



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

## Fiction

- F Kafka
- P Roth
- D Adams
- T Chiang

+ essays ([aeon.co](http://aeon.co), [nautil.us](http://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.



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NEW YORK TIMES BESTSELLER

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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



Clipboard Font Paragraph Editing Styles

Table placement Title Titre 1 sans r A. Titre 2-anr Titre 3-annexe 1 U1-no nun

Comments Editing Share

Dictate Editor Reuse Files Add-ins Open Grammarly

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,<sup>1\*</sup> Kakali Sen,<sup>2</sup> Saikat Mukherjee,<sup>1</sup> Giovanni Granucci,<sup>3</sup> Mario Barbatti<sup>1,4\*</sup>

<sup>1</sup> Aix Marseille University, CNRS, ICR, Marseille, France

<sup>2</sup> STFC Scientific Computing, Daresbury Laboratory, Keckwick Lane, Daresbury, Warrington WA4 4AD, United Kingdom

<sup>3</sup> Department of Chemistry and Industrial Chemistry, University of Pisa, v. G. Moruzzi 13, Pisa, Italy

<sup>4</sup> Institut Universitaire de France, 75231, Paris, France

Corresponding authors: MK: [moumita.kar@univ-amu.fr](mailto:moumita.kar@univ-amu.fr)  
MB: [mario.barbatti@univ.amu.fr](mailto:mario.barbatti@univ.amu.fr); [www.barbatti.org](http://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

Clear All

Abstract

Affiliation

Authors

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Caption

Centered

EndNote Bibliography

EndNote Bibliography + A

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1.1.1.1 Heading 4

Normal

Table text

Title

Emphasis

Footer

# + 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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- 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?

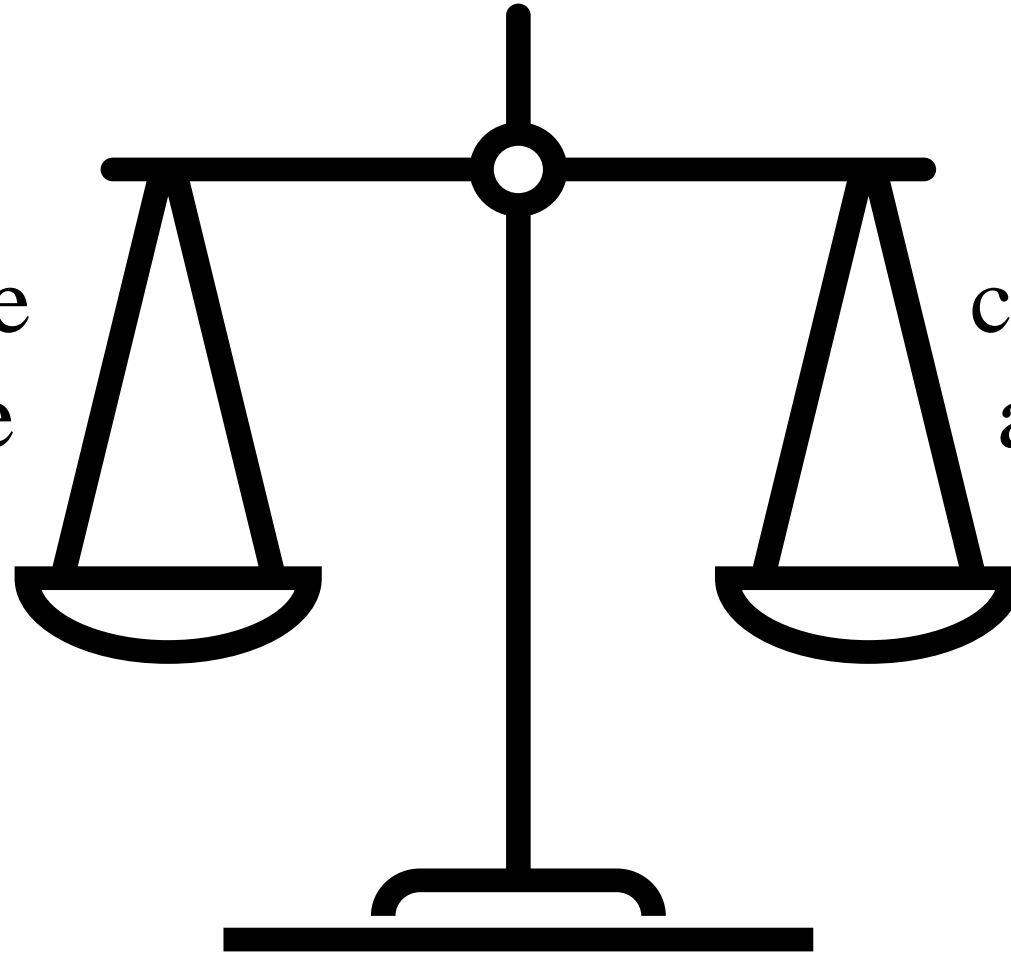
- Low productivity
- Prone to mistakes
- Bad for co-authoring  
(most of my colleagues don't use it)
- Low-level WYSWYG



***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,<sup>23</sup> **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**

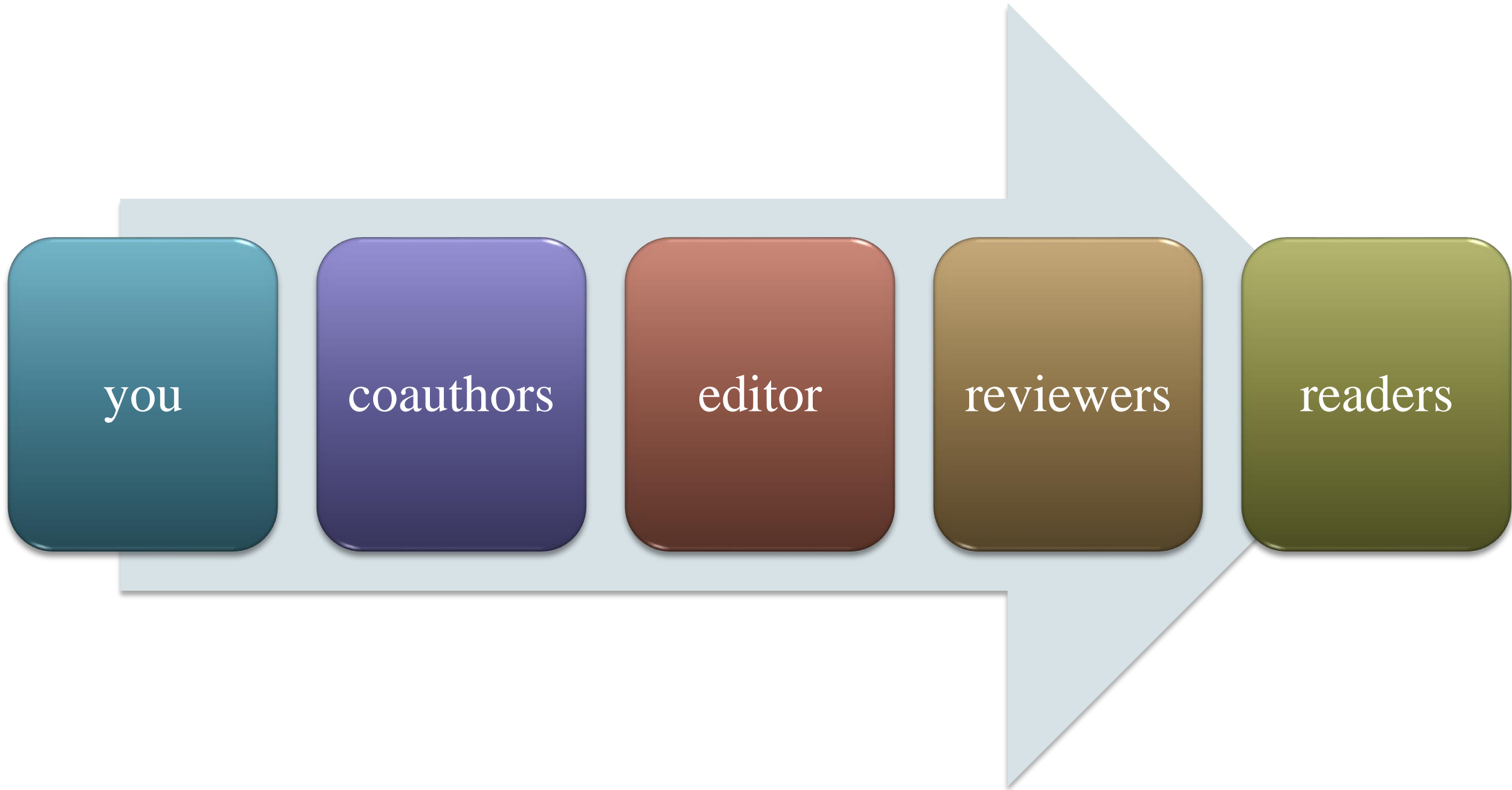
**Conclusion**





***SCIENTIFIC  
WRITING IS  
COLLECTIVE***







***SLIDES AND  
PRESENTATIONS***

# Master your tools

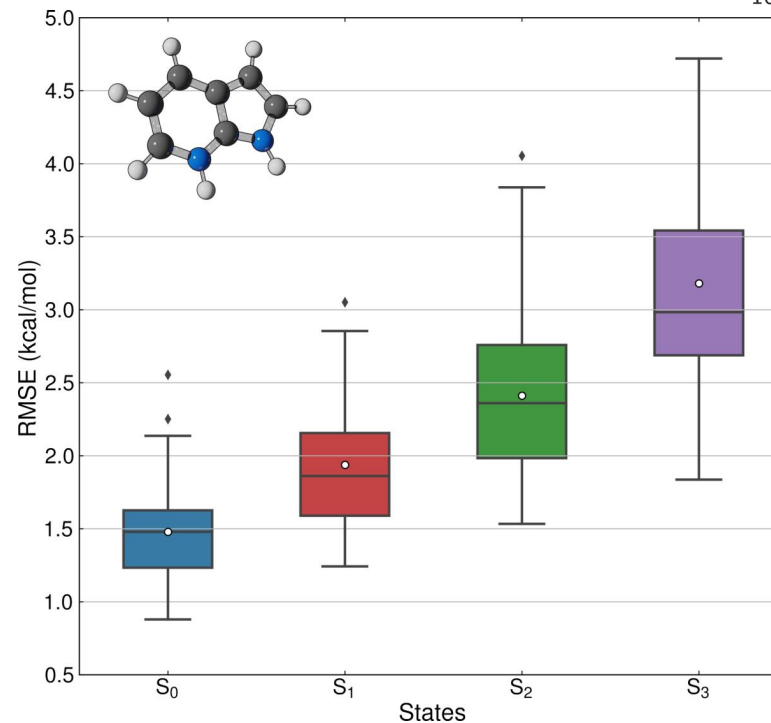
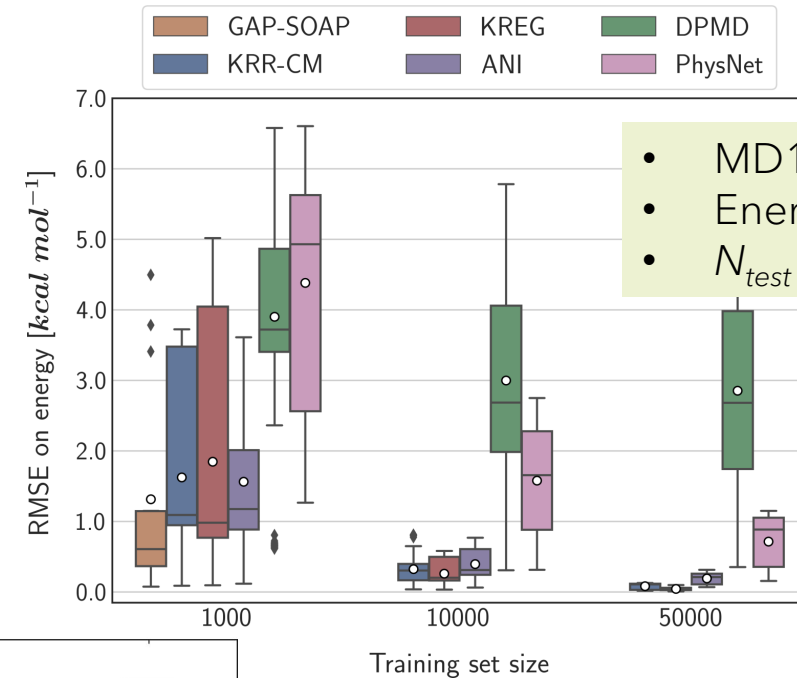
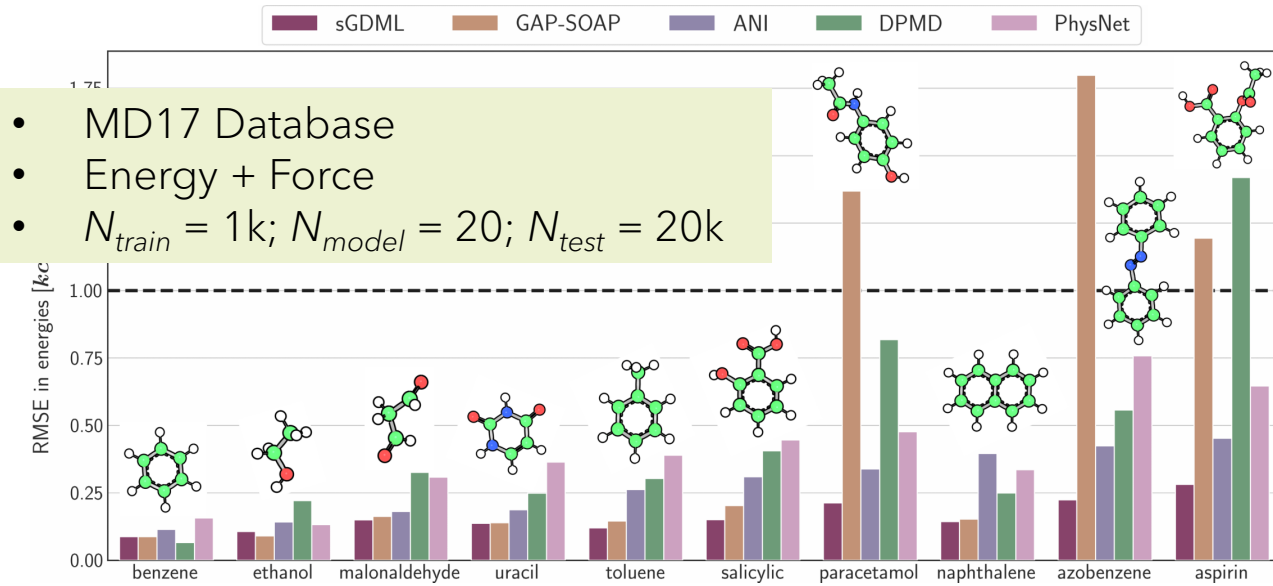
My choice:

