VISTA Seminar

Seminar 67

April 17, 2024

10:00 am – 11:30 am EDT / 3:00 – 4:30 pm BST London / 4:00 pm – 5:30 pm CEST Paris / 10 pm – 11:30 pm CST Beijing

TOC:

Application of NEXMD for Modeling Photolytic Decomposition of Explosives

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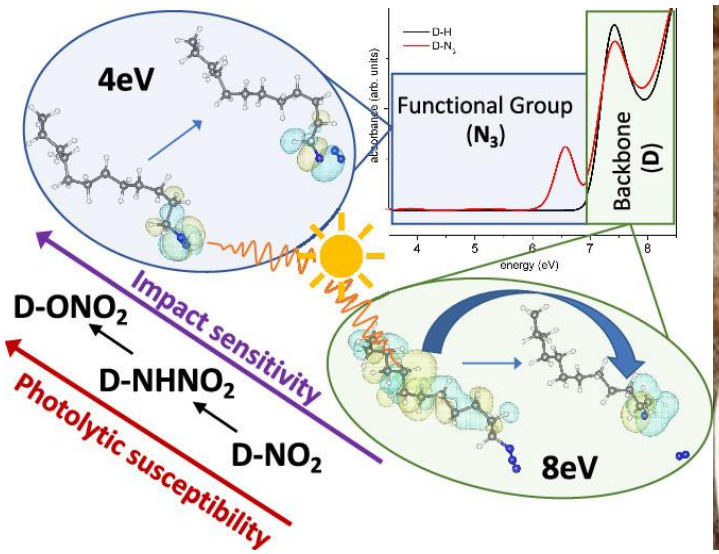

We will give a brief overview of the latest NEXMD software capabilities for modeling nonadiabatic excited state molecular dynamics. Among the recent developments, the open shell electronic structure better enables description of photodegradation. We have applied this methodology for the simulation of photolytic degradation of explosives, which is of interest for environmental remediation of contaminated sites and handling of explosives in sunlight. Specifically, the photolytic degradation of dodecane substituted with various energetic functional groups: azide, nitro, nitrate ester, and nitramine. For the studied molecules, it was found that excitons localize on the energetic functional group, no matter where they were initially formed, and thus, the predominant degradation pathway involves the degradation of the energetic functional group. The relative trends follow what is expected from the relative stability of the energetic functional groups to thermal and sub-shock degradation.

Disentangling the Photophysics of 6-Selenoguanine in Water

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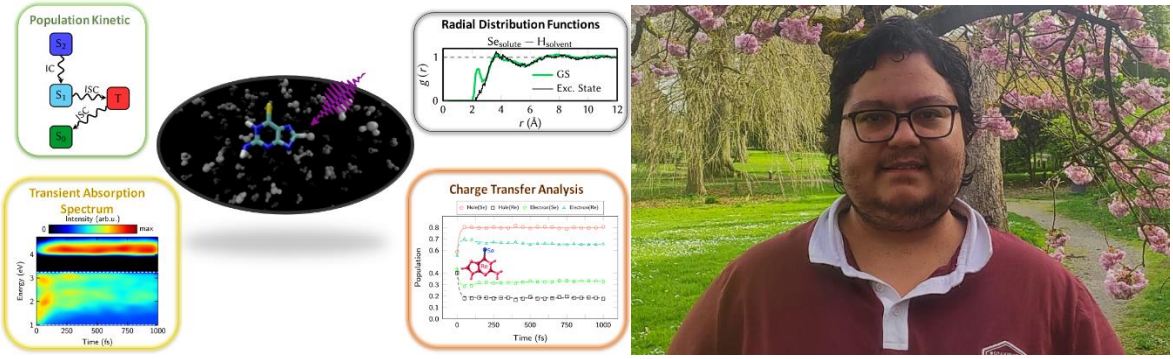

Photodynamics therapy (PDT) is a recognized medicinal technique for the treatment of cancer. In PDT, a photosensitizer (PS) in its lowest triplet state (T_1) interacts with a molecular triplet oxygen ($^3O_2$), yielding the production of $^1O_2$ that damages the tumor cells. The design of new PSs therefore involves a detailed understanding of their photophysics to maximize the triplet states yield. Recent studies have shown that selenium-substituted nucleobases could be good candidates as PSs for PDT [1] due both their near-unity triplet yields, thanks to a high spin-orbit coupling, and a red-shifted absorption spectrum into the visible as compared to thiobases, allowing for a deeper penetration into human tissue. With this in mind, we herein undertake a first-principles surface-hopping dynamics with an electrostatic embedding quantum mechanics/molecular mechanics (QM/MM) scheme to study the ultrafast excited-state relaxation mechanism of 6-selenoguanine in water [2]. We find the predominant relaxation mechanisms and also explain the reasons of why the T_1 lifetime of the 6SeGua is shorter than its thiobase analogue (6tGua). The transient absorption (TA) spectrum is also simulated and the extracted time constants are in very good agreement with previous experimental data [1].

References

[1] K. Farell, et al. J. Am. Chem. Soc. 2018, 140, 36, 11214. DOI: 10.1021/jacs.8b07665.
[2] D. Valverde, et. al. J. Am. Chem. Soc. Au 2022, 2, 7, 1699-1711. DOI: 10.1021/jacsau.2c00250.

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 67
Time: Apr 17, 2024 10:00 AM Eastern Time (US and Canada)

Join Zoom Meeting
https://buffalo.zoom.us/j/97349702914?pwd=YWo3SjI3MUtjS29MVWl2R3E3a3A2Zz09

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