


$10^{th}$ User's Conference of IT4Innovations

# Structural Models for Carbon Nanodots:

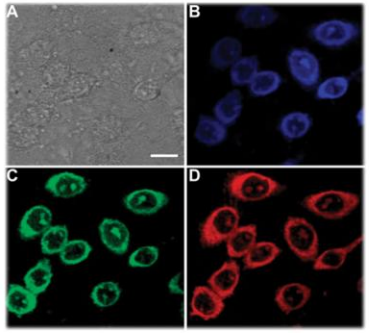
# Graphitic, Nitrogen-doped and Graphyne-Based systems

Zaira Carboni, Ph.D. Student

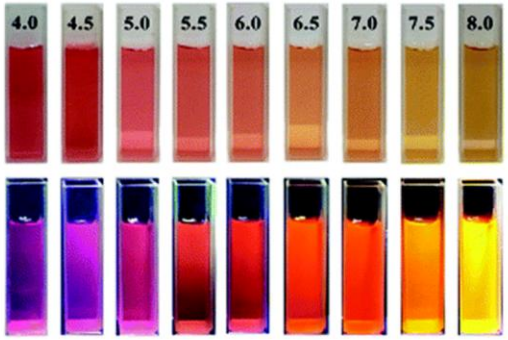
# Carbon Dots

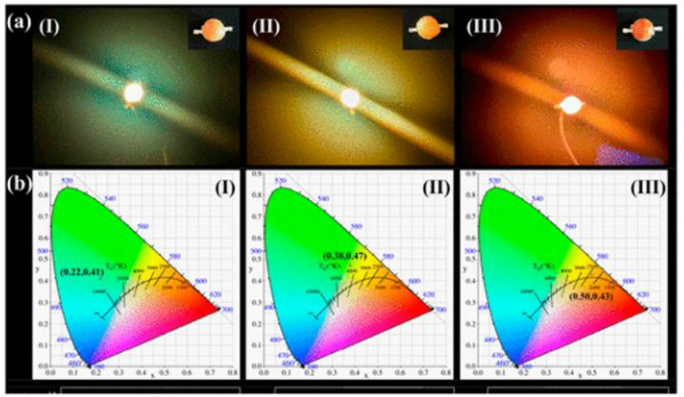
- Zero-Dimensional Carbon-Based Nanomaterials
- Tunable photoluminescence and high quantum yield
- Biocompatible and cost-effective
- Highly versatile

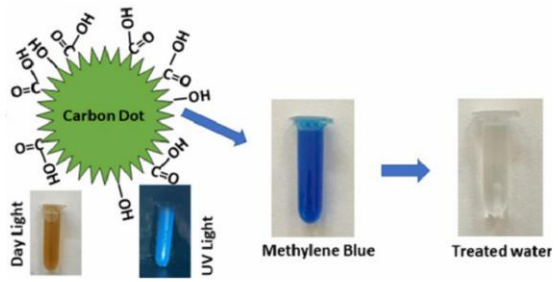
Bioimaging




Sensing



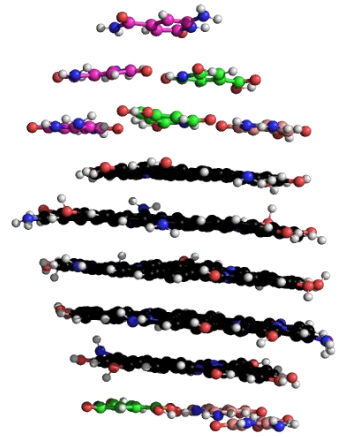




Optoelectronics

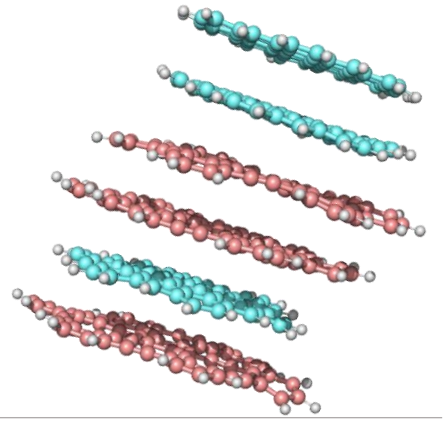
Enviromental

# Overview

- Comparative Molecular Dynamics Study of **Hydroxyl-Functionalized** and **Nitrogen-Doped** Carbon Dots Interacting with **Molecular Fluorophores**