- PowerPoint
- MathType
- Grammarly
- Endnote

# Laws of slide composition

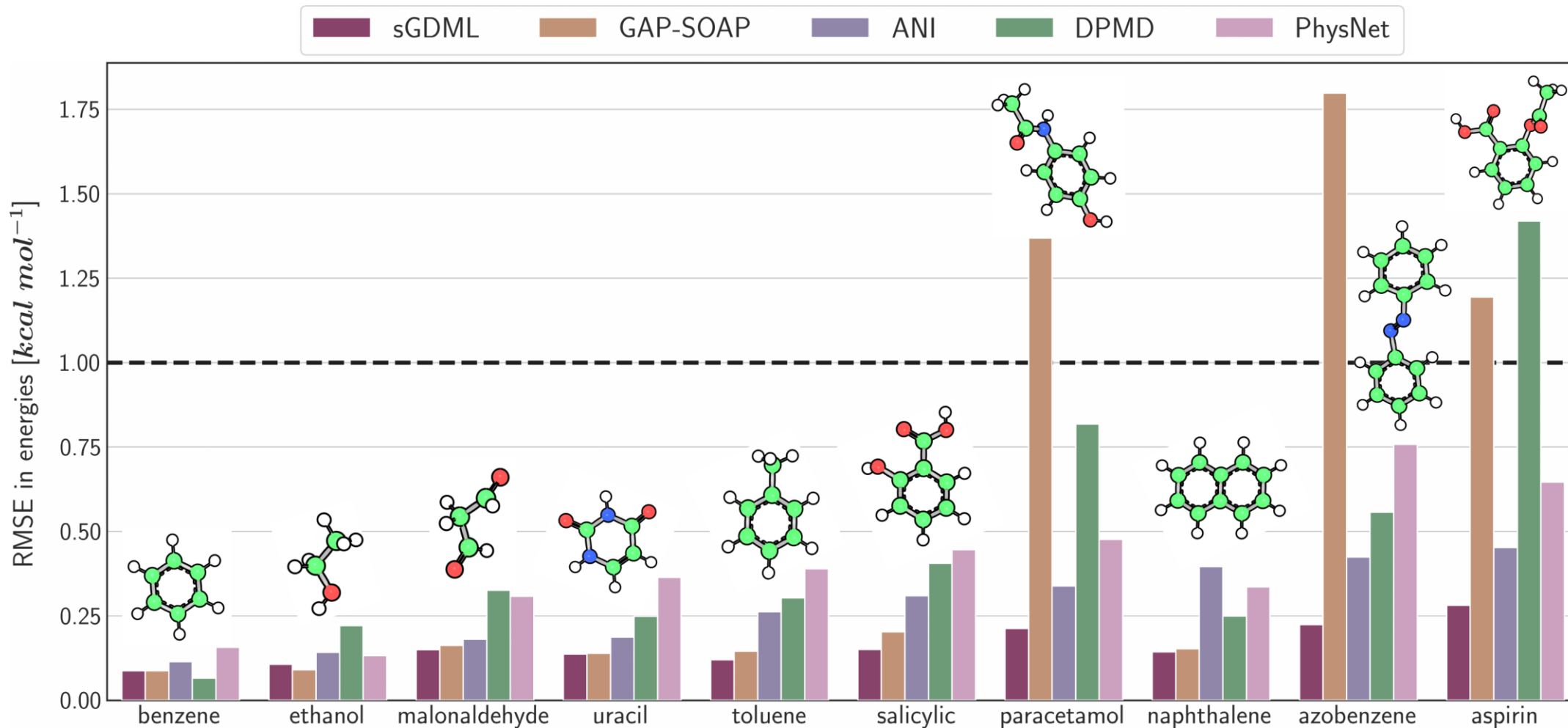
1. Background can have any color as long it's white.
2. Font size in PTs must be at least half the age of the oldest person in the public.
3. One slide fits one and only one piece of info. Slides are for free. Don't save their number.

*COULD HAVE DONE*



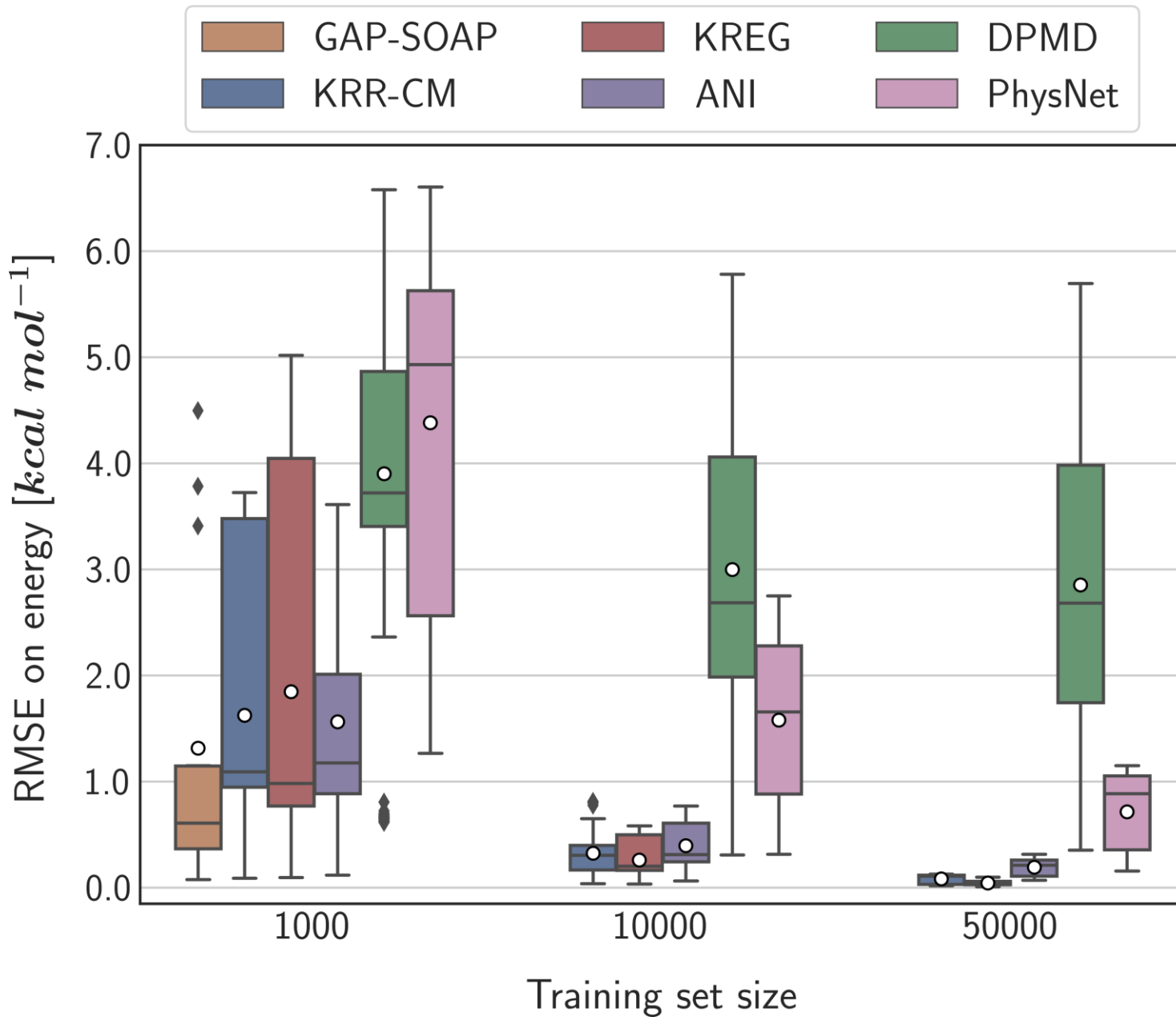
KREG x RI-ADC(2)/cc-pVDZ  
DC-FSSH: 50 trajs; 0.5 fs; 300 ps

