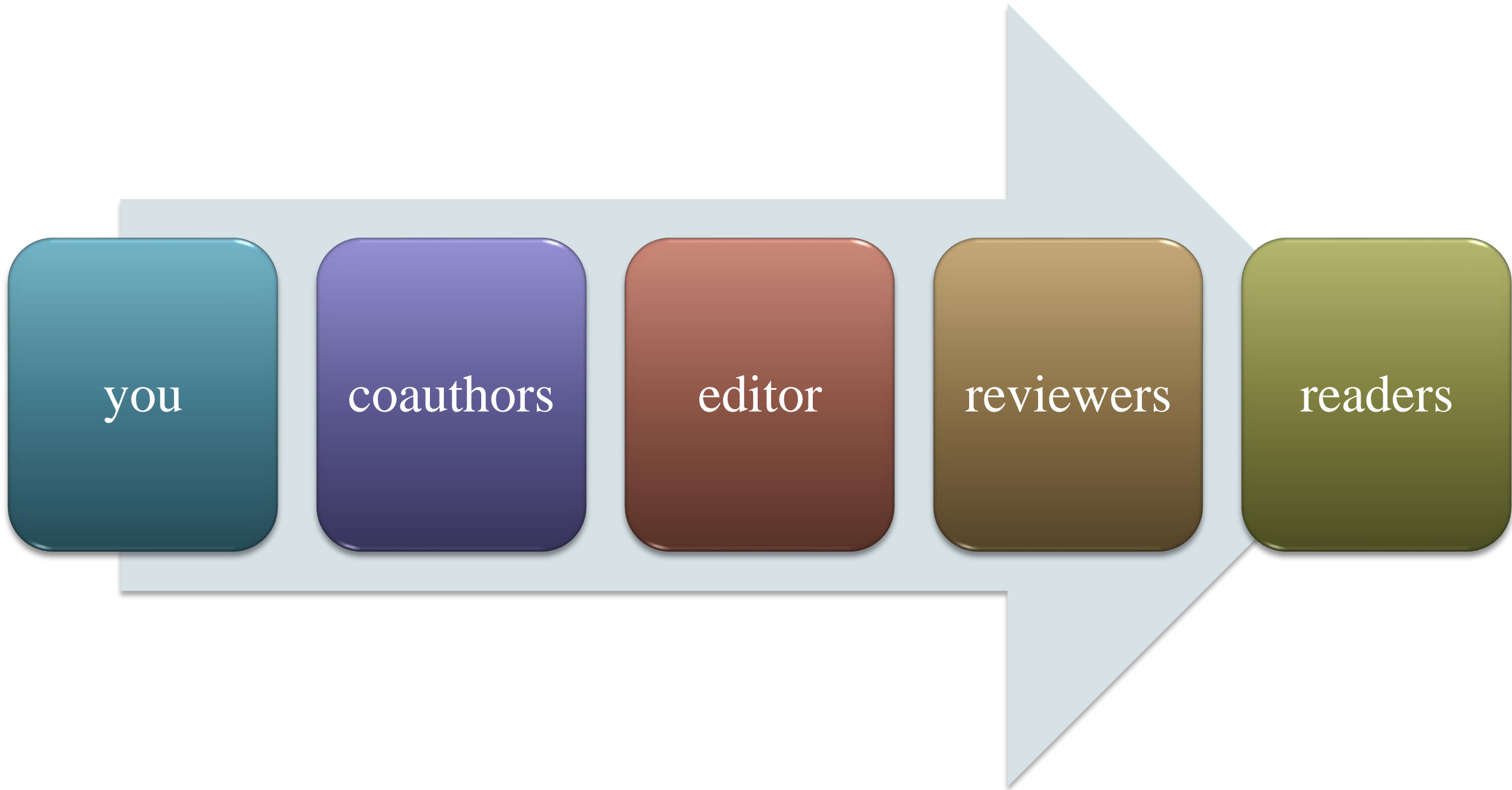
Results

Discussion

Conclusion



***SCIENTIFIC
WRITING IS
COLLECTIVE***





***SLIDES AND
PRESENTATIONS***

Master your tools

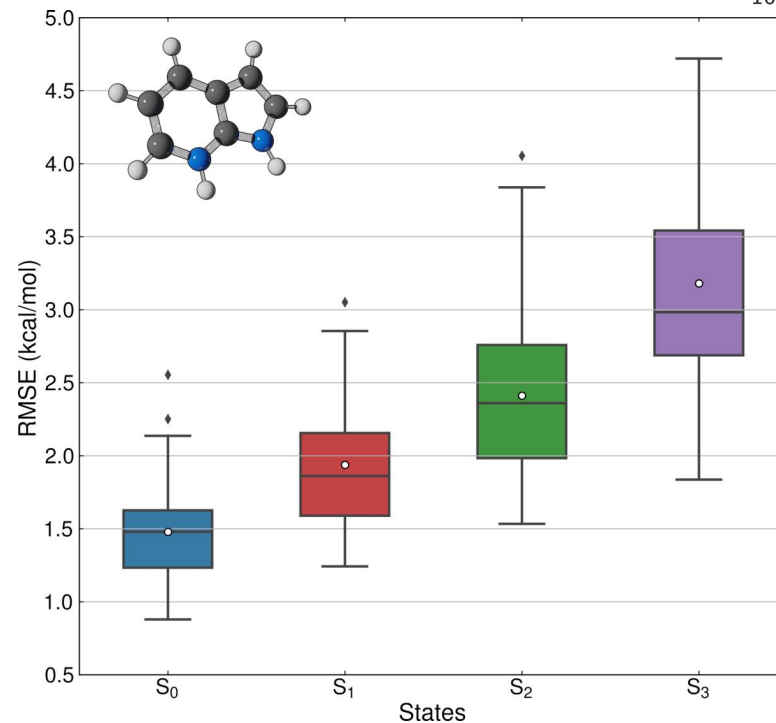
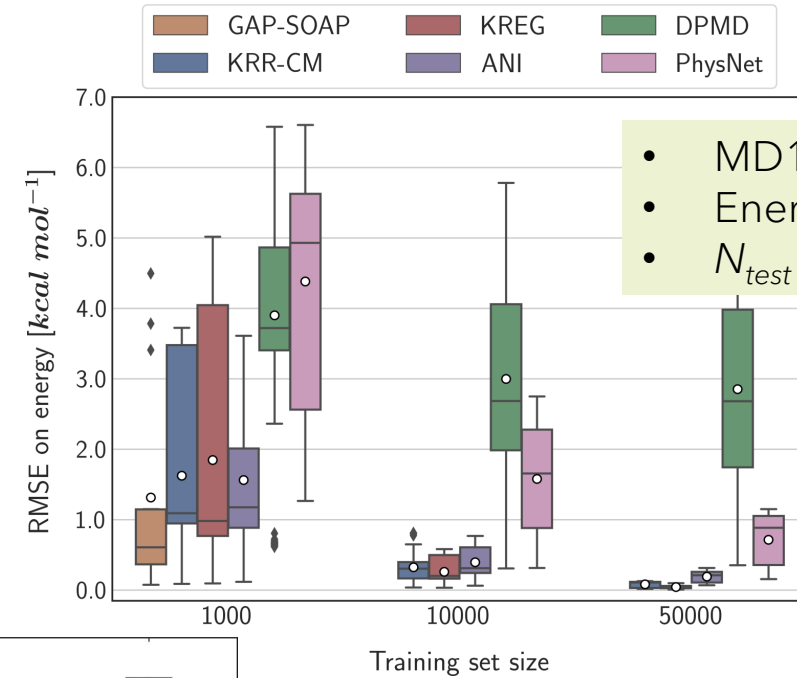
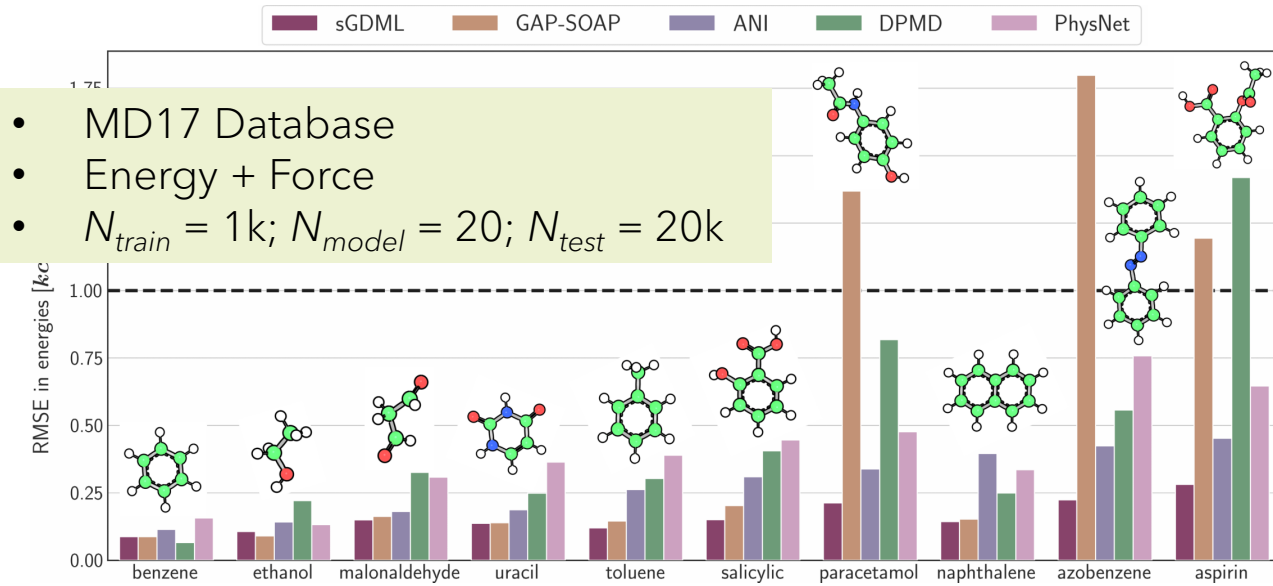
My choice:

- PowerPoint
- MathType
- Grammarly
- Endnote

Laws of slide composition

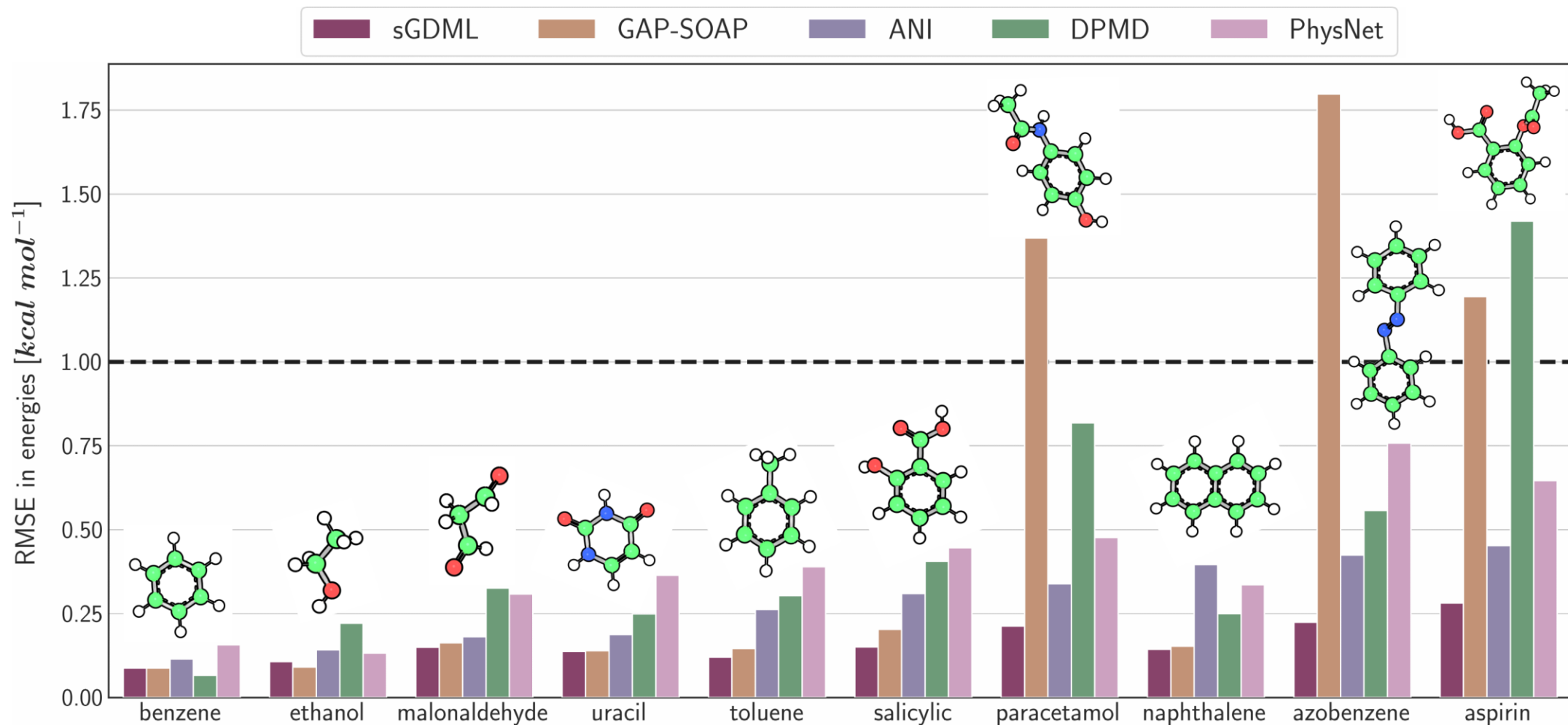
1. Background can have any color as long it's white.
2. Font size in PTs must be at least half the age of the oldest person in the public.
3. One slide fits one and only one piece of info. Slides are for free. Don't save their number.