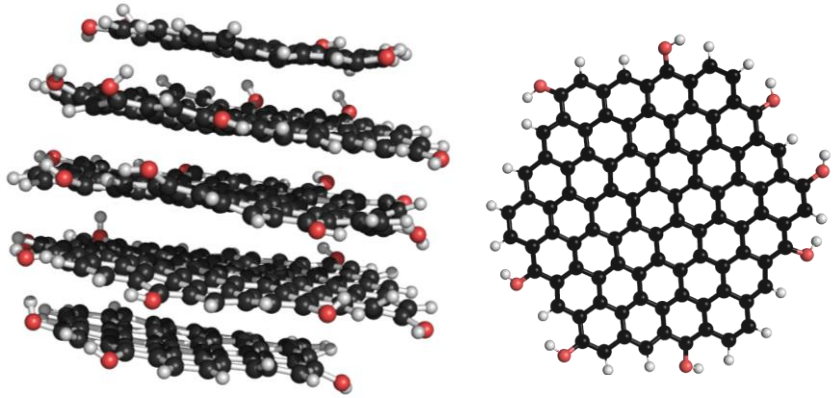


- Exploration of **Graphene–Graphyne** Hybrid Structures

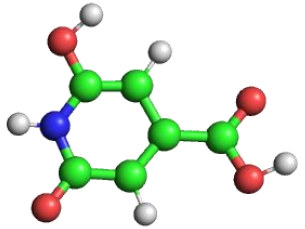


# Comparative Molecular Dynamics Study of **Hydroxyl-Functionalized** and **Nitrogen-Doped** Carbon Dots Interacting with **Molecular Fluorophores**