***BETTER***

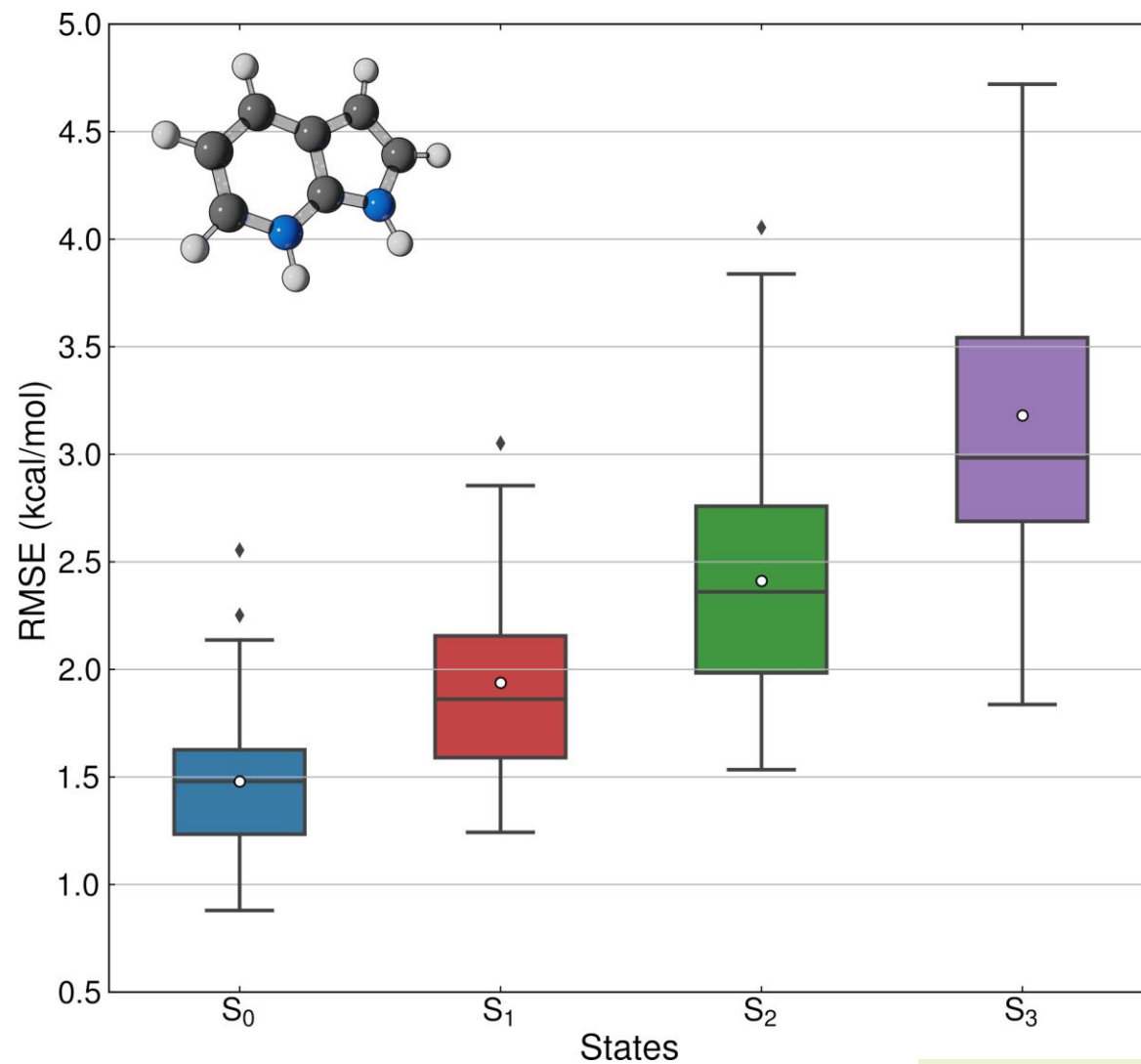


- MD17 Database
- Energy + Force
- $N_{train} = 1k$ ;  $N_{model} = 20$ ;  $N_{test} = 20k$





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



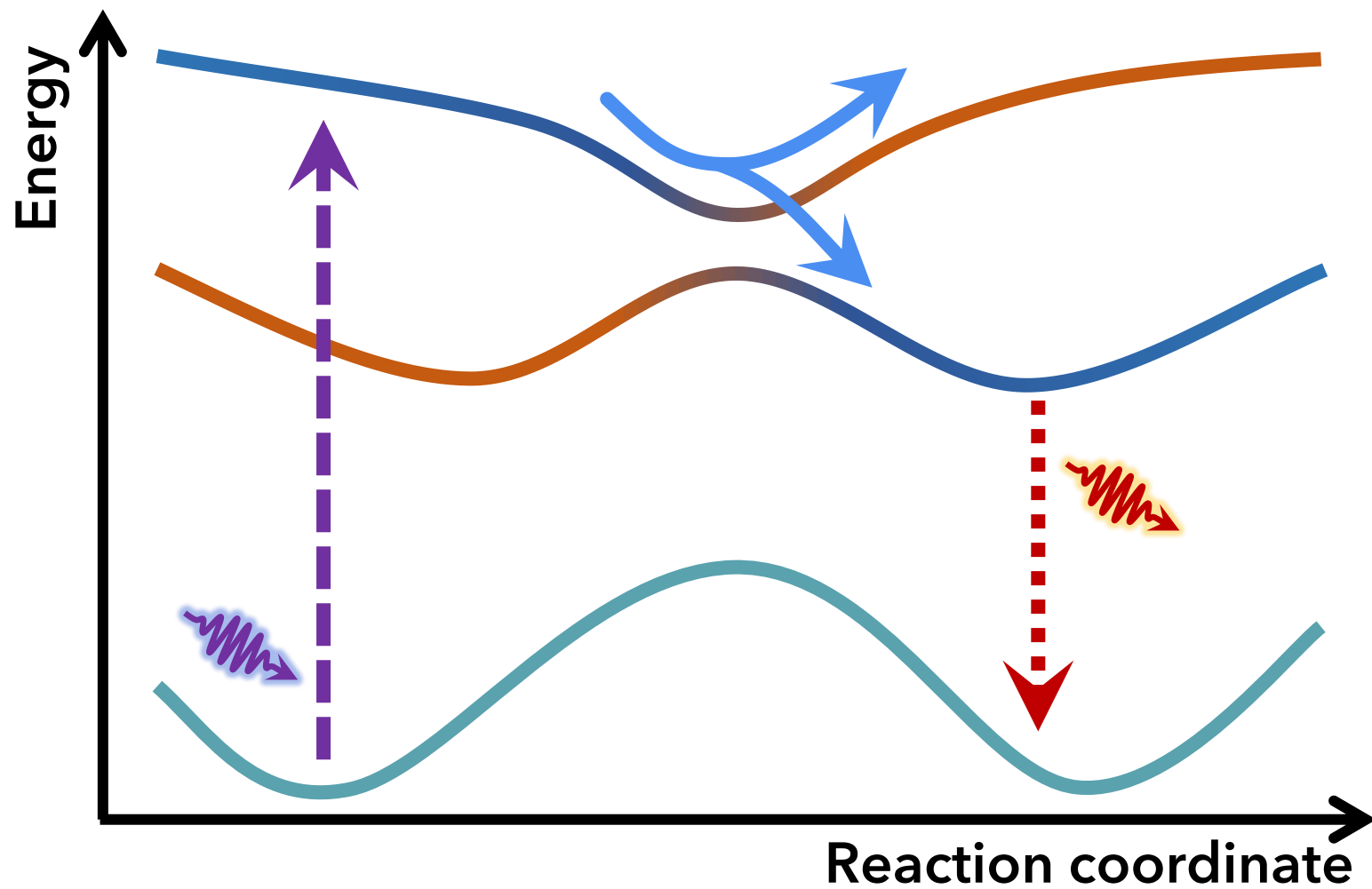
- KREG x RI-ADC(2)/cc-pVDZ
- DC-FSSH: 50 traj; 0.5 fs; 300 ps

# Master animations

Use animations to tell the public where to focus.

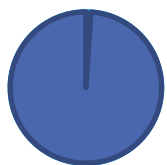
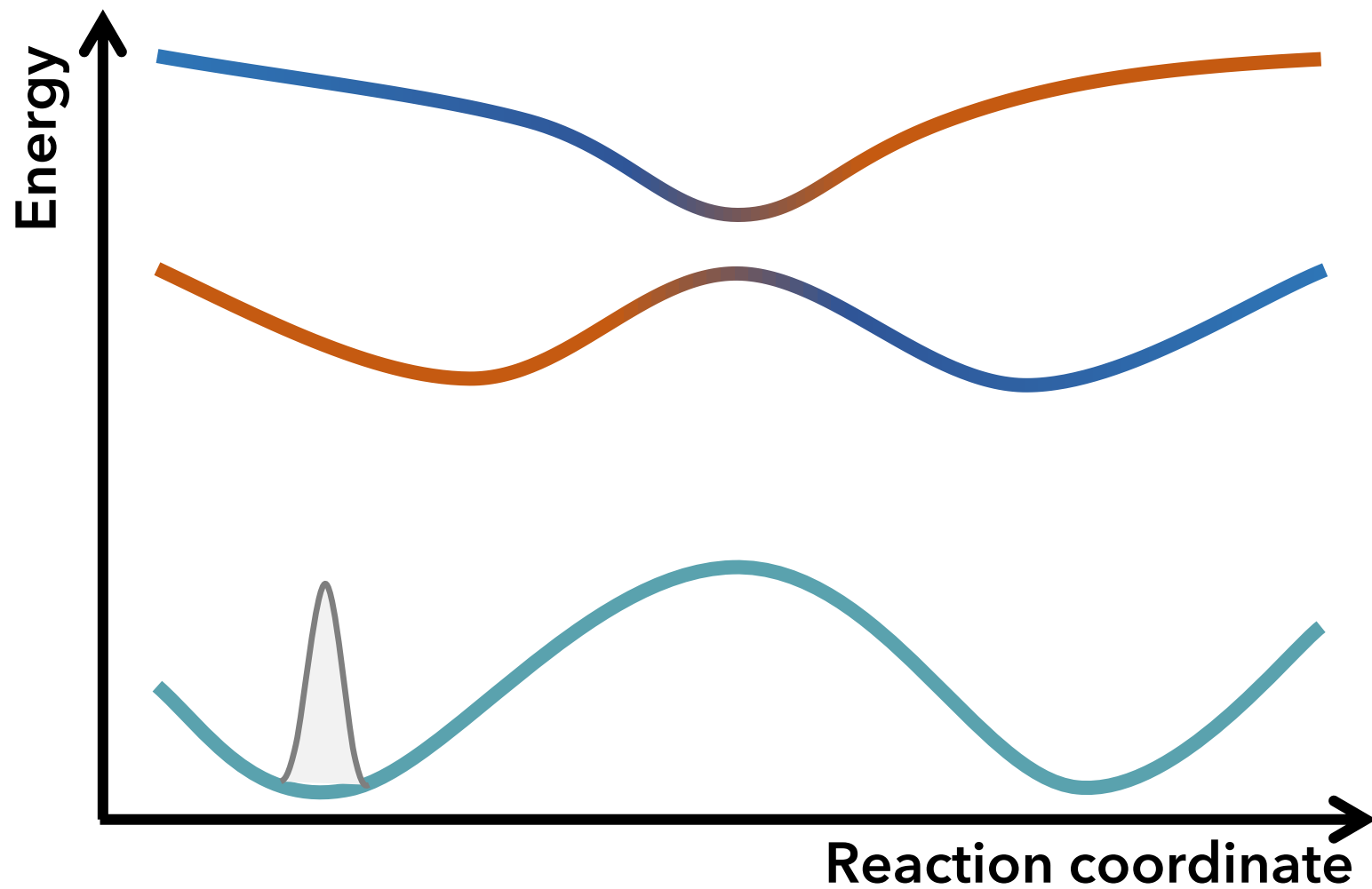
*COULD HAVE DONE*