COULD HAVE DONE

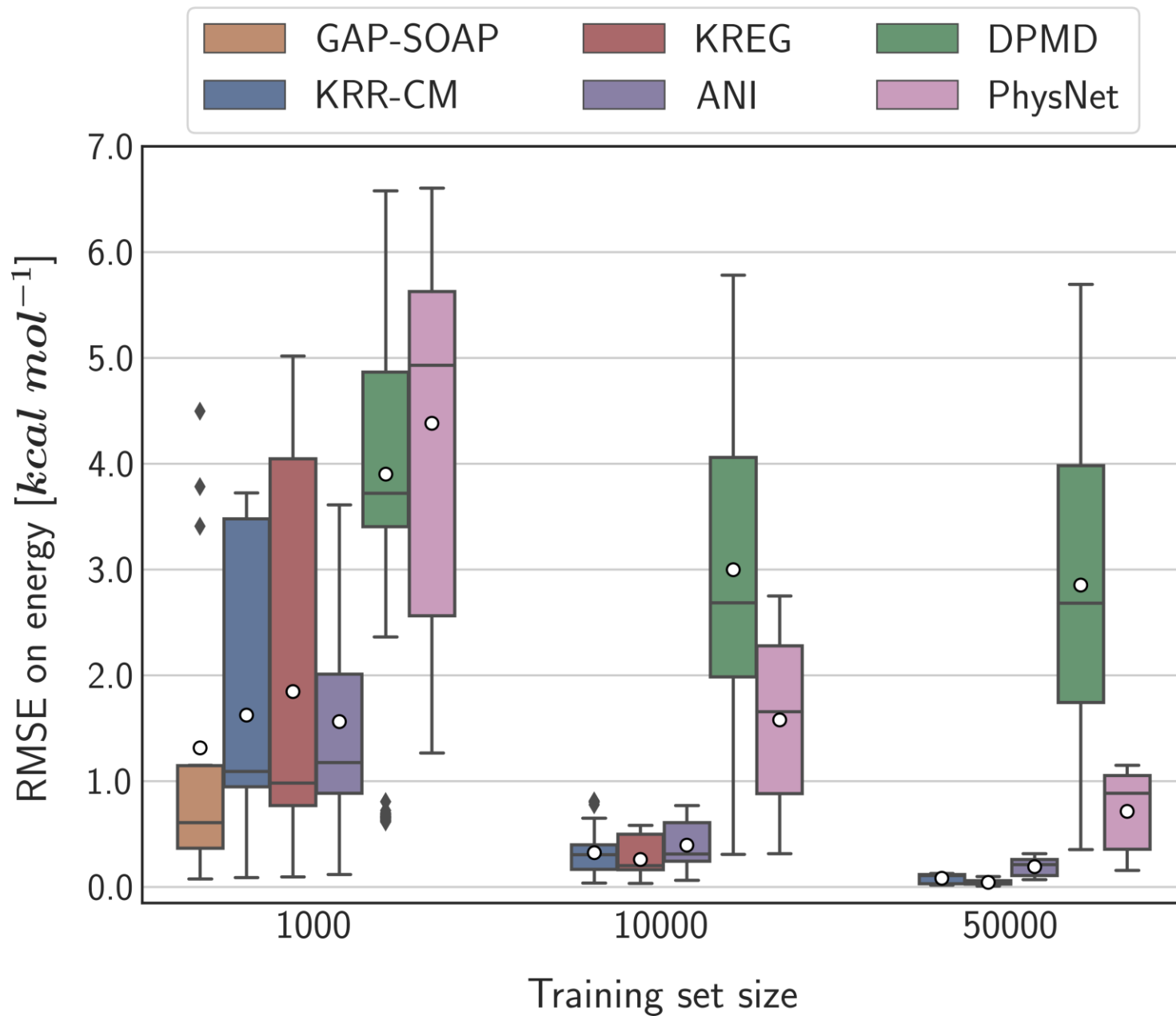


KREG x RI-ADC(2)/cc-pVDZ
DC-FSSH: 50 trajs; 0.5 fs; 300 ps

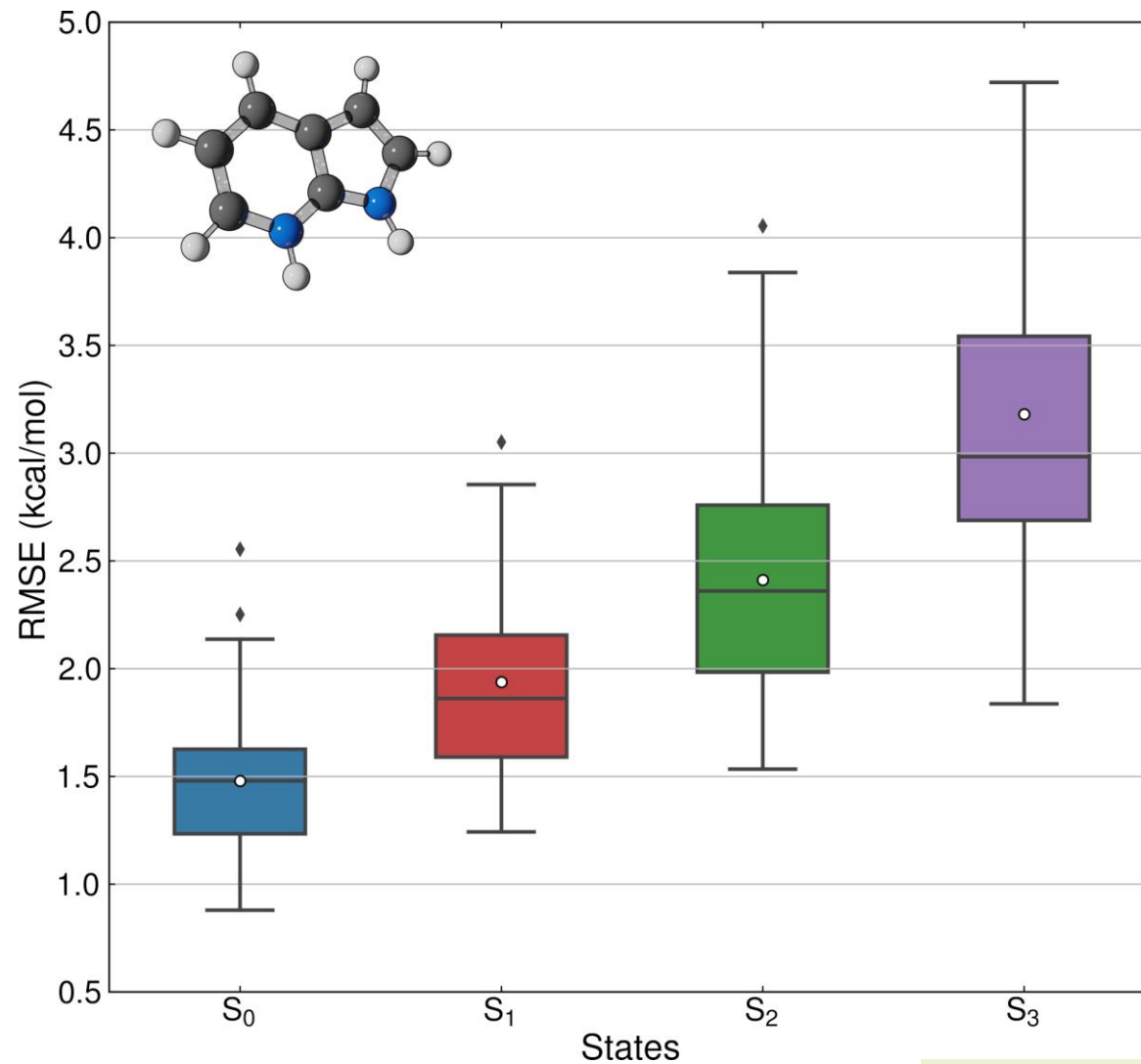
BETTER



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



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



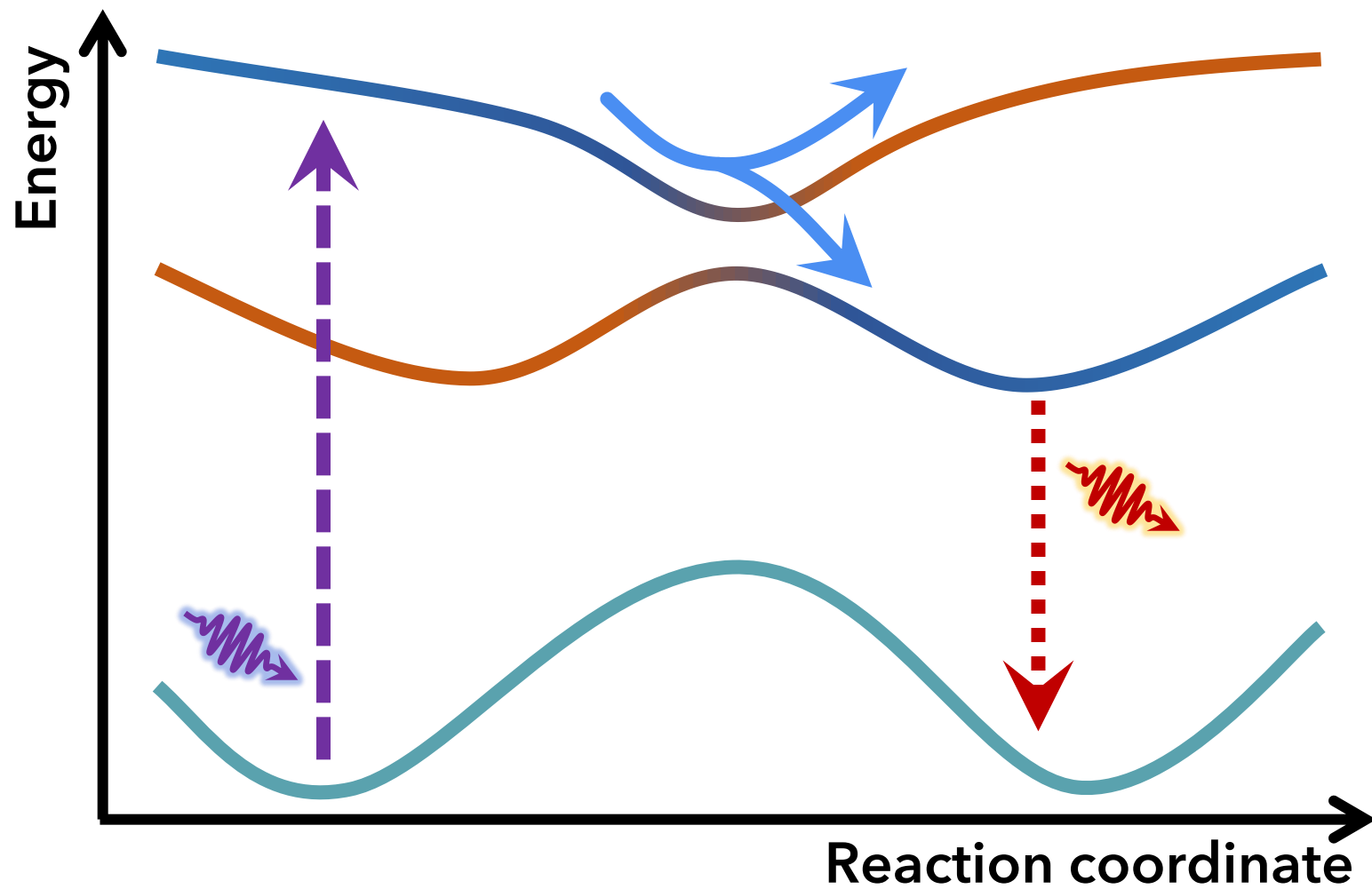
- KREG x RI-ADC(2)/cc-pVDZ
- DC-FSSH: 50 traj; 0.5 fs; 300 ps

Master animations

Use animations to tell the public where to focus.

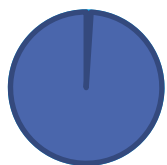
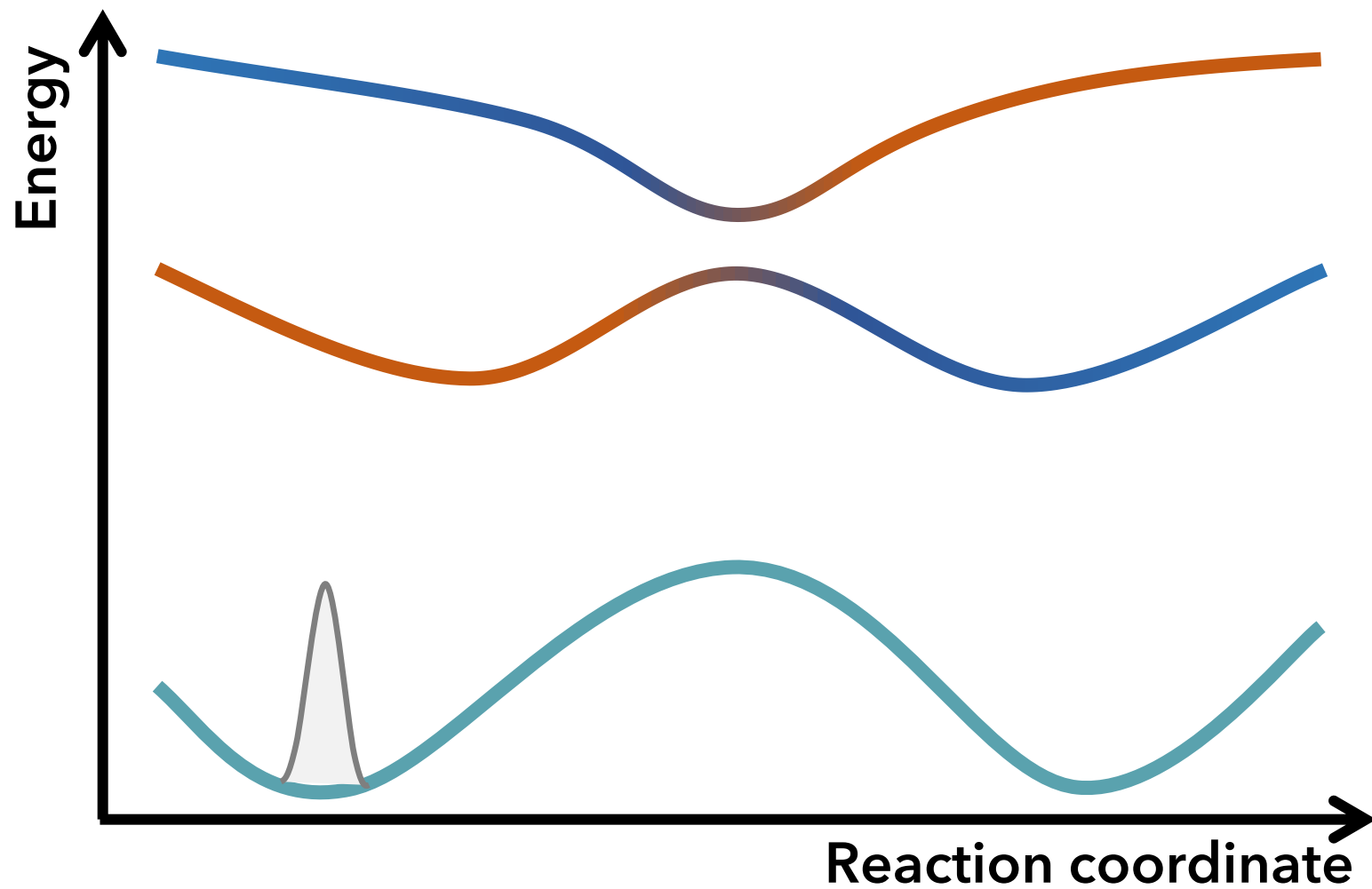
COULD HAVE DONE

