nanoHUB.org:
Real users, Real stories, My story

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Outline

I. **NUITNS: Nanodiamond Fluorescence Project**

- **nanoHUB.org:** An Approach for Teaching Computational Chemistry to Engineering Undergraduate Students
- Objective
- Introduction
- Model Complexes
- Results and Impact

II. **Calibrating MM force fields and QM Methods for Supramolecular Complexes**

- Fundamental Aspects
- Significance of Study
- Summary

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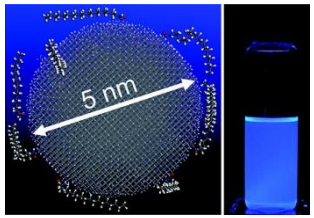
Part I

Objective:

- Introduce students to semiempirical electronic structure methods within the QC-Lab modeling program at the nanoHUB.org website.

Introduction:

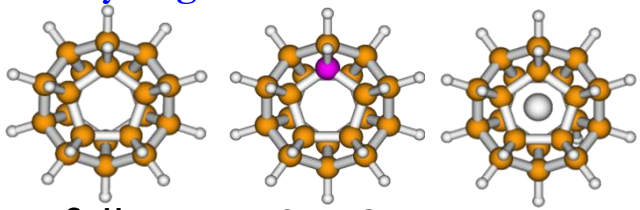
- Doped nanodiamonds (**NDs**) are promising as fluorescent markers and drug delivery platforms in therapeutic applications. Typical **NDs** have 5000 atoms and are 3nm in diameter.



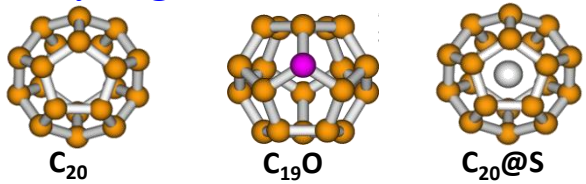
J. Am. Chem. Soc. **2009,** 131, 4594-4595.

Studied Complexes

Hydrogenated Nanodiamonds



Dehydrogenated Nanodiamonds



Approach:

- Use electronic structure calculations to study hydrogenated (**HNDs**) and dehydrogenated (**DHDs**) **NDs**.
- Chemical functionalization based on structural and physical properties investigated.
- Optical properties of the final geometries estimated using the semiempirical electronic method CNDO/INDO.

Results / Impact:

- NUITNS educational outreach developed tutorials and laboratory assignments for the nanoHUB.org website.
- Assignments benchmarked for Winter Quantum Mechanics and Spectroscopy course at NU.
- Students (≥ 40) used nanoHUB.org to supplement NU learning experience
- Assignments transferred to www.nanoHUB.org.
- Manuscript submitted to *J. Chem. Edu.*

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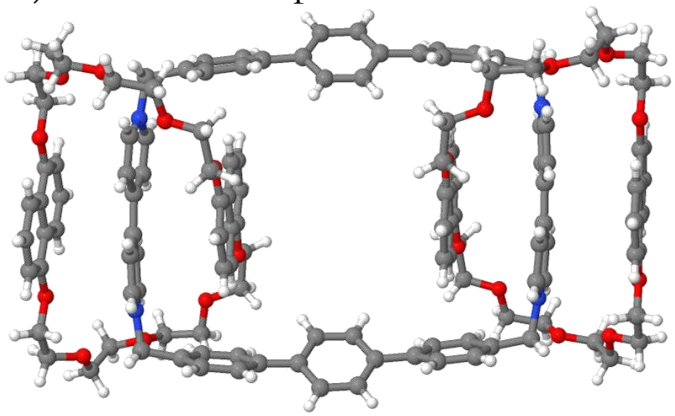
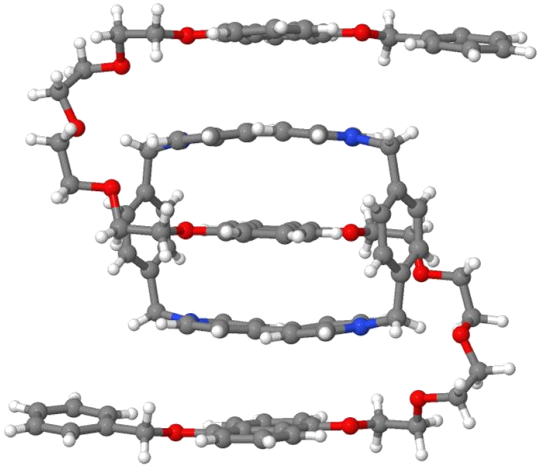
Part II

Supramolecular Complexes

a) Catenane complex



b) Rotaxane complex



Introduction:

Catenanes and rotaxanes are promising molecules for molecular switches and machines. We want to develop MM methods to describe these machines, and calibration is essential.

Fundamental Aspects:

-Benchmark calibrations of QM methods and MM force fields.

-What is the nature of noncovalent intermolecular forces?

Significance of Study:

-QM studies provide an accurate benchmark description to determine force fields of larger and sophisticated complexes.

-Results will suggest if MM is suitable for larger supramolecular complexes.

Supramolecular complexes "*noncovalent interactions*" based on:

- π-π stacking
- C-H···O hydrogen bonding
- C-H···π

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Summary

- We have assessed the ability of various *ab initio* QM methods to calibrate MM force fields.
- Relative to the *ab initio* optimized structures, geometries and energetics are described fairly well with MM3 force fields.
- Differences between QM methods, HF and MP2, energetic results arise to the latter's van der Waals attraction contributions.
- The MM3 force field provides a reasonably good balance between accuracy and description.
- Results are encouraging and suggest the possibility of using the computationally efficient MM3 force field for simulating larger complexes.
- The nanoHUB.org resources (*presentations, coursework assignments and lectures*) have enriched my postdoctoral learning experience tremendously.

Contributors

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