# Nonadiabatic dynamics

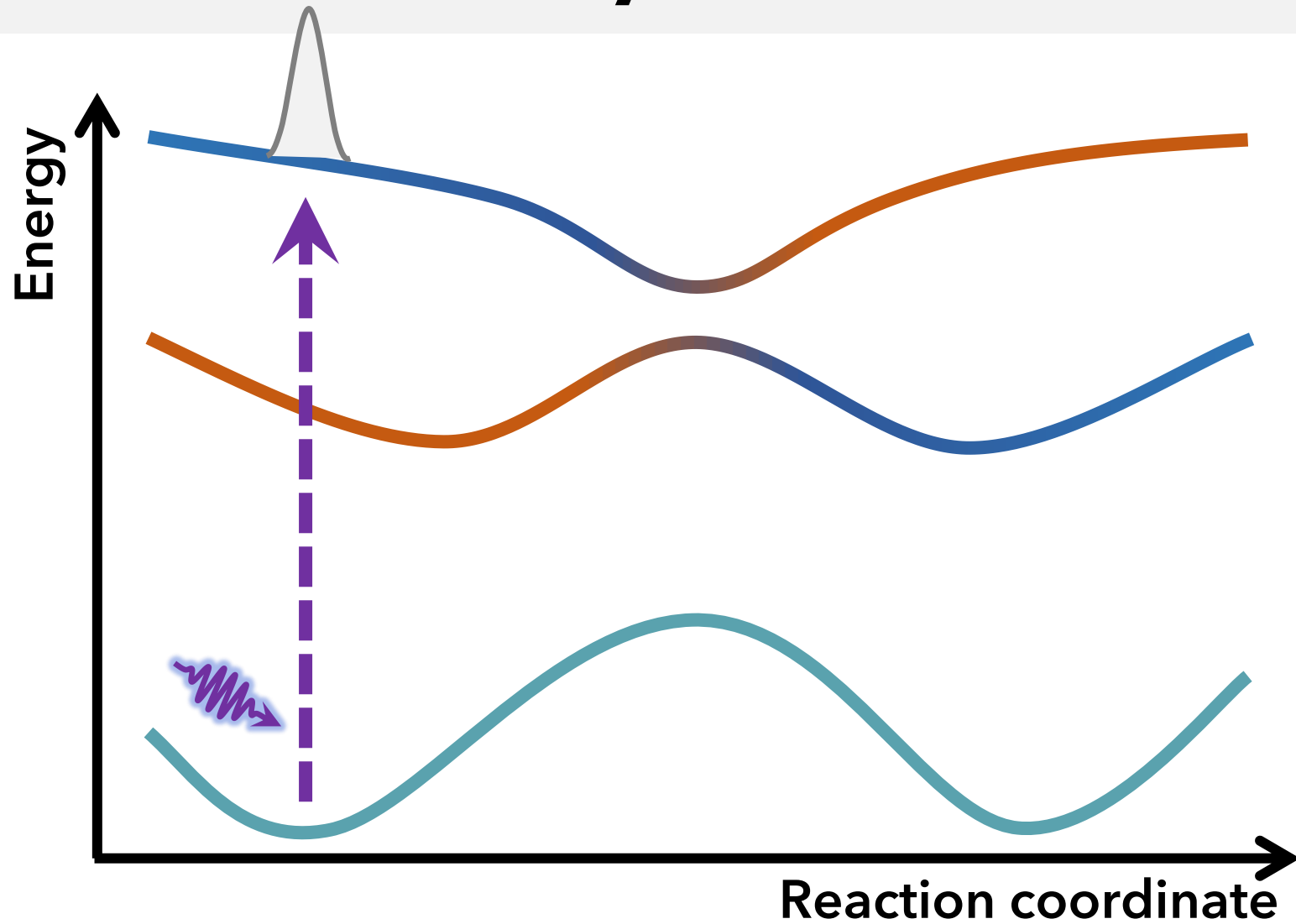


***BETTER***

# Nonadiabatic dynamics

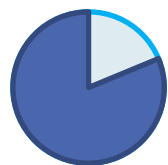
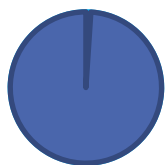
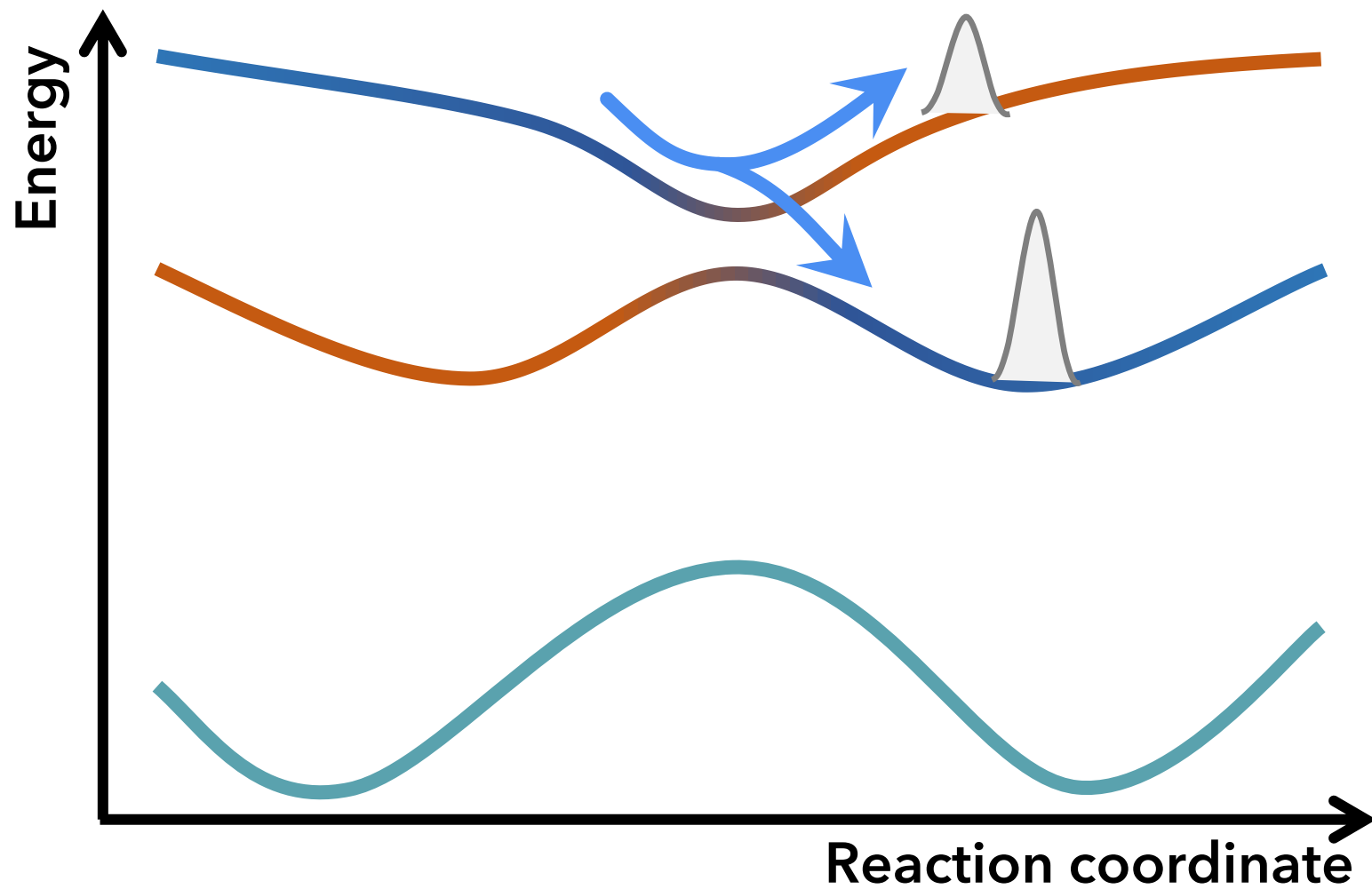