Nonadiabatic dynamics

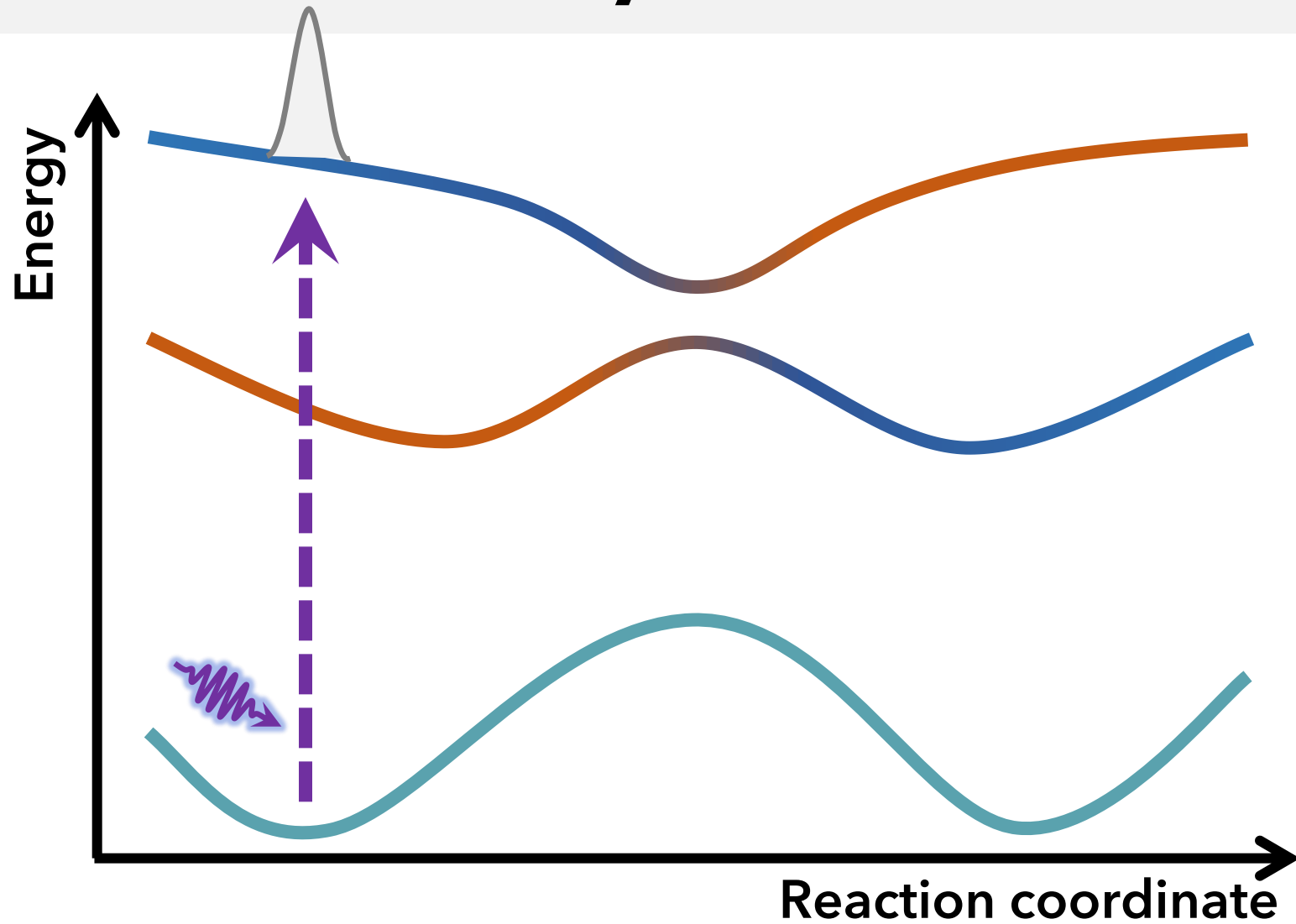


BETTER

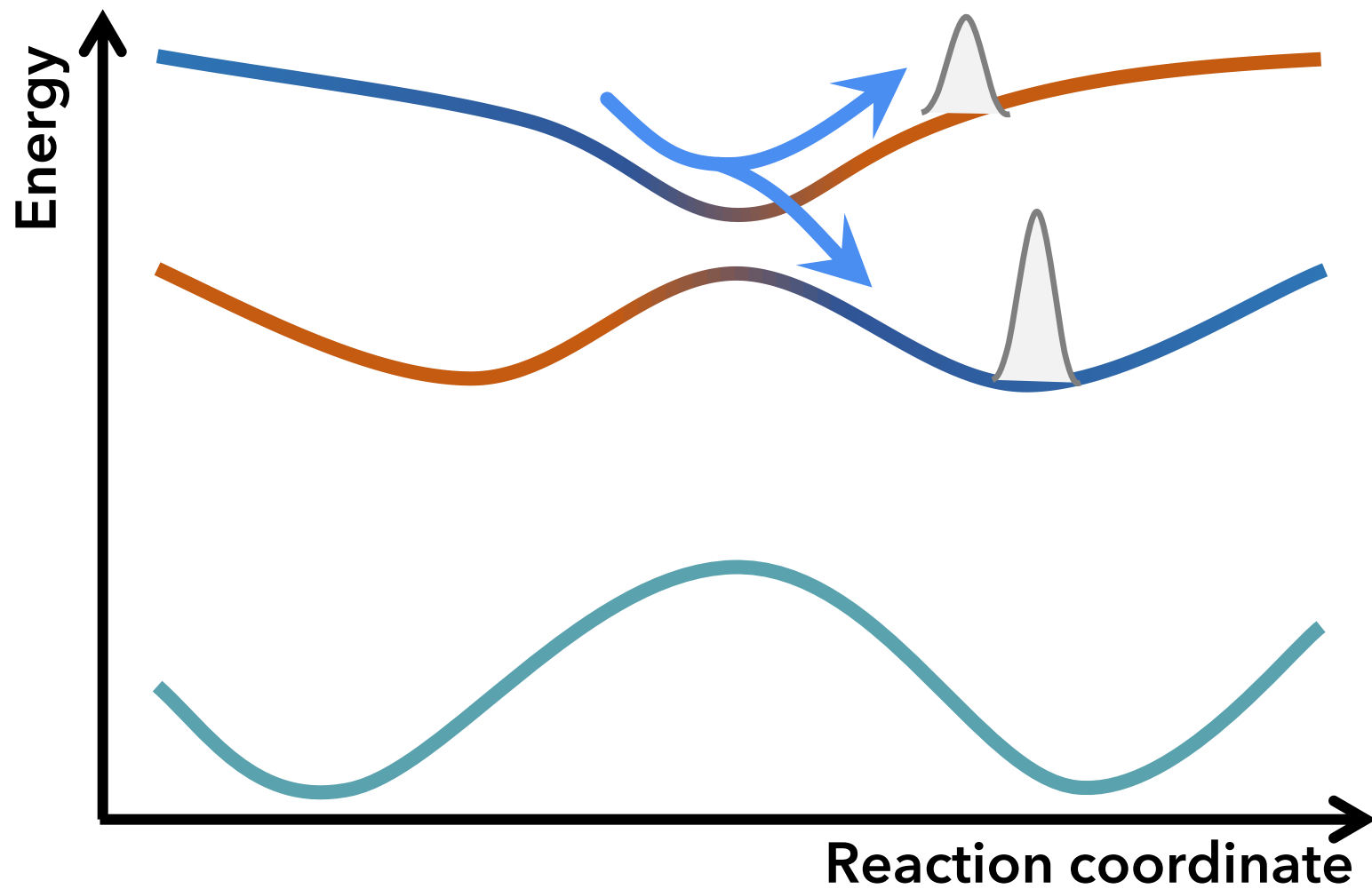
Nonadiabatic dynamics



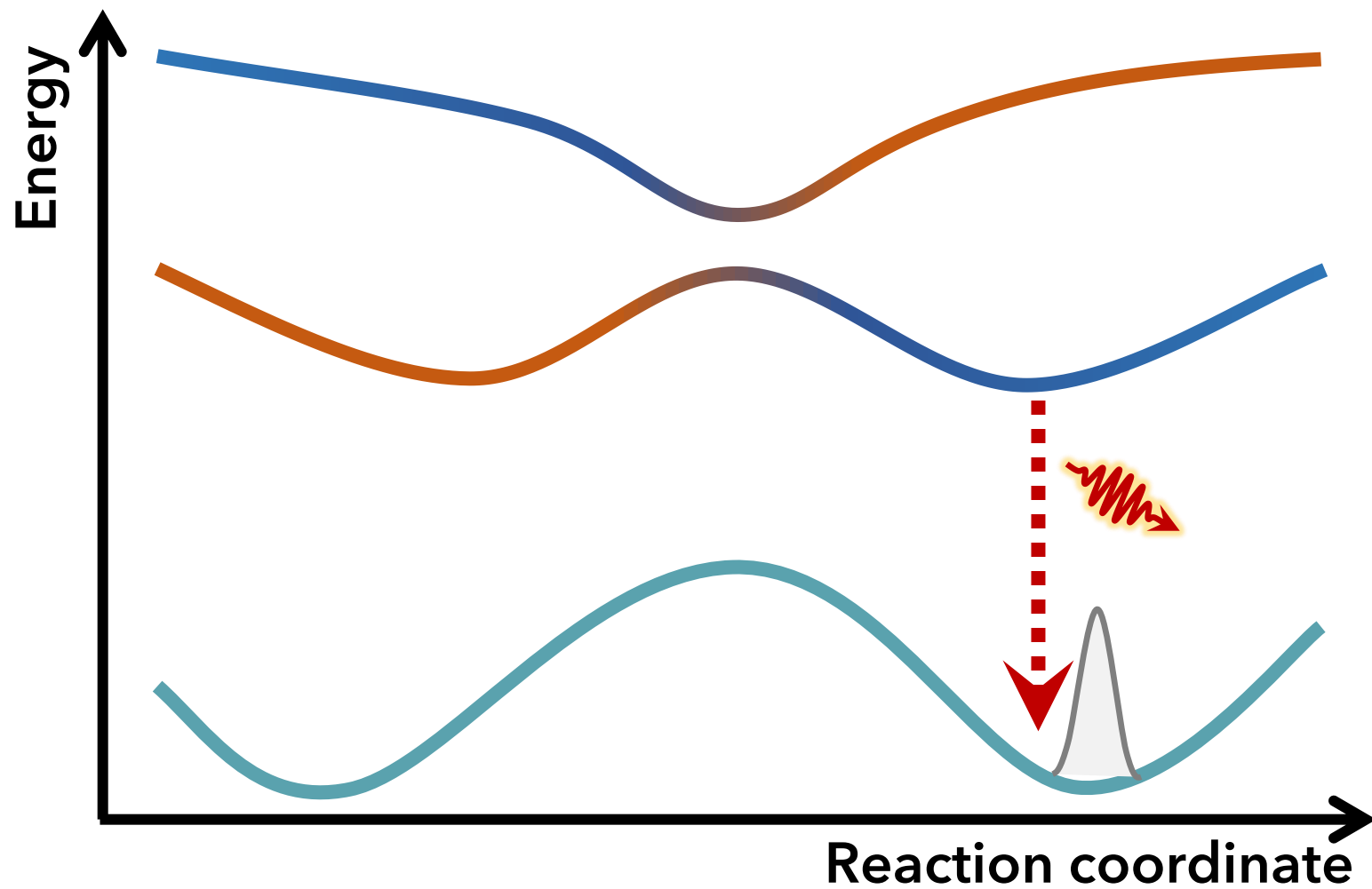
Nonadiabatic dynamics



Nonadiabatic dynamics



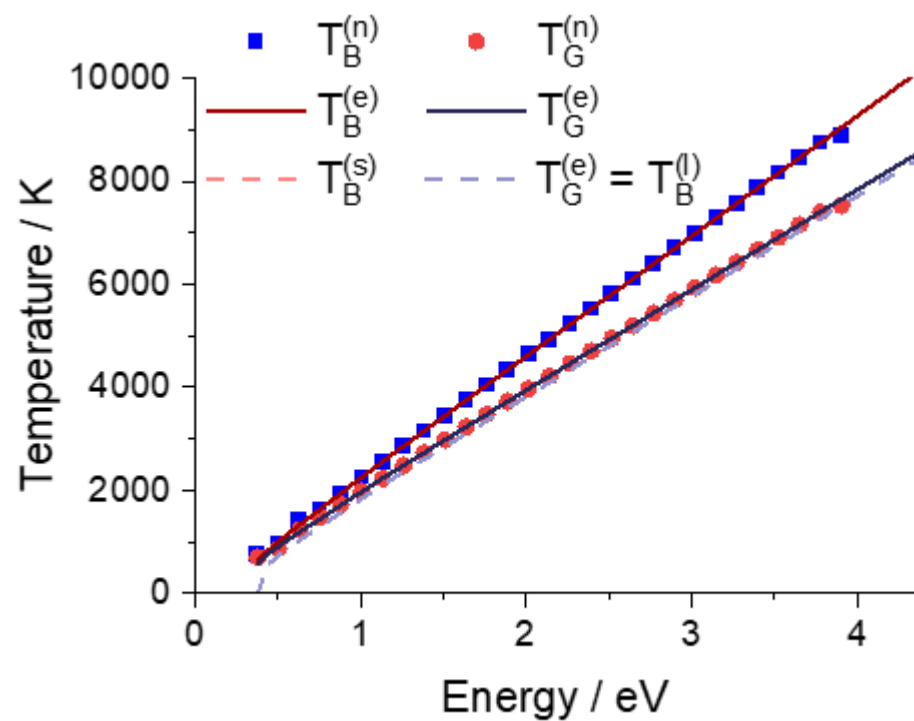
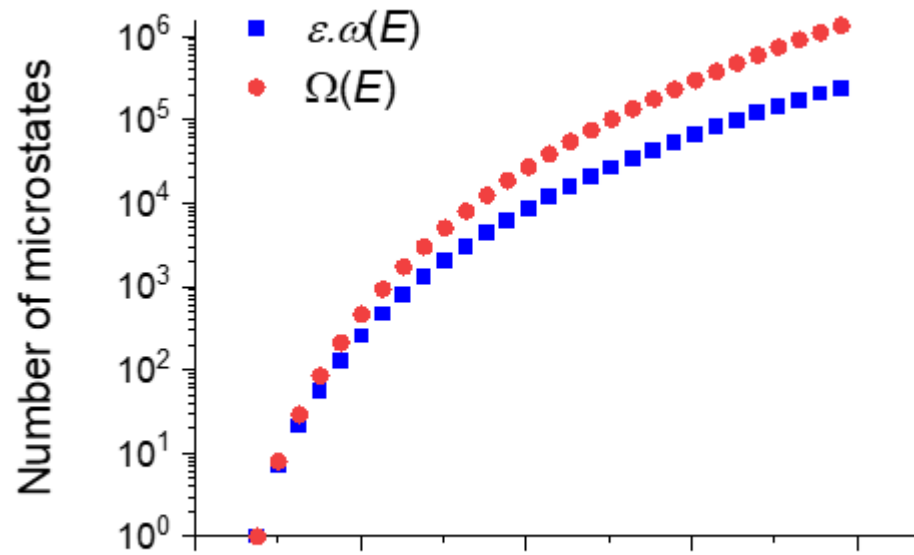
Nonadiabatic dynamics





