Benchmarking a Computational Workflow Modeling Near-Infrared-Emitting Graphene Quantum Dots

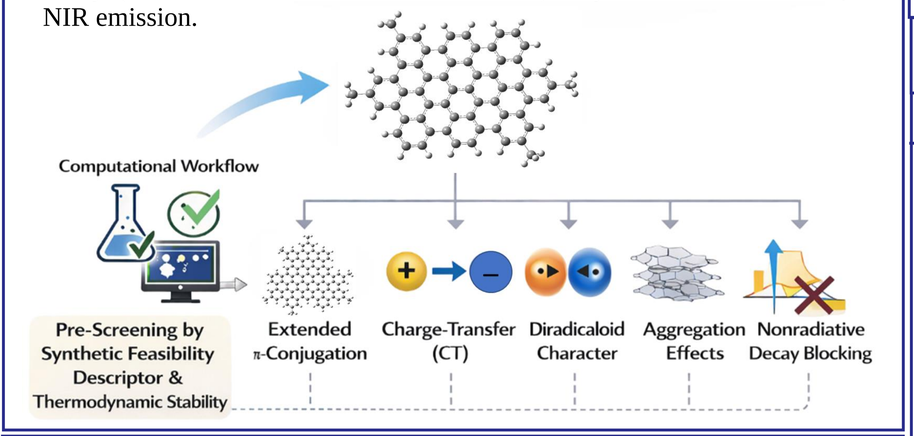
Muhammad Hammad Ali[a], Benjamin G. Janesko*

[a],*Department of Chemistry & Biochemistry, Texas Christian University, Fort Worth, Texas 76129, United States

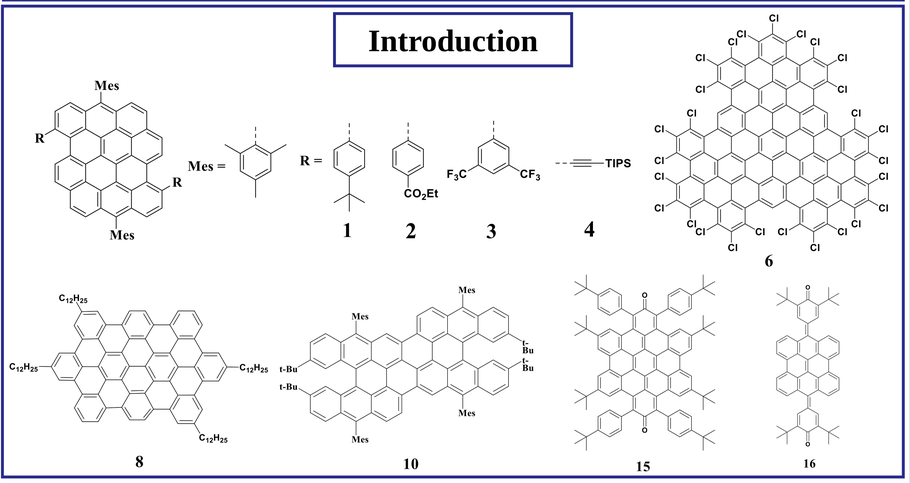
[a]*Presenter: m.hammad.ali@tcu.edu* **Advisor: b.janesko@tcu.edu*

Abstract

- Graphene quantum dots (GQDs) are emerging nanocarbon materials with tunable electronic structures and strong NIR emission, making them promising for bioimaging applications.
- The chromophores responsible for GQDs' NIR emission are often poorly characterized, limiting rational design and clinical applications.
- Extended π-conjugation, charge-transfer excitations, the presence of diradicaloids, stacking of multiple GQD layers, and blocking of nonradiative decay (as seen in non-aromatic fluorescence) may all contribute to GQDs' NIR emission.



Introduction



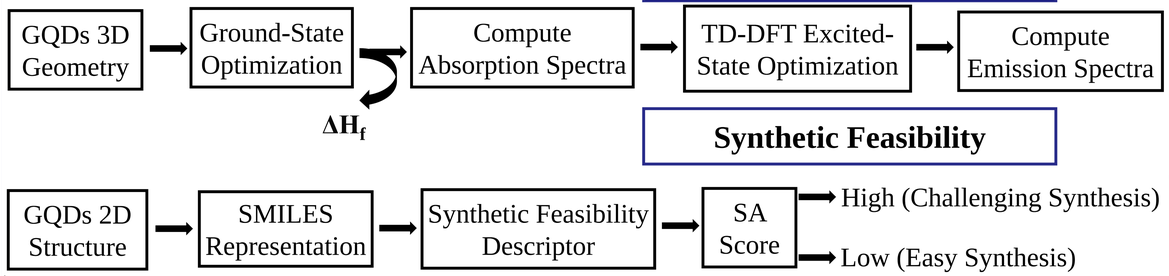
Problem Statement

- The chromophores responsible for NIR emission in GQDs remain poorly characterized.

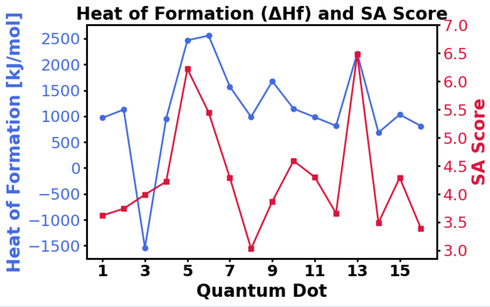
Objective

- Identify the chromophores responsible for near-infrared (NIR) emission in GQDs.
- Evaluate the performance of TD-DFT functionals for predicting absorption and emission wavelengths.
- Develop an efficient computational workflow for modeling NIR-Emitting GQDs.