# Nonadiabatic dynamics

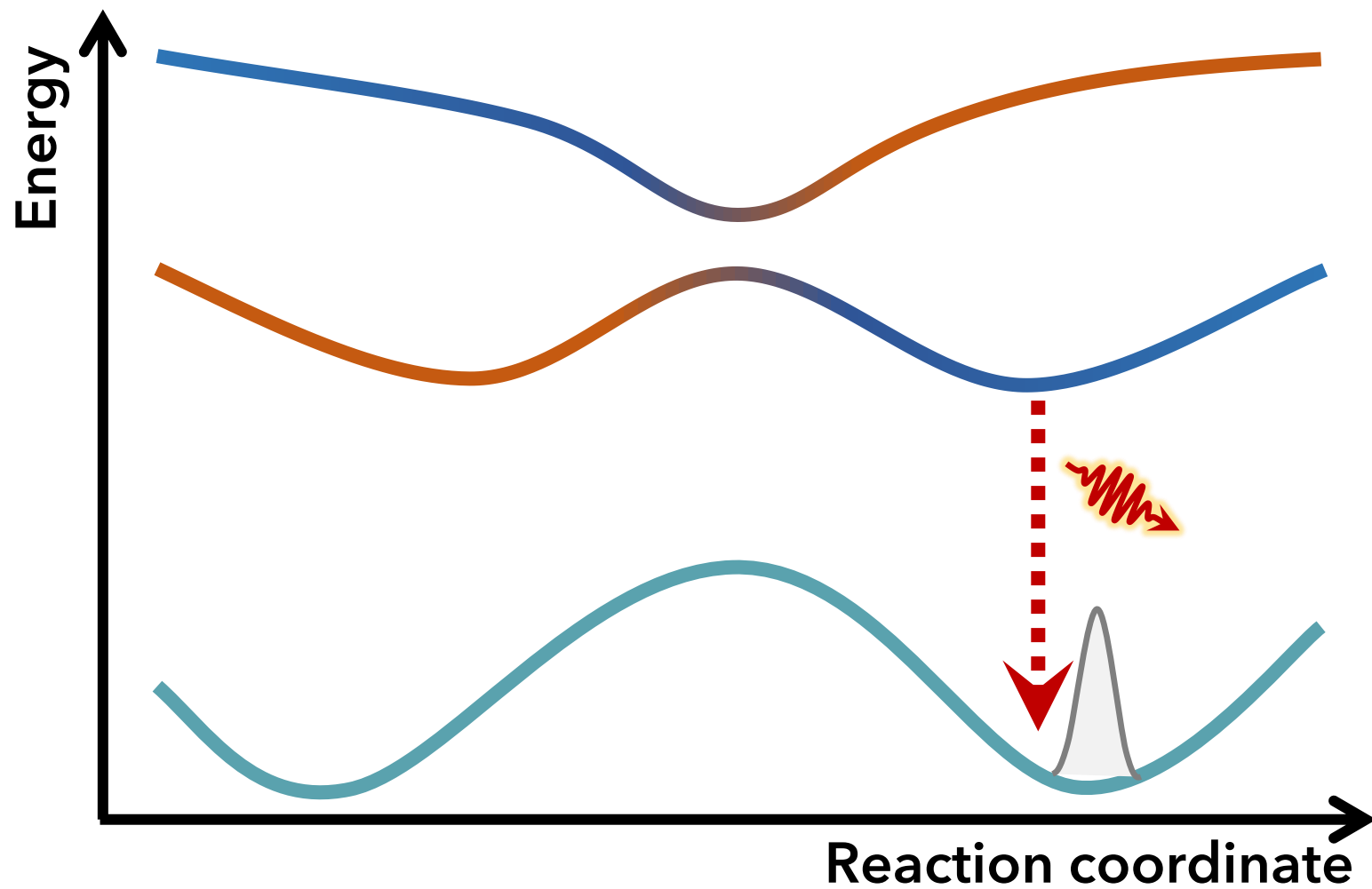




# Nonadiabatic dynamics



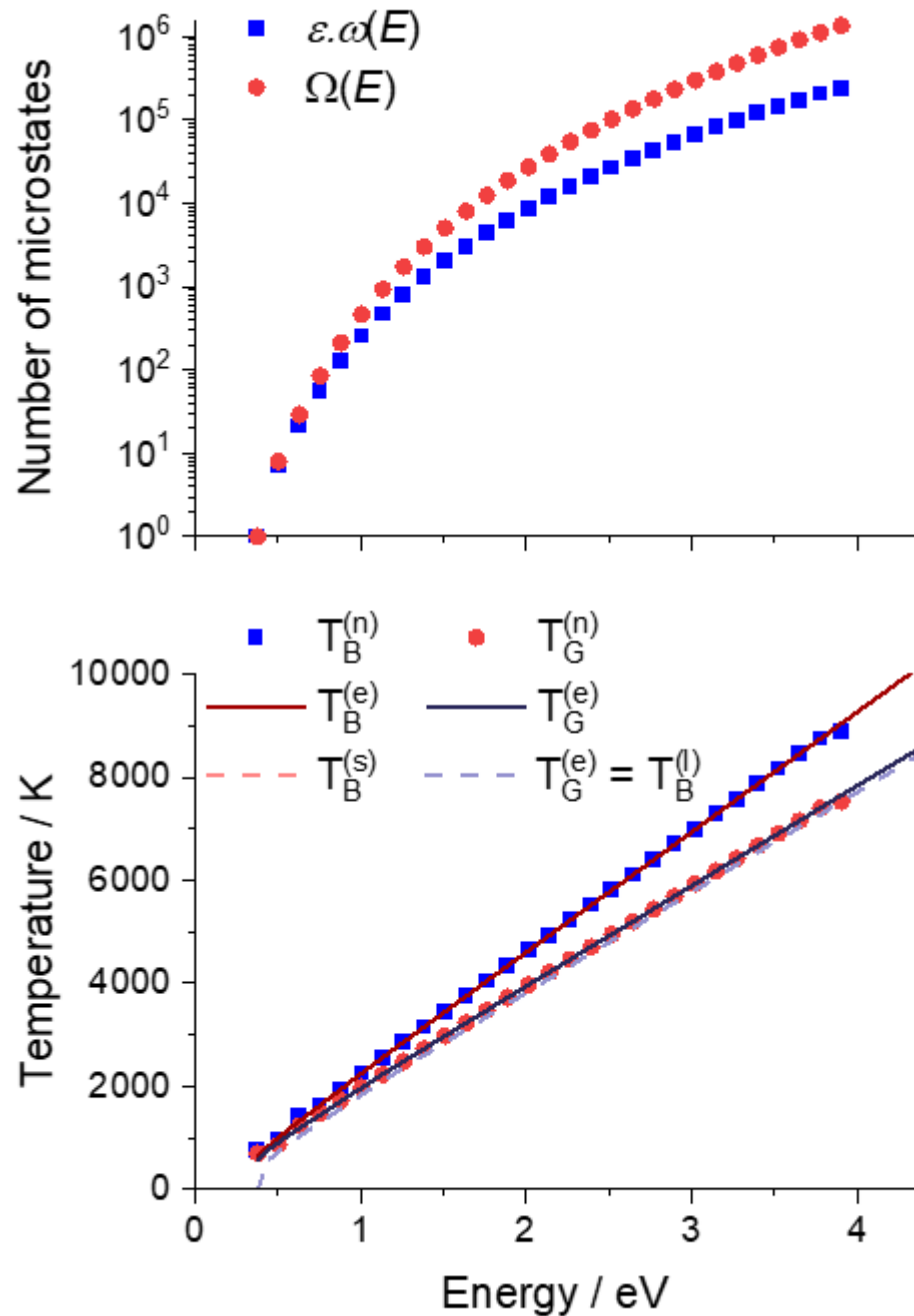
# Nonadiabatic dynamics





***DIFFERENT MEDIA,  
DIFFERENT  
APPROACHES***

The figure as  
appearing in the paper

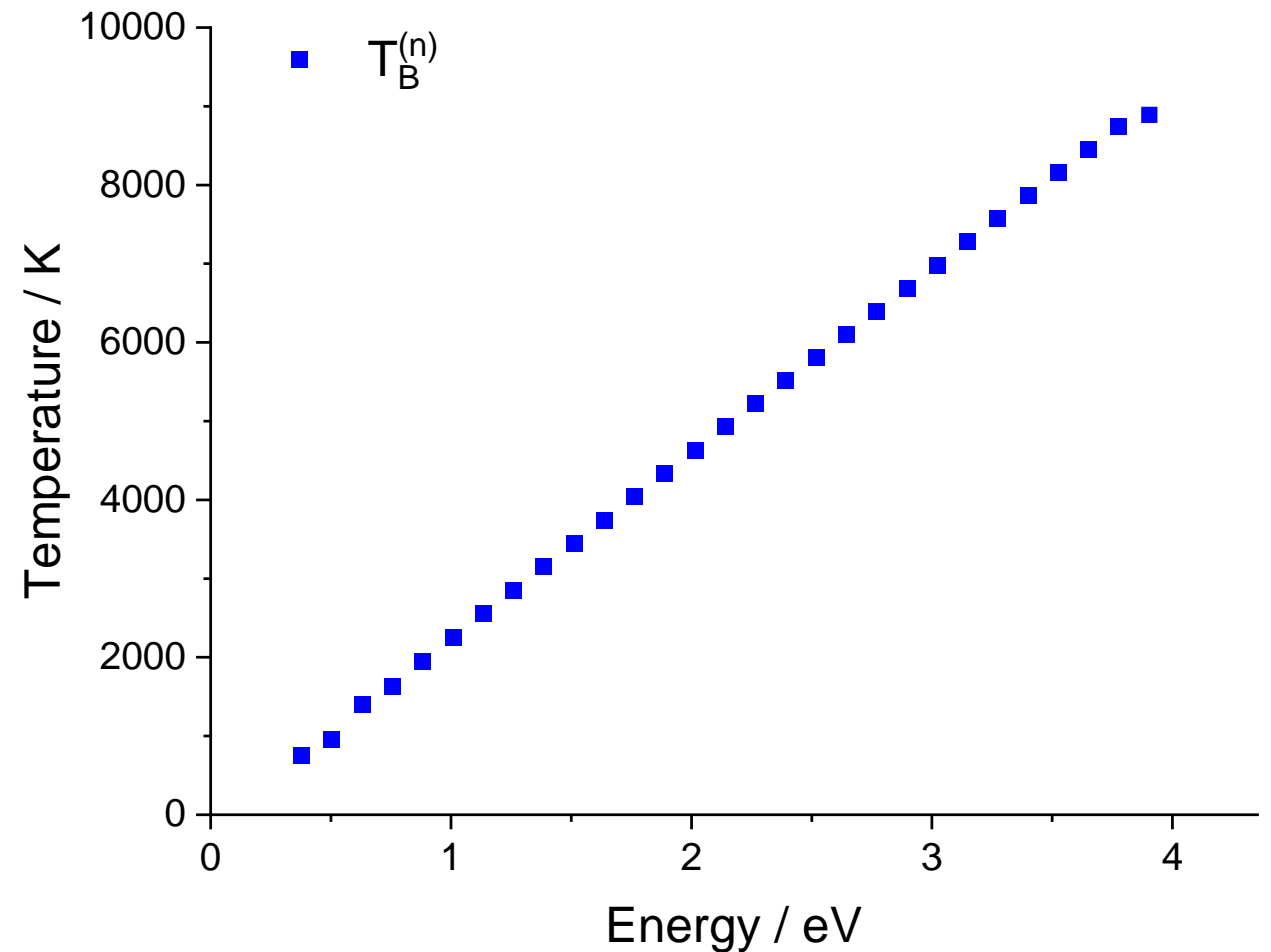


# Boltzmann

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

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

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

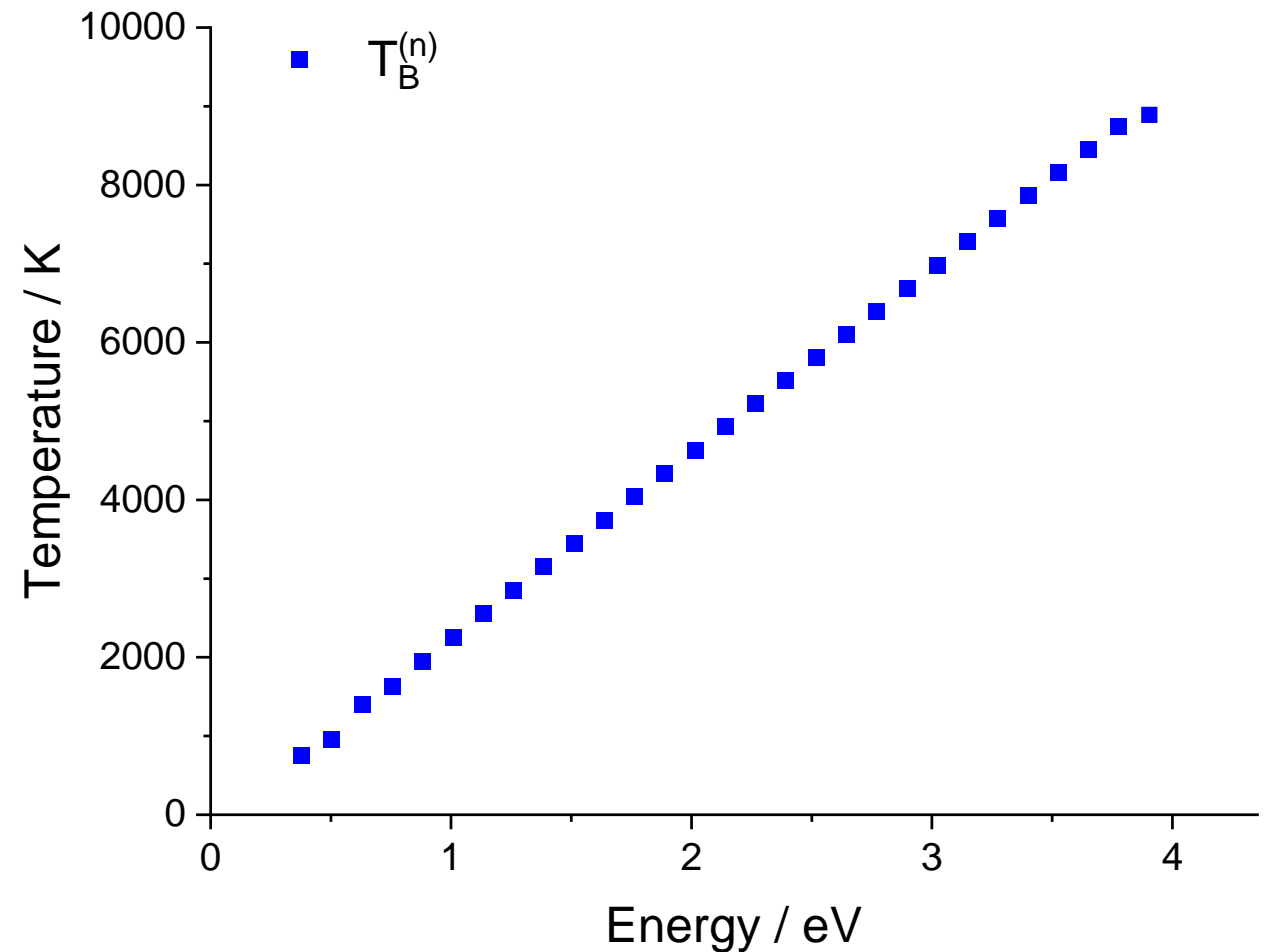


$$S_B(E_M) = k_B \ln \left[ \frac{(M + N - 1)!}{(N - 1)!M!} \right]$$

Stirling's approximation

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

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