***DIFFERENT MEDIA,
DIFFERENT
APPROACHES***

The figure as
appearing in the paper

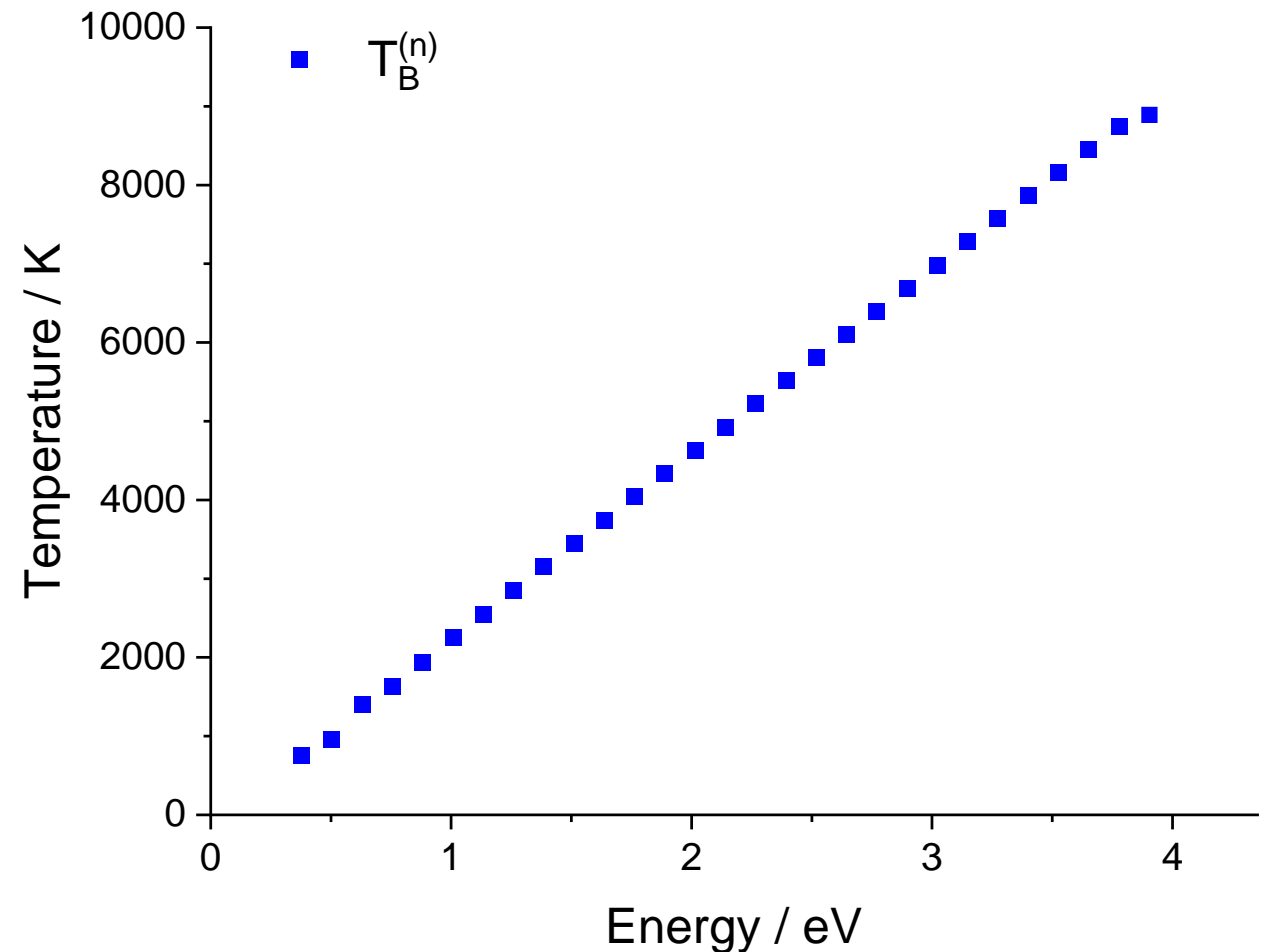


Boltzmann

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

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

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

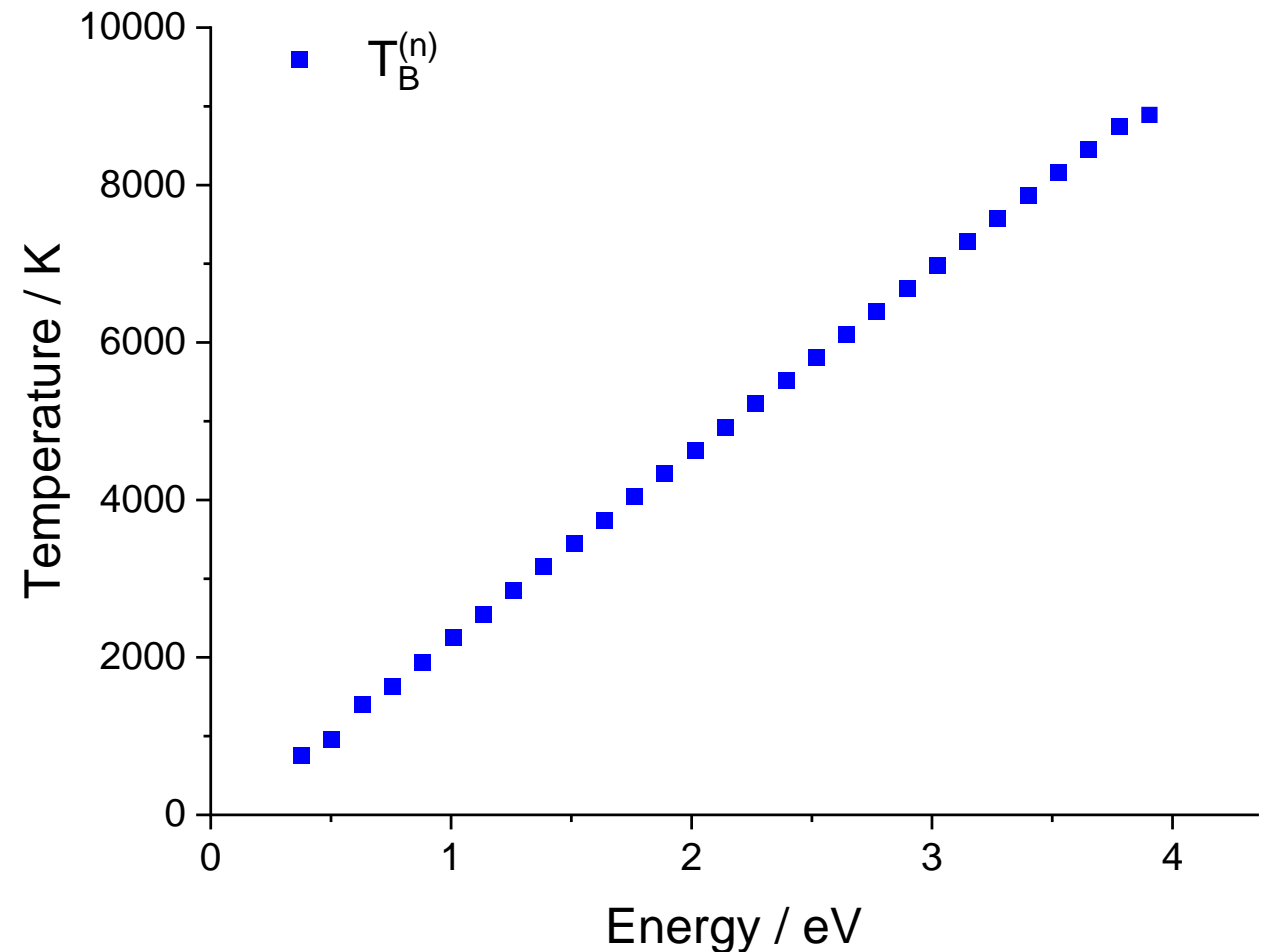


$$S_B(E_M) = k_B \ln \left[\frac{(M + N - 1)!}{(N - 1)!M!} \right]$$

Stirling's approximation

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

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



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

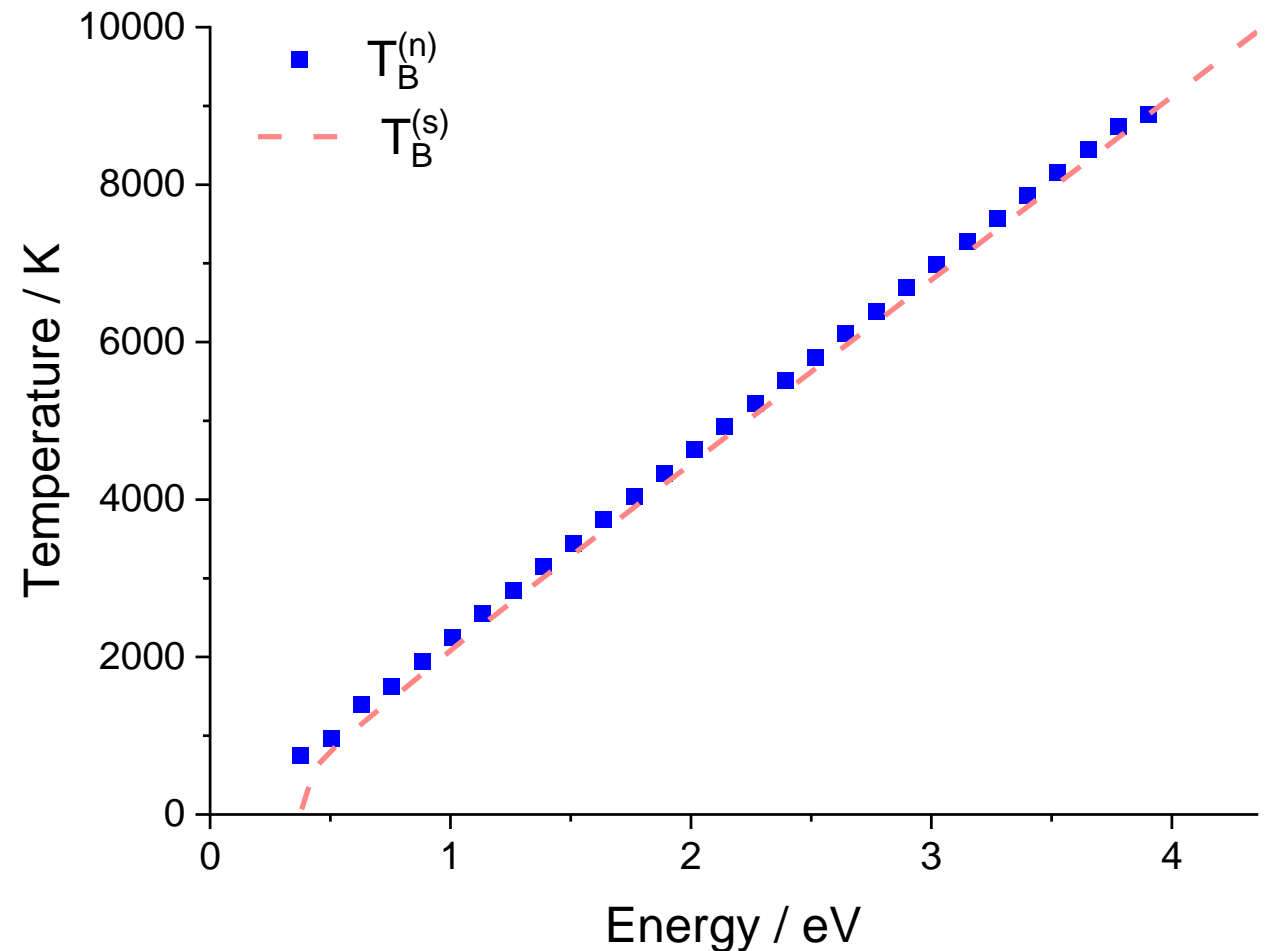
