# Graph theory meets Born Oppenheimer molecular dynamics and replica-exchange Monte Carlo simulation

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Analysis based on graph theory is applied nowadays to different problems encountered in a wide variety of fields such as biology, computer science, physics, mathematics, and chemistry, among others. It allows a comprehensive understanding of the different interactions and processes that take place in the investigated system. In this seminar, I will discuss how graph theory can be used to analyze a set of Born-Oppenheimer molecular trajectories. The first part of the talk will be dedicated to explaining a developed methodology [1] and the second part will focus on how it is used to understand the complex dynamics dissociation in the gas phase of three systems: the protonated cyclo Gly-Gly and the naphthalene and azulene cations. Finally, I will show how this methodology can be extended to the analysis of a set of replica-exchange Monte-Carlo trajectories. To this end, the phase change diagram of $C_{28}H_{0-12}$ and $C_{60}H_{0-20}$ systems will be discussed. The effect of hydrogenation on carbon clusters will be highlighted.

## References

[1] Ariel F. Perez-Mellor and Riccardo Spezia. Determination of kinetic properties in unimolecular dissociation of complex systems from graph theory based analysis of an ensemble of reactive trajectories. *The Journal of Chemical Physics*, 155(12):124103, 2021.