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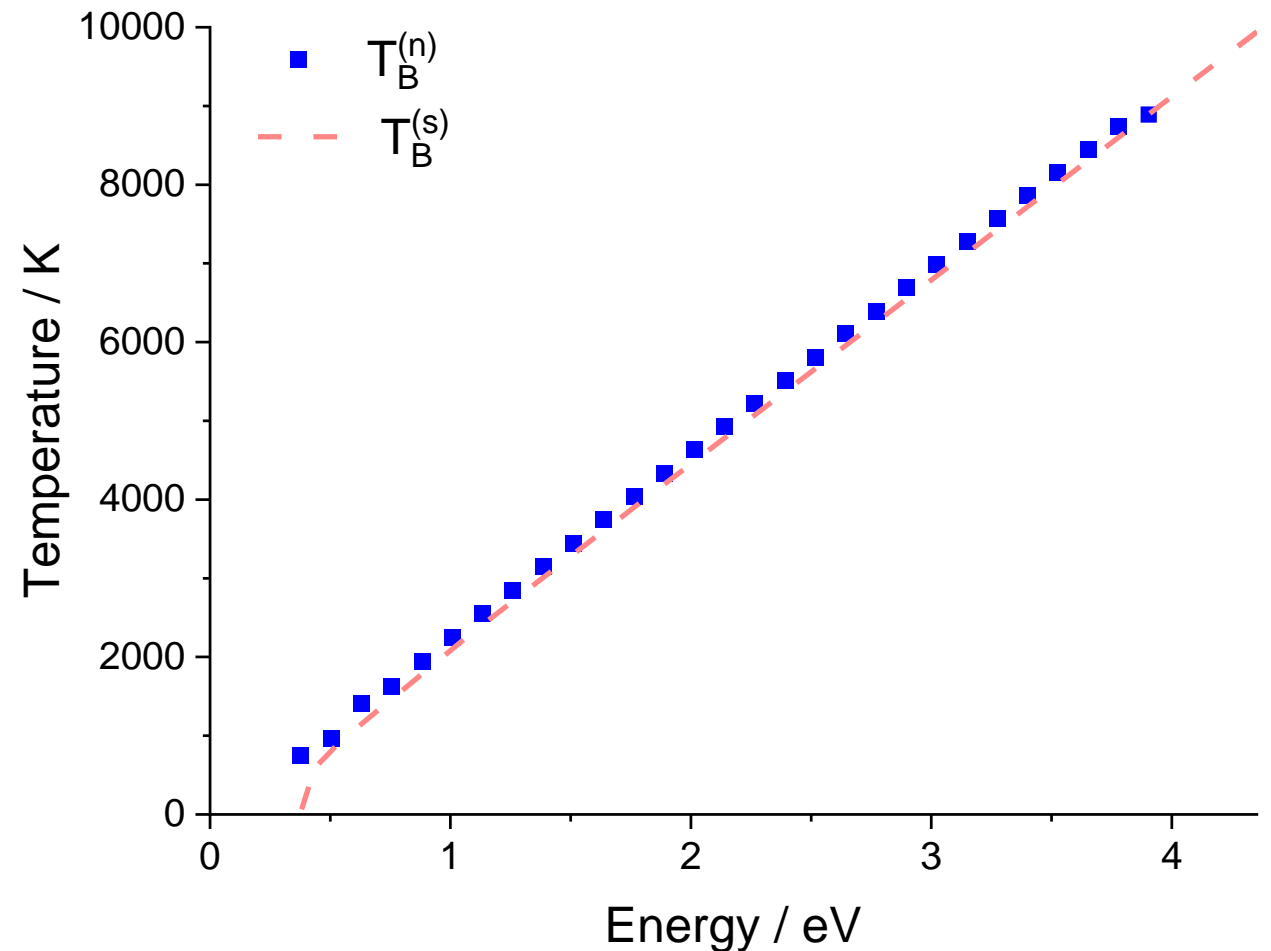
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$N \gg 2$  approximation

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



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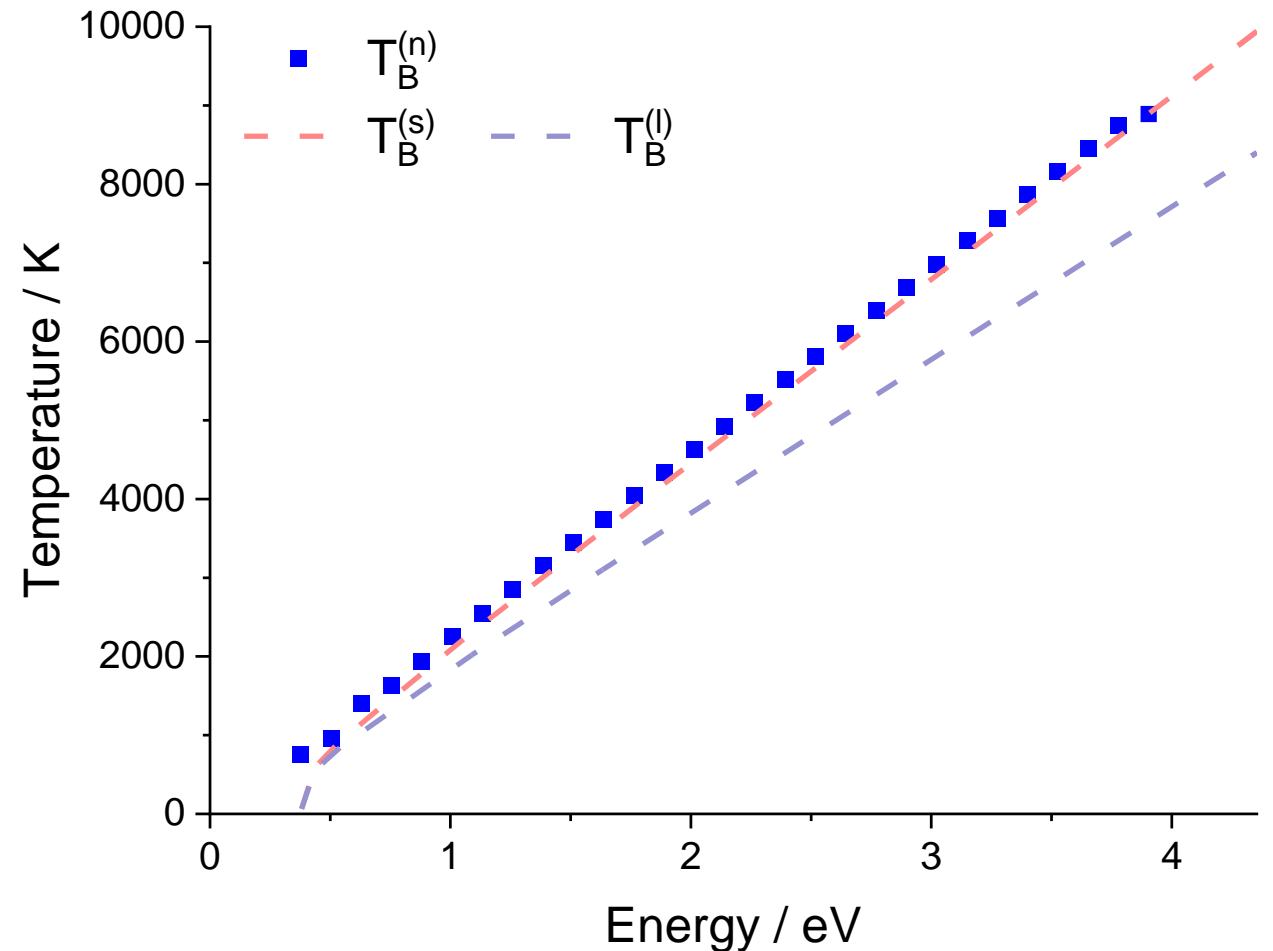
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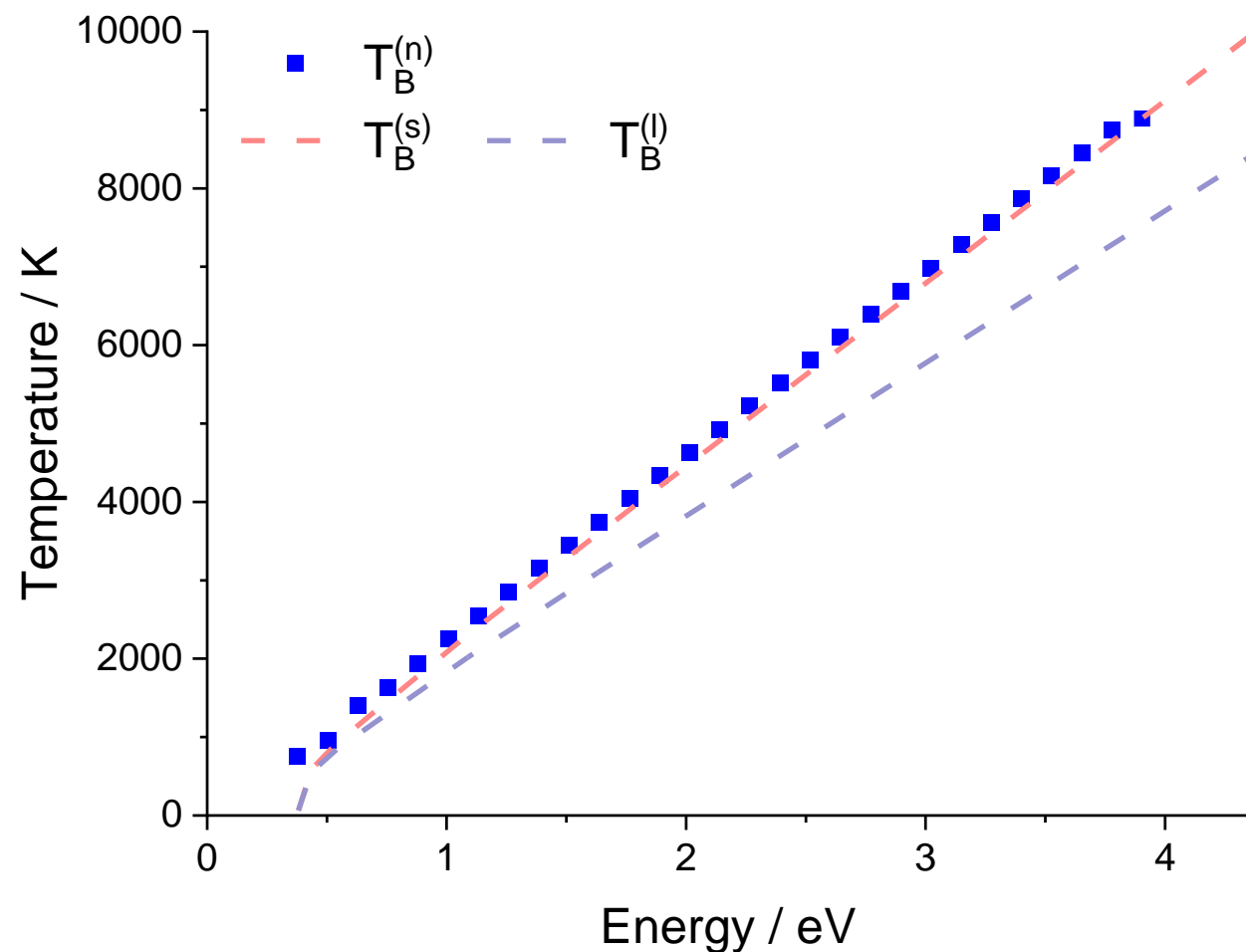


# Gibbs volume

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

Hockey-stick identity

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



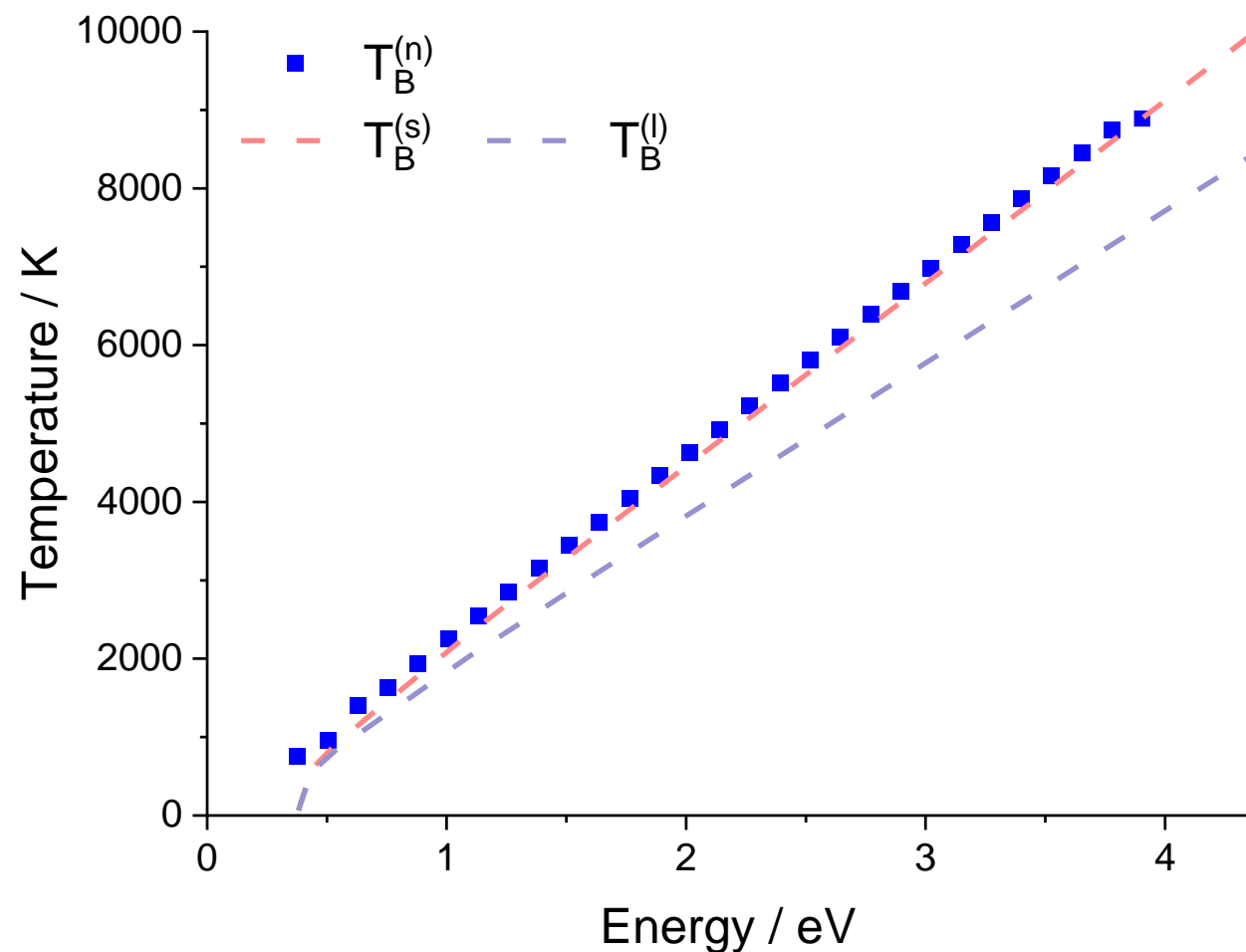
Hockey-stick identity: [en.wikipedia.org/wiki/Hockey-stick\\_identity](https://en.wikipedia.org/wiki/Hockey-stick_identity)

