Dig Deeper into the Nanoverse: Computer Simulations Lending a Hand to Experiments in Bio-Nanotechnology

Ugur Can Topkiran[1], Alina Valimukhametova[1], Anton V. Naumov[1]

[1]Department of Physics and Astronomy, Texas Christian University

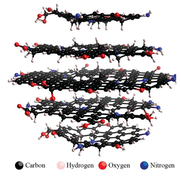
Abstract

With novel materials getting smaller and their size falling to the nanometer scale, it becomes harder to fully characterize them by only using the experimental apparatus at hand. Therefore, taking advantage of computational methods proves to be trustworthy in filling those gaps and in aiding our experimental data to get a better understanding of the nanomaterials' structural and electronic properties. Graphene quantum dots (GQDs) have recently become one of the flagships of carbon nanotechnology due to their remarkable physical properties and, when functionalized, their ability to become water soluble, biocompatible, and capable of fluorescence in the visible and near-infrared. This makes them perspective carriers for therapeutic delivery and image-tracking. In order to assess the advantages of their utilization for a variety of bioapplications, we have investigated the optical properties of doped GQDs and their interactions with biomolecules using a variety of molecular simulation approaches. The true atomic ground state of the N-GQD is achieved by performing first-principle calculations based on density functional theory (DFT). DFT calculations also unrevealed the contributions of each functional group within the structure to HOMO–LUMO band edges. The adsorption of biomolecules and genes on the GQD surface has been further investigated with regard to the GQD structure, complementing experimental results that verify gene and drug complexation.

Introduction

Experimental characterization:

- **Can give you structural and optical structure**
- **You cannot decompose the electronical excitation to orbital or atomic scale**



Avogadro Geometric Optimization:

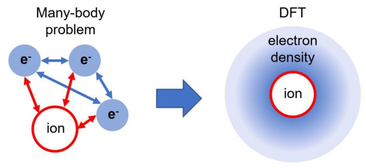
- **Quick geometric optimization tool**
- **Valance charge based**
- **Great for really big structures**

Going down to electron scale with first-principle calculations:

- **Can show electronic properties**
- **Almost perfect but high work-power**
- **Harder to work on big systems**

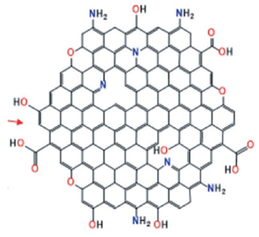
Graphene Quantum Dots in Bio-Nanotechnology:

- **biocompatible and biodegradable**
- **nanoscale size**
- **NIR flurescence**
- **drug delivery vehicles**
- **Easy synthesis and use**