Computational Methodology

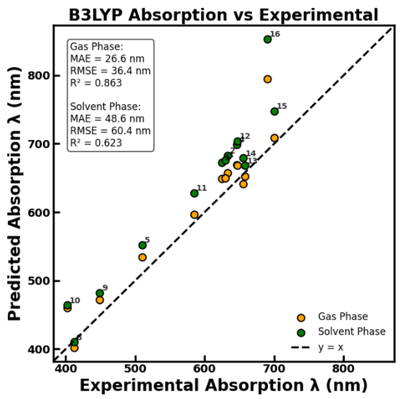


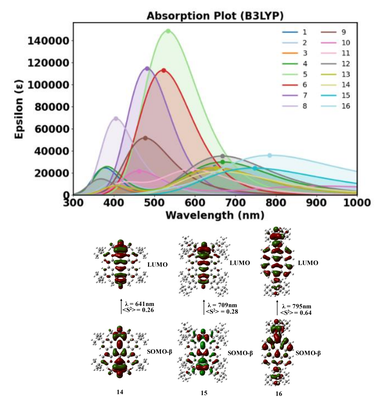
Synthetic Feasibility

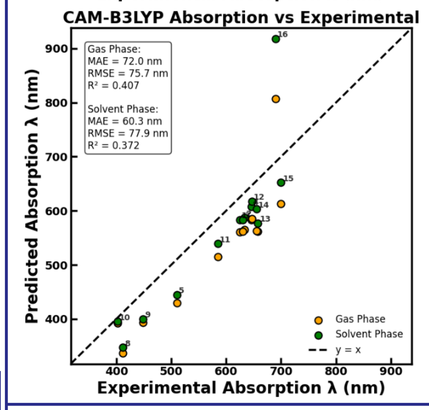


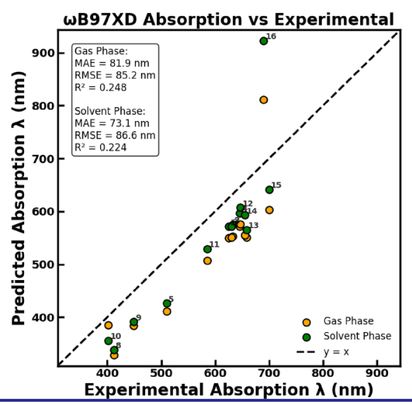
TD-DFT Benchmarking of Absorption & Emission

Absorption Benchmarking

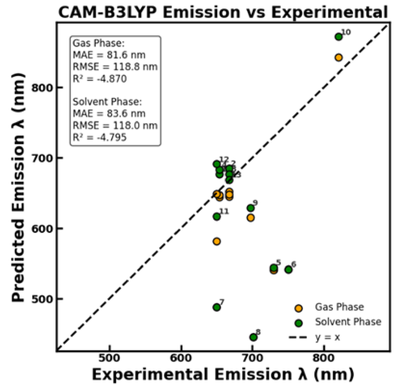




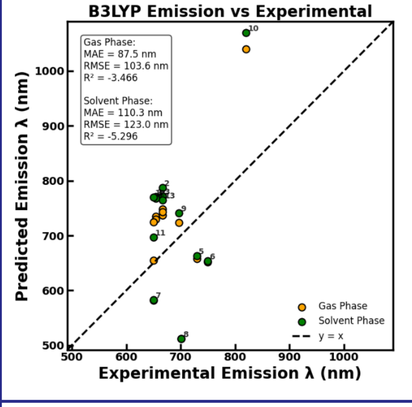


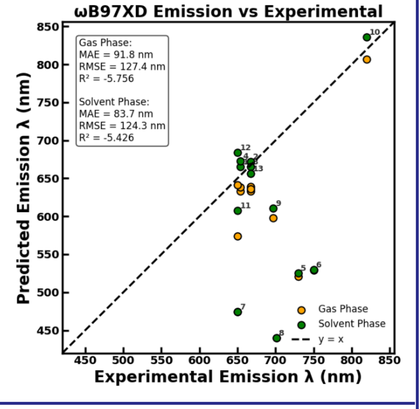


Emission Benchmarking



Quantum Dots	λ_{emiss} (nm) (Gas)	λ_{emiss} (nm) (Exp)	Excited State ($f_0 \neq 0$)
1	644	654	1
2	652	667	1
3	645	667	1
4	647	654	1
5	541	730	2
6	542	750	1
7	488	650	2
8	446	701	1
9	615	697	1
10	843	820	1
11	582	650	1
12	649	650	1
13	648	667	1





Conclusion &Future Work

- Developed a computational workflow for predictive modeling and high-throughput design of NIR-emitting GQDs.
- B3LYP accurately predicts absorption, while CAM-B3LYP provides reliable emission wavelengths for NIR GQDs.
- NIR emission arises from π-conjugation, charge-transfer character, diradical effects, and aggregation/stacking interactions.
- Future work will extend this protocol to design new NIR-emitting graphene nanostructures with well-characterized chromophores.

References & Acknowledgements

1. Ali, M. H.; Janesko, B. G.; Rana, M. M.; Saleem, U.; Gajula, N. M. Benchmarking a Computational Workflow Modeling Near-Infrared-Emitting Graphene Quantum Dots. The Journal of Physical Chemistry C 2026.

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