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

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

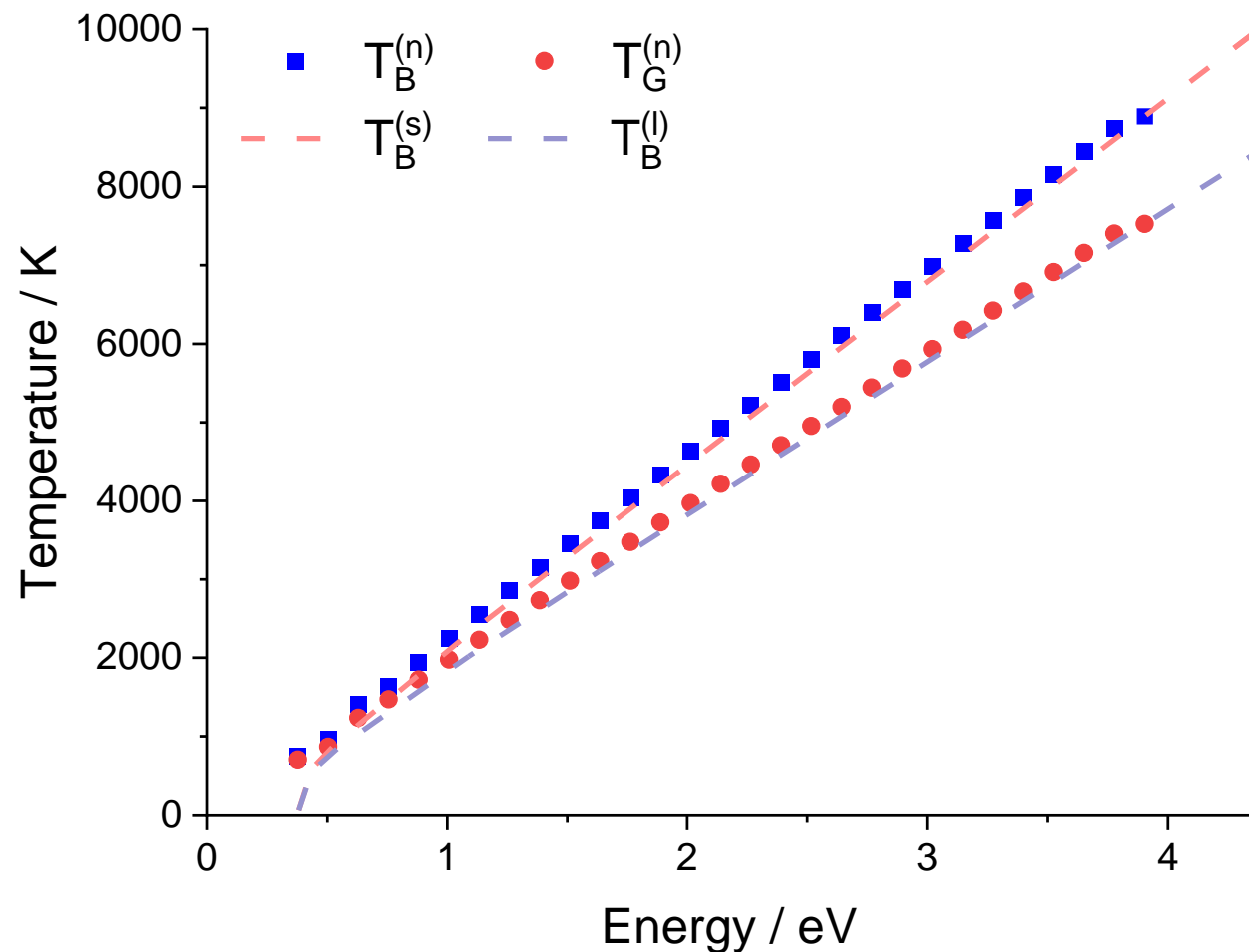


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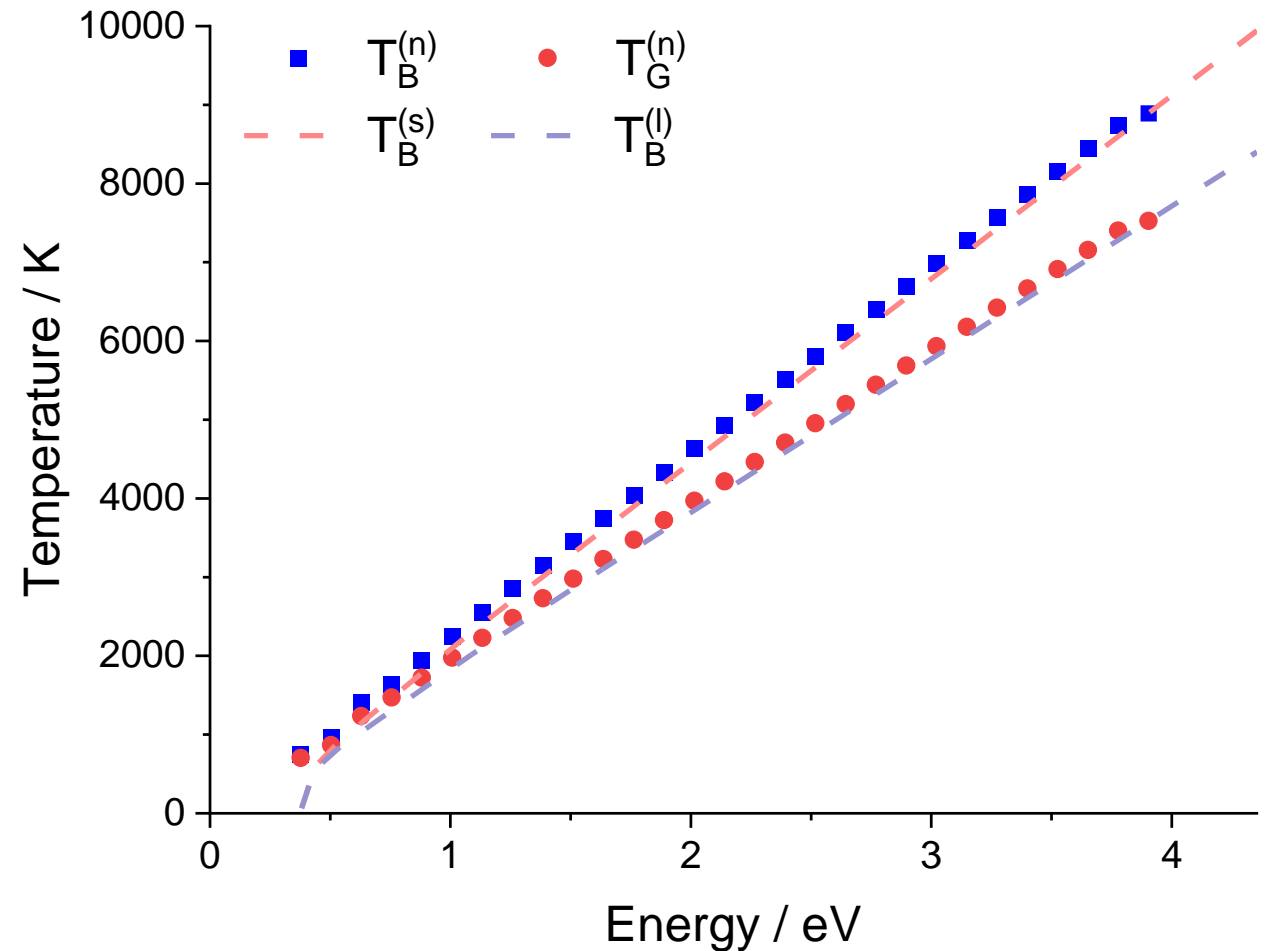
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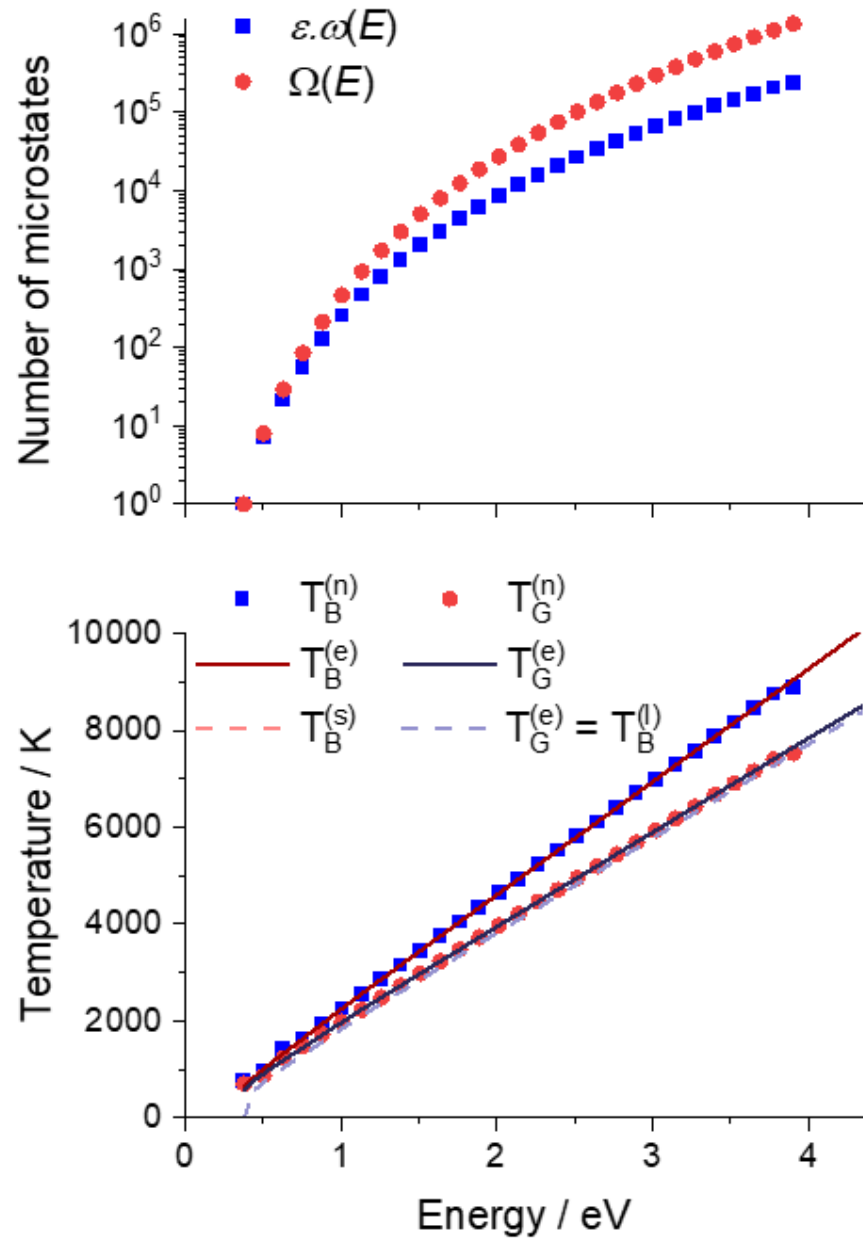
Stirling's approximation