Stirling's approximation

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$N \gg 2$ approximation

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



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

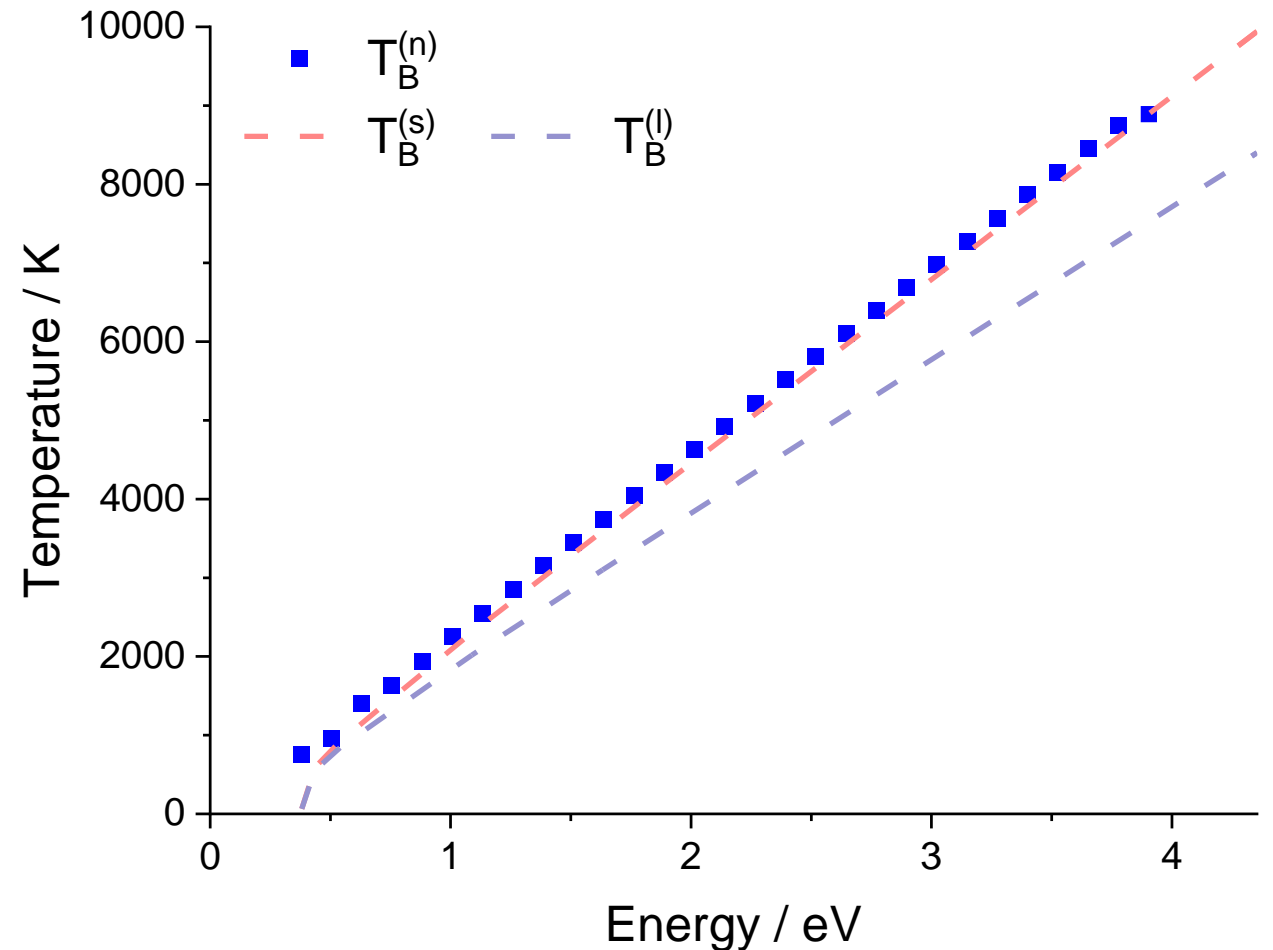
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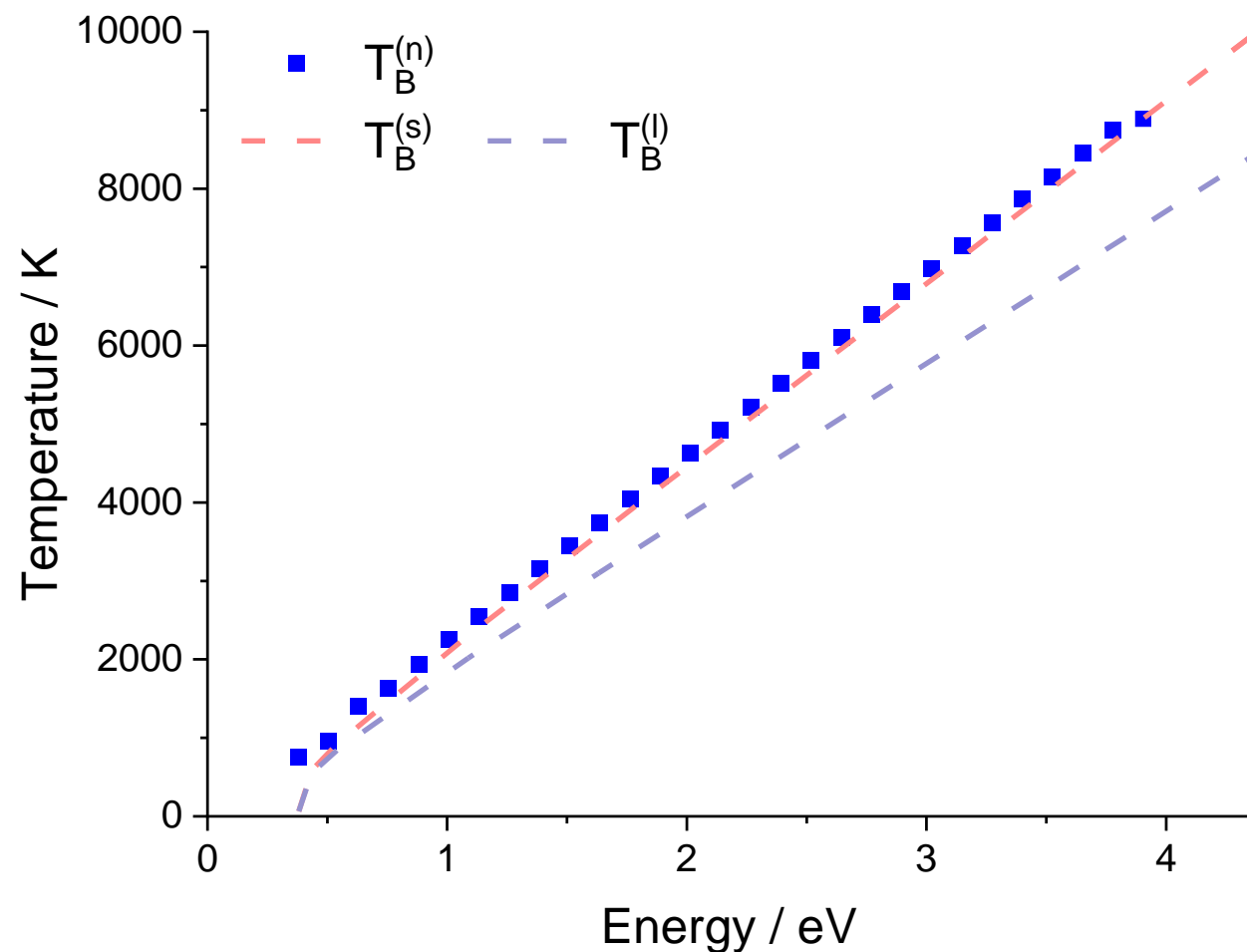


Gibbs volume

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

Hockey-stick identity

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



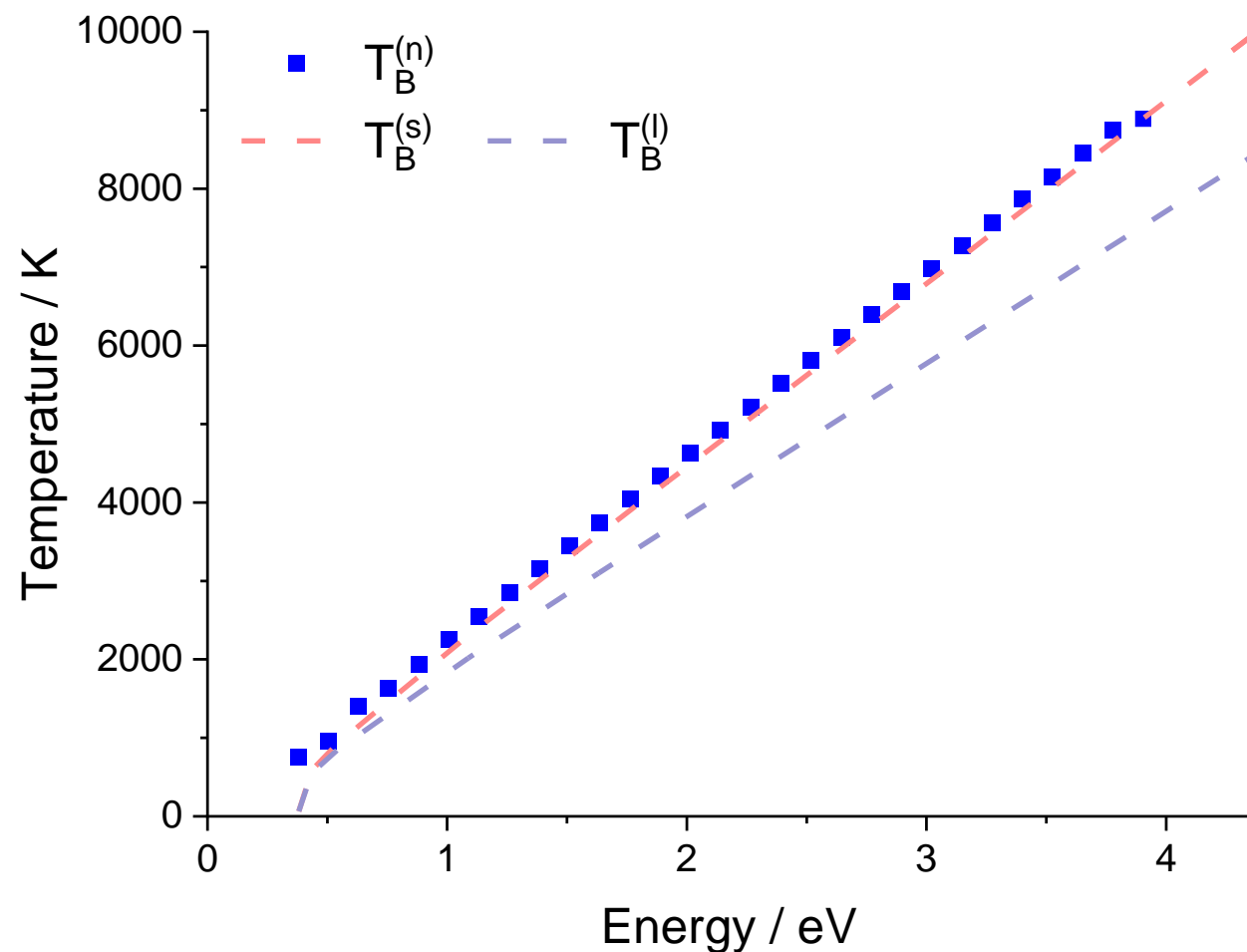
Hockey-stick identity: en.wikipedia.org/wiki/Hockey-stick_identity

