

# **VISTA Seminar**

## **Seminar 32**

**March 2, 2021**

**10:00 am – 11:30 am EST / 3:00 – 4:30 pm GMT / 4:00 pm – 5:30 pm  
Paris**

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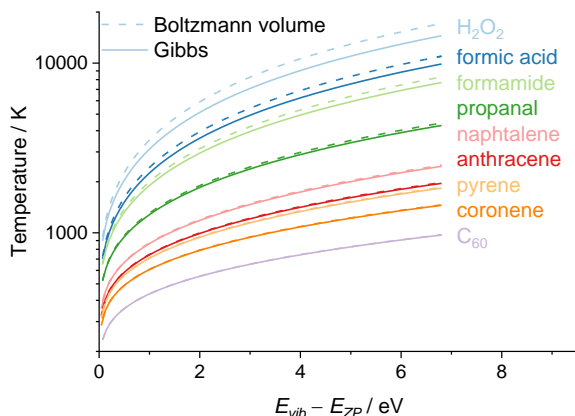
## What is the temperature of an isolated molecule in a vacuum?

Mario Barbatti

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Defining the temperature of an isolated molecule in a vacuum is helpful for many purposes like understanding radiative cooling, sampling nuclear ensembles, and assigning interstellar molecules. Nevertheless, such a molecular temperature concept has not been well defined so far.

In this VISTA talk, I will discuss how the temperature of an isolated molecule can be derived within the quantum harmonic approximation using statistical thermodynamics. I will examine the effects of the entropy functional choice, evaluate various approximations, and show that we can estimate the molecular temperature as a function of the vibrational energy as<sup>1</sup>

$$T(E_{vib}) = \left[ \ln \left( \frac{E_{vib} + E_{ZP}}{E_{vib} - E_{ZP}} \right) \right]^{-1} \frac{2E_{ZP}}{(3N_{at} - 6)k_B}.$$

Moving beyond this practical aspect, this diving into the heart of statistical physics allows us to learn a big deal about the thermodynamics of finite systems and even devise an experiment to settle the current debate on which entropy—Boltzmann or Gibbs volume—is the correct one.

### References

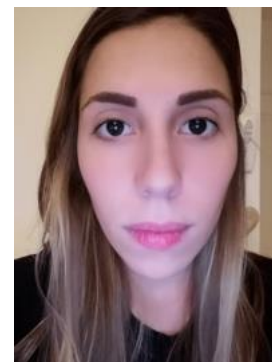
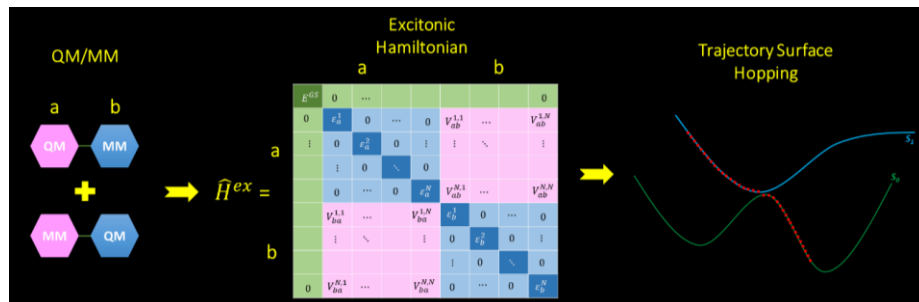
- (1) Barbatti, M. Defining the Temperature of an Isolated Molecule. ChemRxiv **2022**, DOI: [10.26434/chemrxiv-2022-5kr7s](https://doi.org/10.26434/chemrxiv-2022-5kr7s).

## Surface hopping dynamics with Frenkel exciton model in a semiempirical framework

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The electronic excitation energy transfer (EET) is a fundamental process, in which electronic excitation is transferred from a donor fragment to an acceptor. This process normally starts with a chromophore (the donor) being optically excited, and then the excitation is transferred to a nearby acceptor. The study of EET and other aspects of nonadiabatic dynamics in multichromophoric systems calls for employing some sort of “divide and conquer” strategy. In this respect, one of the most successful schemes is offered by the Frenkel exciton model, where the electronic excited states of the multichromophoric system are represented by linear combinations of localized excitations. We present an implementation of the Frenkel exciton model in the framework of the semiempirical floating occupation molecular orbitals-configuration interaction (FOMO-CI) electronic structure method, aimed at simulating the dynamics of multichromophoric systems, in which excitation energy transfer can occur, by an efficient approach.[1] The nonadiabatic molecular dynamics is here dealt with by the surface hopping (SH) method, but the implementation we proposed is compatible with other dynamical approaches. The application of our implementation is carried out on a self-assembled monolayer (SAM) of 4-(biphenyl-4-ylazo)-biphenyl-4-thiol (ABPT), where the excitonic interaction among 12 azobenzene chromophores was considered during the SH dynamics. However, the Frenkel exciton model is designed to describe local excitations, which makes its use not suitable for systems where, for instance, charge transfer effects play an important role. In order to improve on this shortcoming, we propose an extended exciton model in which charge transfer states and/or multiple excitations are taken into account by including QM calculations carried out on dimers.

### References

[1] Sangiogo Gil, E.; Granucci, G.; Persico, M., Surface hopping dynamics with Frenkel exciton model in a semiempirical framework. *J. Chem. Theory Comput.* **2021**, *17* (12), 7373-7383.

## How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 32

Time: Mar 2, 2022 10:00 AM Eastern Time (US and Canada)

Join Zoom Meeting

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