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

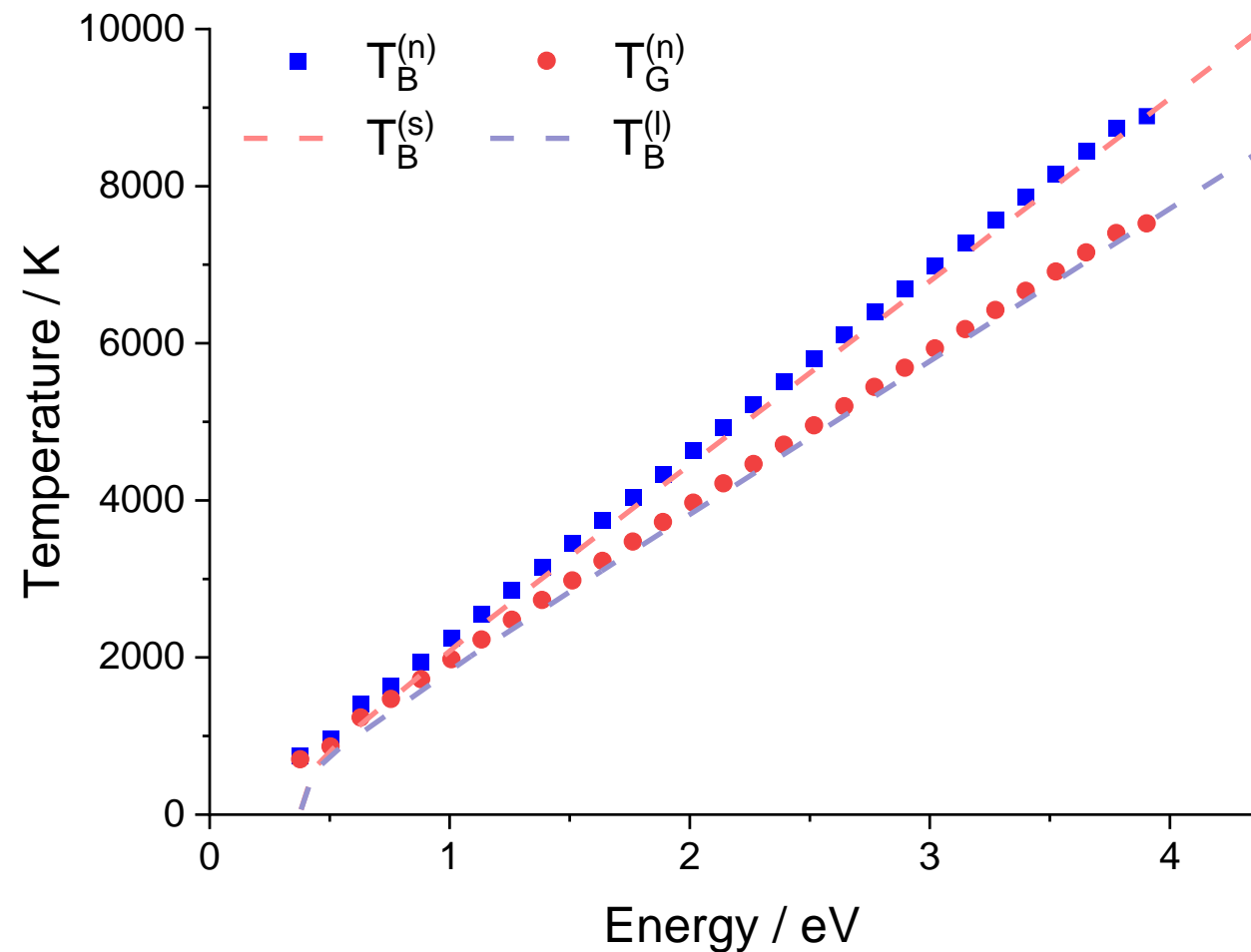
$$T_G^{(s)} = T_B^{(l)}$$

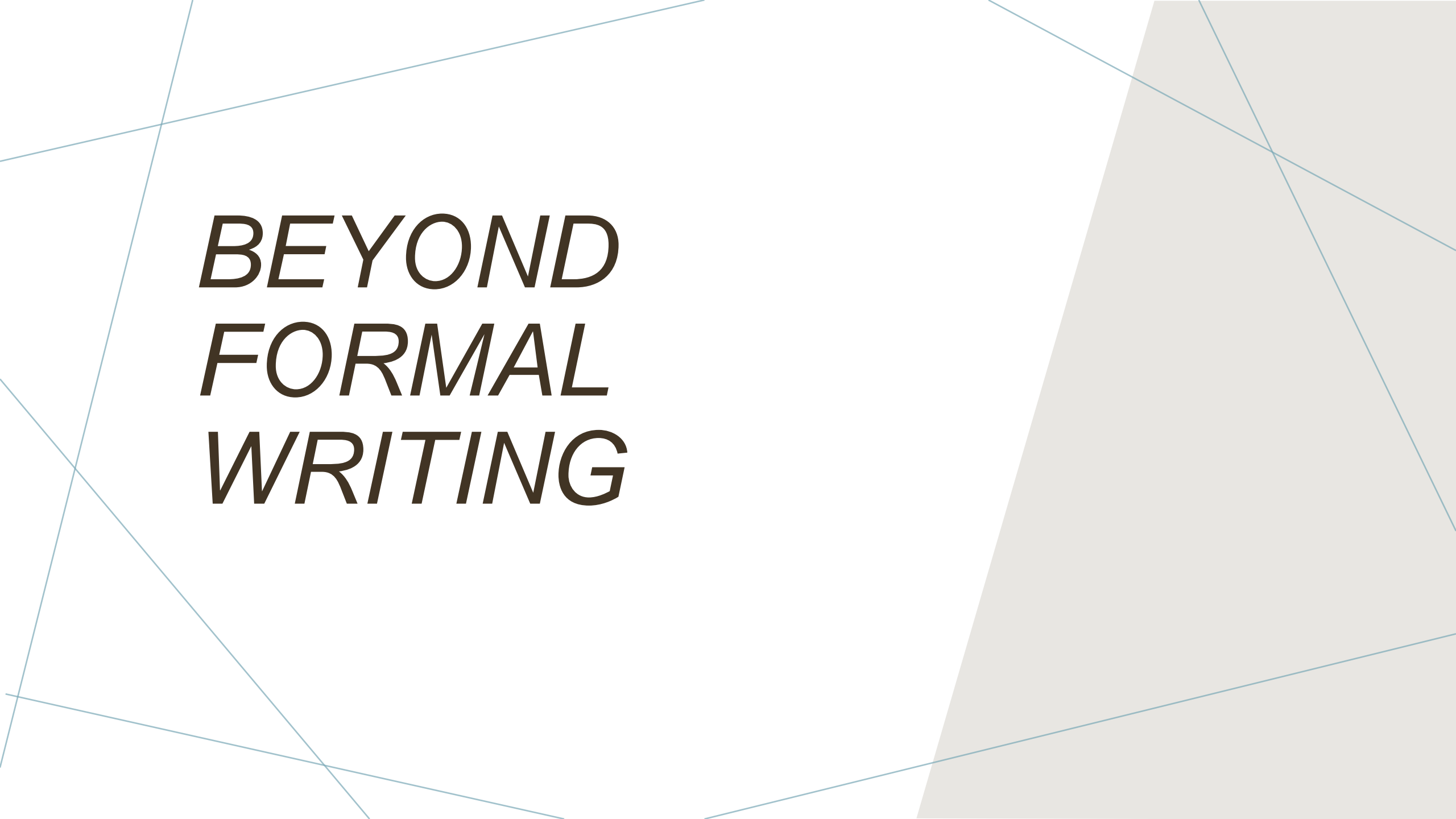


# Good for a paper



# 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](https://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](http://www.barbatti.org)



New  
adventures!

Available on Amazon  
Kindle and paperback








# One Billion Faces







Short Stories


MARIO BARBATTI





# New adventures!




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OPINION

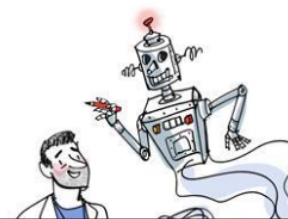
## Authorship in the time of ChatGPT

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](https://tinyurl.com/cwchatgpt)

# New adventures!

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

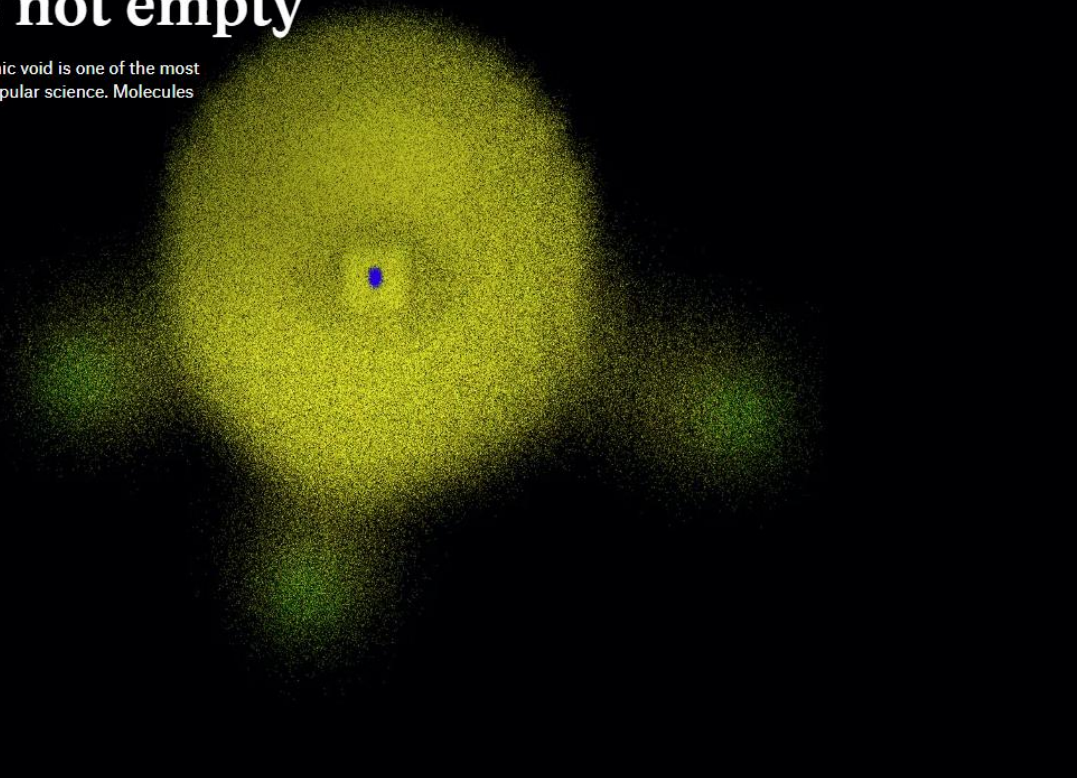
MENU / Q / f o t v

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](https://tinyurl.com/emptyatom)

# New adventures!

## 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](https://tinyurl.com/qmeasure)



**Thank you**



**[www.barbatti.org](http://www.barbatti.org)**



**[mario.barbatti@univ-amu.fr](mailto:mario.barbatti@univ-amu.fr)**



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