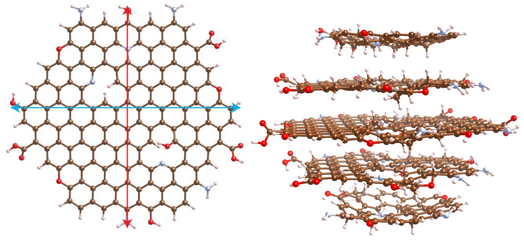


Atomic Structure of NGQDs

Experimental Result



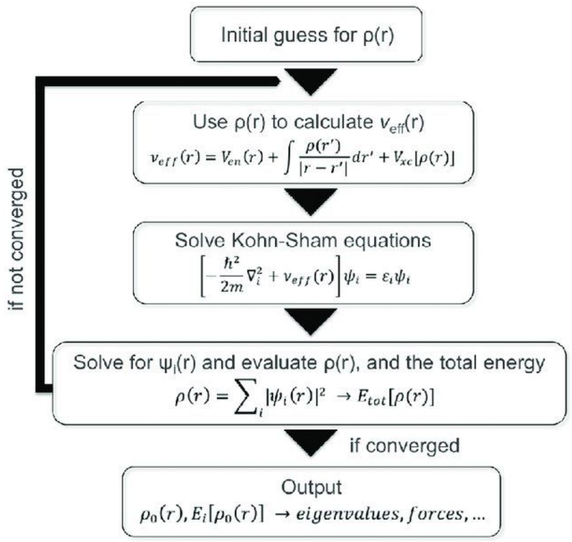
Top View



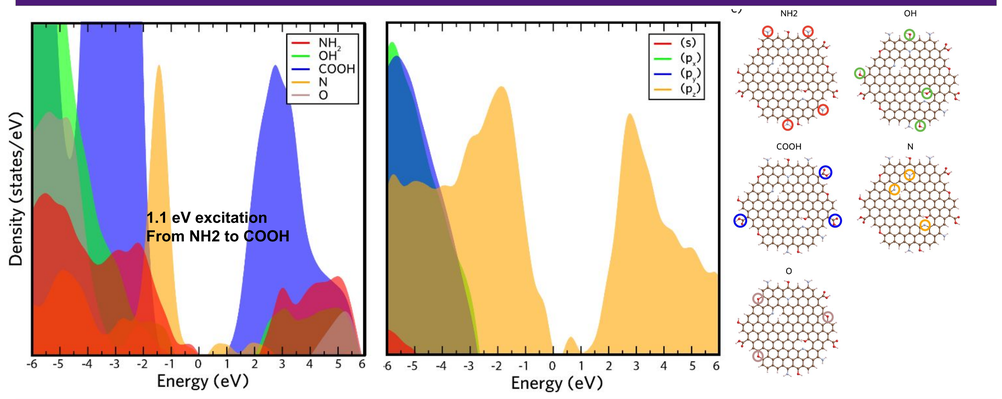
$d_{vertical}$: 23.5 Å $d_{horizontal}$: 25.0 Å

- **Single flake Structure of NGQD optimized in DFT and its multilayer form optimized in Avogadro.**

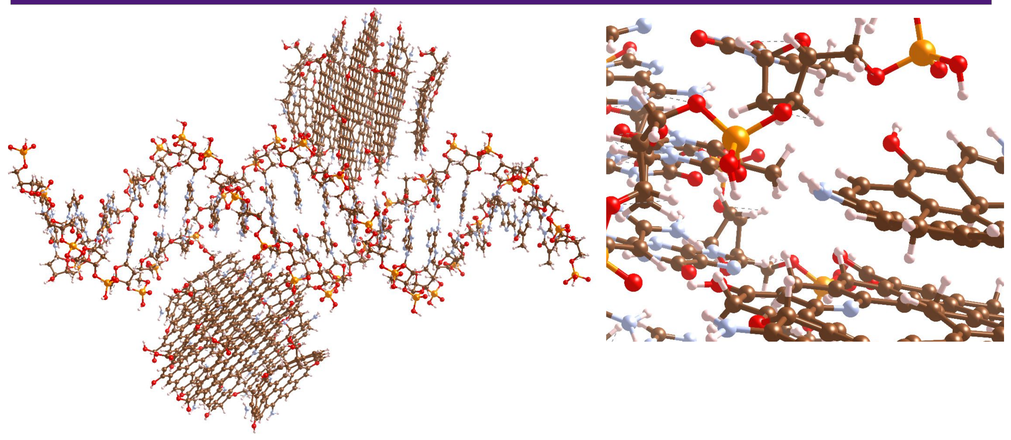
Self-Consistent Scheme



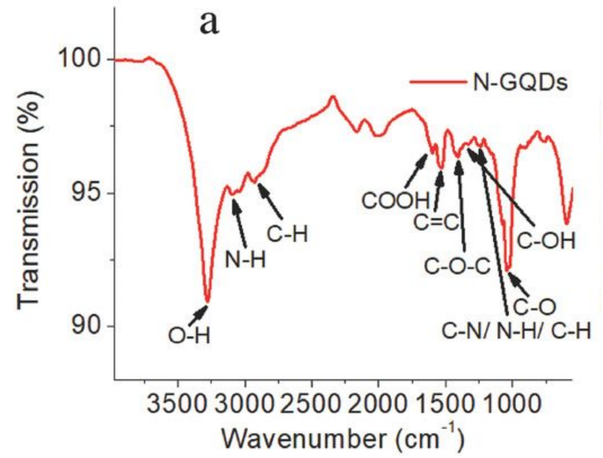
Electronic Properties Calculated with DFT



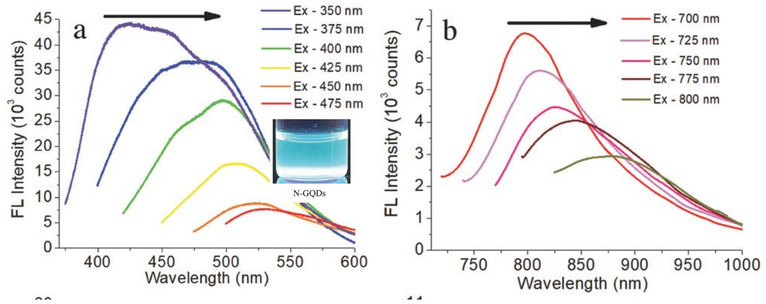
Interactions of NGQDs and Bio-Molecules



NGQD FTIR Spectrum



FL Intensity of NGQDs in Visible and NIR



- **Excitation-dependent emission in a) visible, b) NIR**

Conclusion

- **Although experimental result has the final say, in our current level of technology; it lacks capabilities go smaller**
- **When simple geometric optimization tool like Avogadro are giving us amazing results in the bigger structure, we need first principle calculations to look at the electronic or optical properties of a material.**
- **After one's experimental results, using available computational tools will not only increase our understanding of the material, but will open new doors as we are digging deeper into the nanoverse**

References

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