Gibbs volume

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

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

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

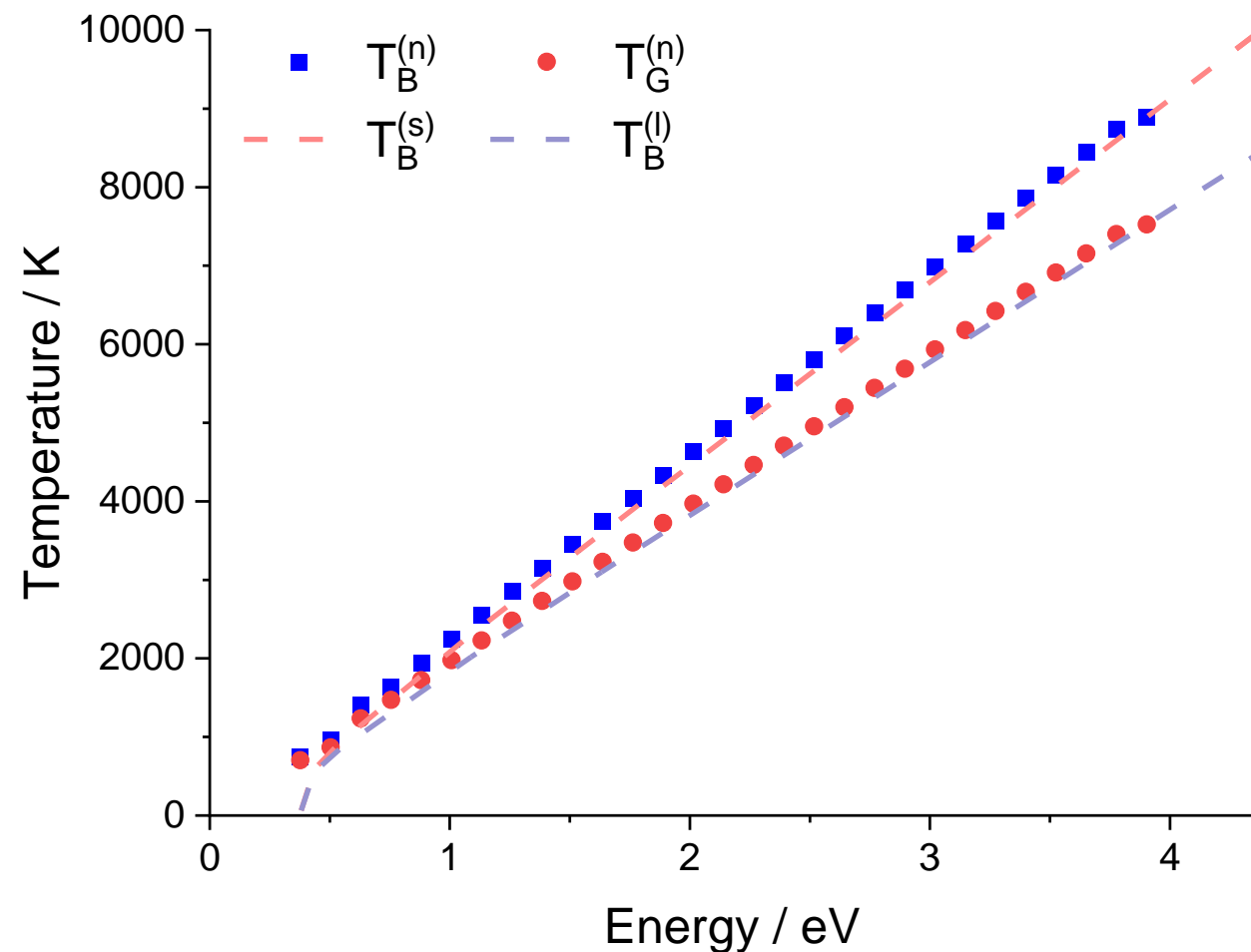


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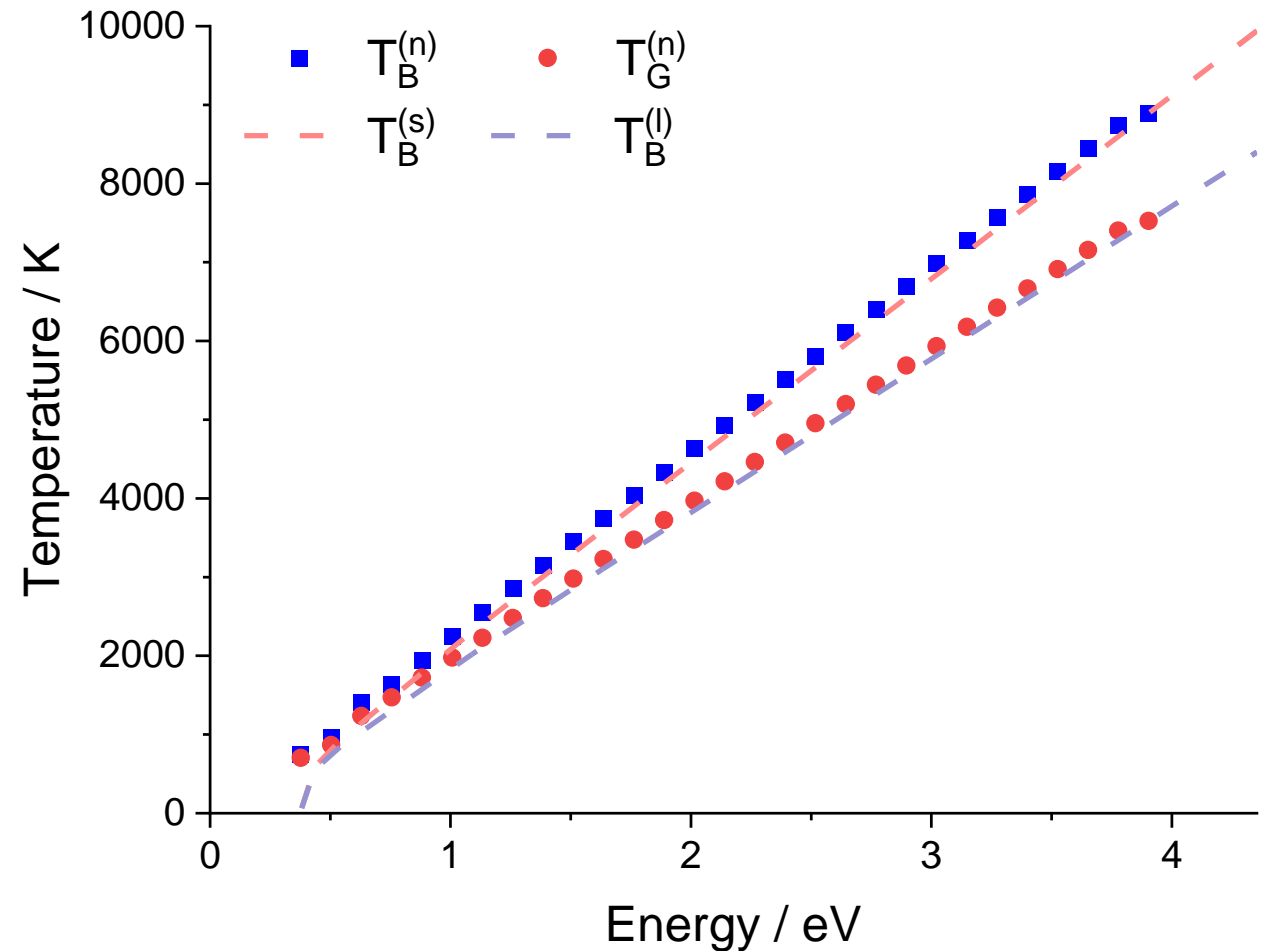
$$S_G(E_M) = k_B \ln \left[\frac{(M + N)!}{N!M!} \right]$$

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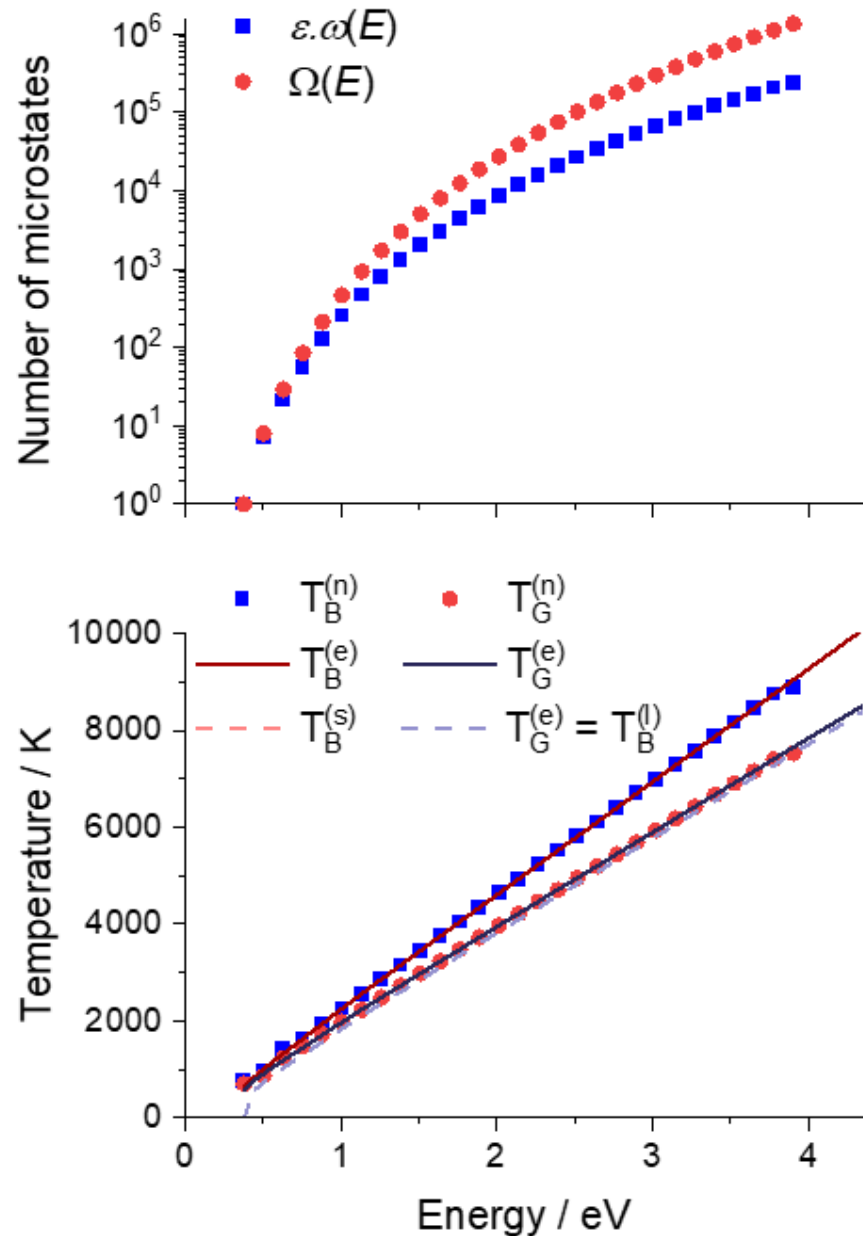
Stirling's approximation

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

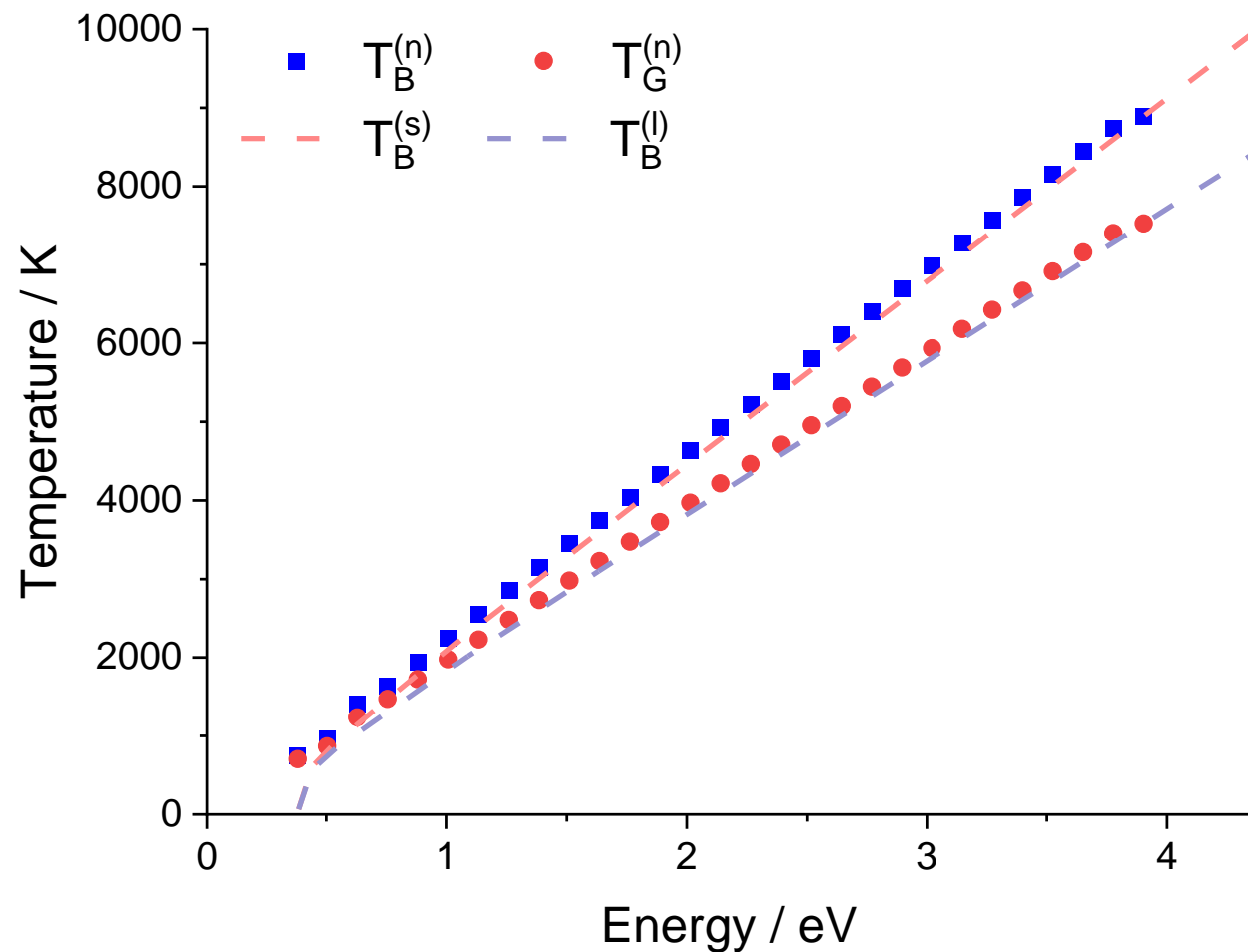
$$T_G^{(s)} = T_B^{(l)}$$

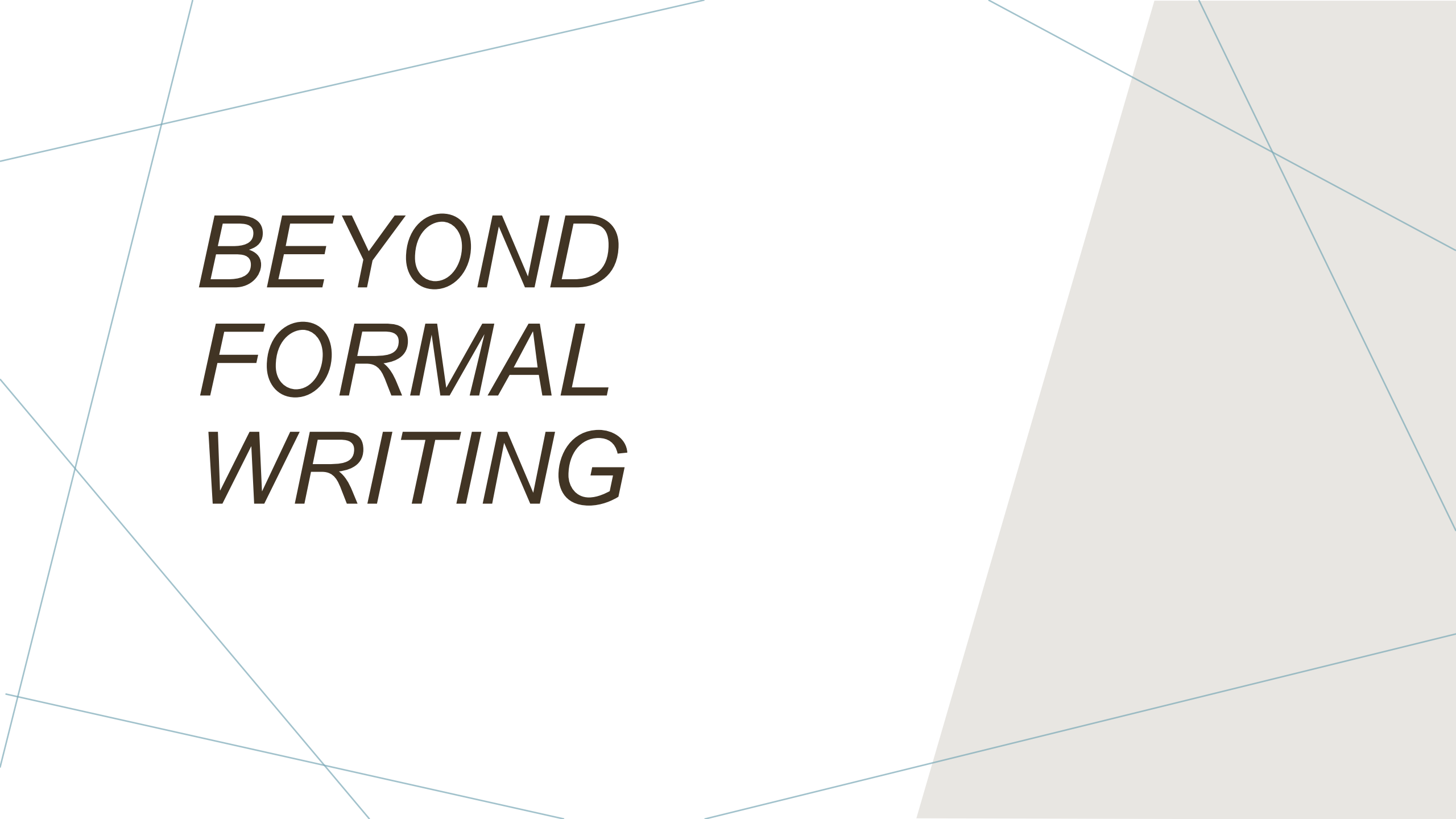


Good for a paper



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!

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Short Stories


MARIO BARBATTI





New adventures!




chemistryworld.com/opinion/scientific-authorship-in-the-time-of-chatgpt/4017232.art...       

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OPINION

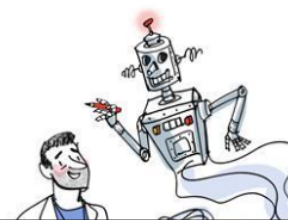
Authorship in the time of ChatGPT

BY MARIO BARBATTI | 12 APRIL 2023



What should we expect from our students?

Maybe two decades ago, my friend Thomas was working on his PhD thesis in quantum gravity. He had some awfully complicated equations to solve and started using a software



tinyurl.com/cwchatgpt

New adventures!

aeon.co/essays/why-the-empty-atom-picture-misunderstands-quantum-theory

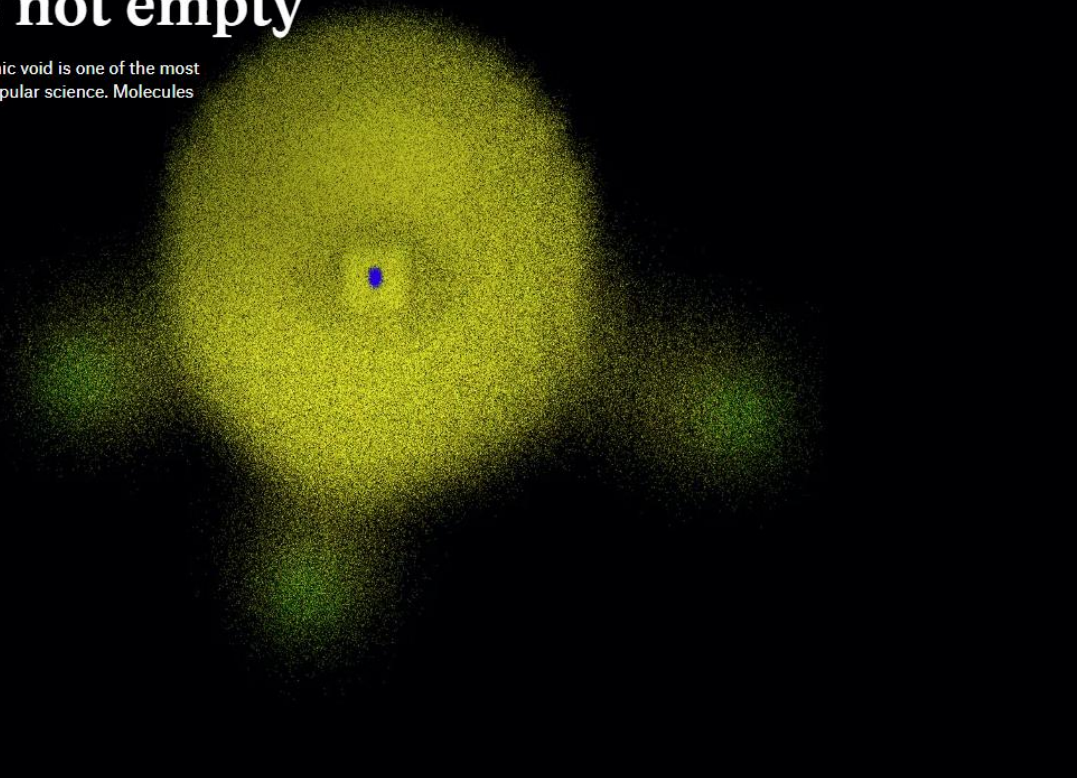
MENU / Q / f o t v

aeon

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We are not empty

The concept of the atomic void is one of the most repeated mistakes in popular science. Molecules are packed with stuff



Electronic and nuclear quantum clouds in an ammonia molecule. The molecule is approximately 400,000 femtometres wide. There are approximately a trillion femtometres in a millimetre. Image supplied by the author

[Mario Barbatti](#) is a theoretical chemist and physicist researching light and molecule interactions. He is professor of chemistry at Aix Marseille University in France and a senior member of Institut Universitaire de France.

The camera zooms in on the person's arm to reveal the cells, then a cell nucleus. A DNA strand grows on the screen. The camera focuses on a single atom within the strand, dives into a frenetic cloud of rocketing particles, crosses it, and leaves us in oppressive darkness. An initially imperceptible tiny dot grows smoothly, revealing the atomic nucleus. The narrator lectures that the nucleus of an atom is tens of thousands of times smaller than

tinyurl.com/emptyatom



www.barbatti.org



mario.barbatti@univ-amu.fr



[@MarioBarbatti](https://twitter.com/MarioBarbatti)