## Graphitic Carbon Dot with Hydroxyl-group on the surface: VMD Builder

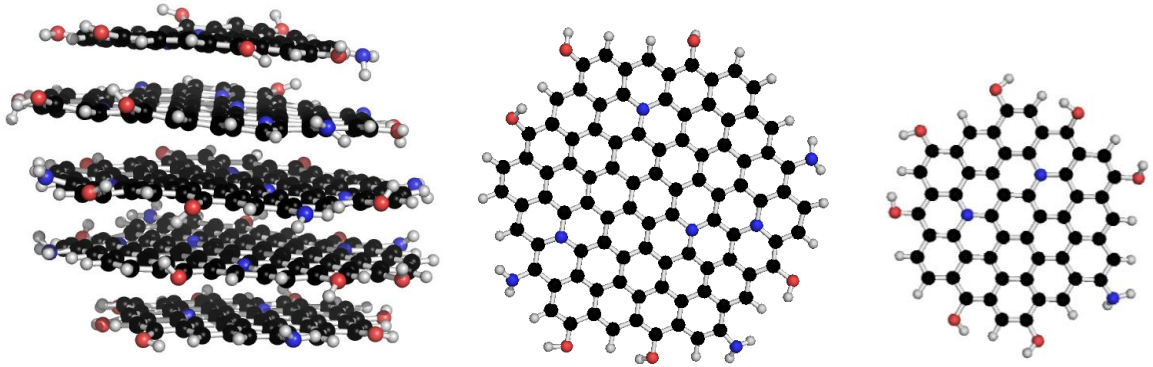


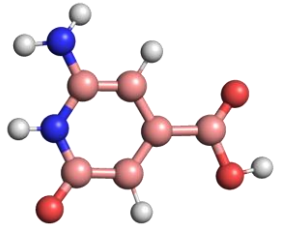
## Molecular fluorophores: Gaussview



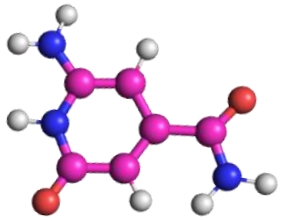
Citrazinic Acid:
CZA

## Graphitic N-doped Carbon Dot:
## VMD Builder + Gaussview + Self assembly





Citrazinic Acid Amine:
CZA-A

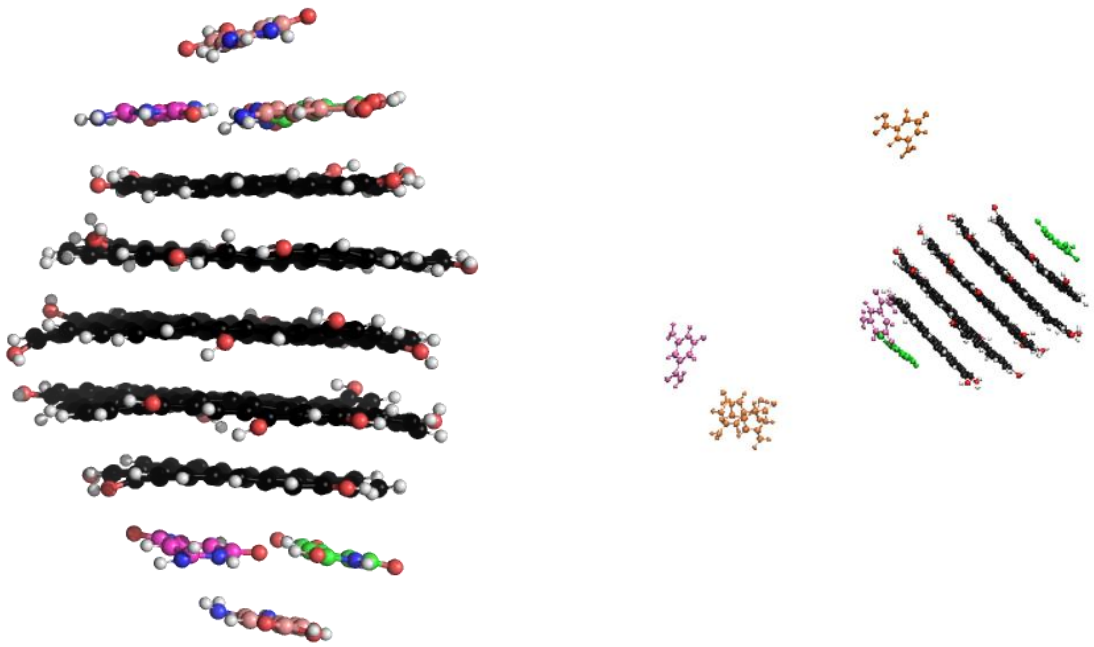


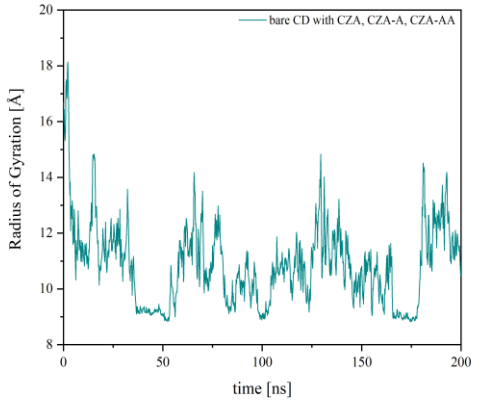
Citrazinic Acid Amine Amide
CZA-AA

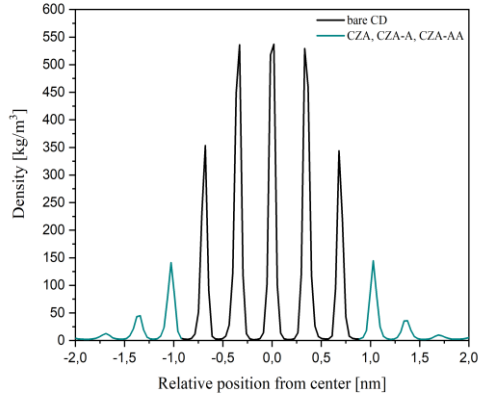
# Graphitic Carbon Dot with Hydroxil-group on the surface

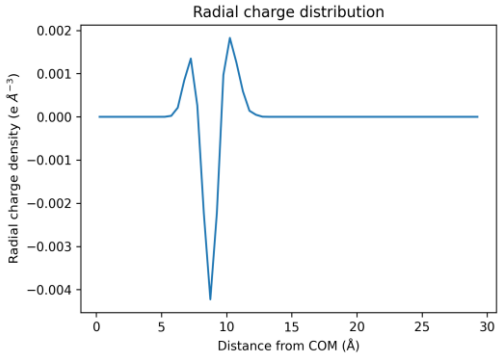
$d_l \approx 0.34\ nm$

$u \approx 0.06\ nm$





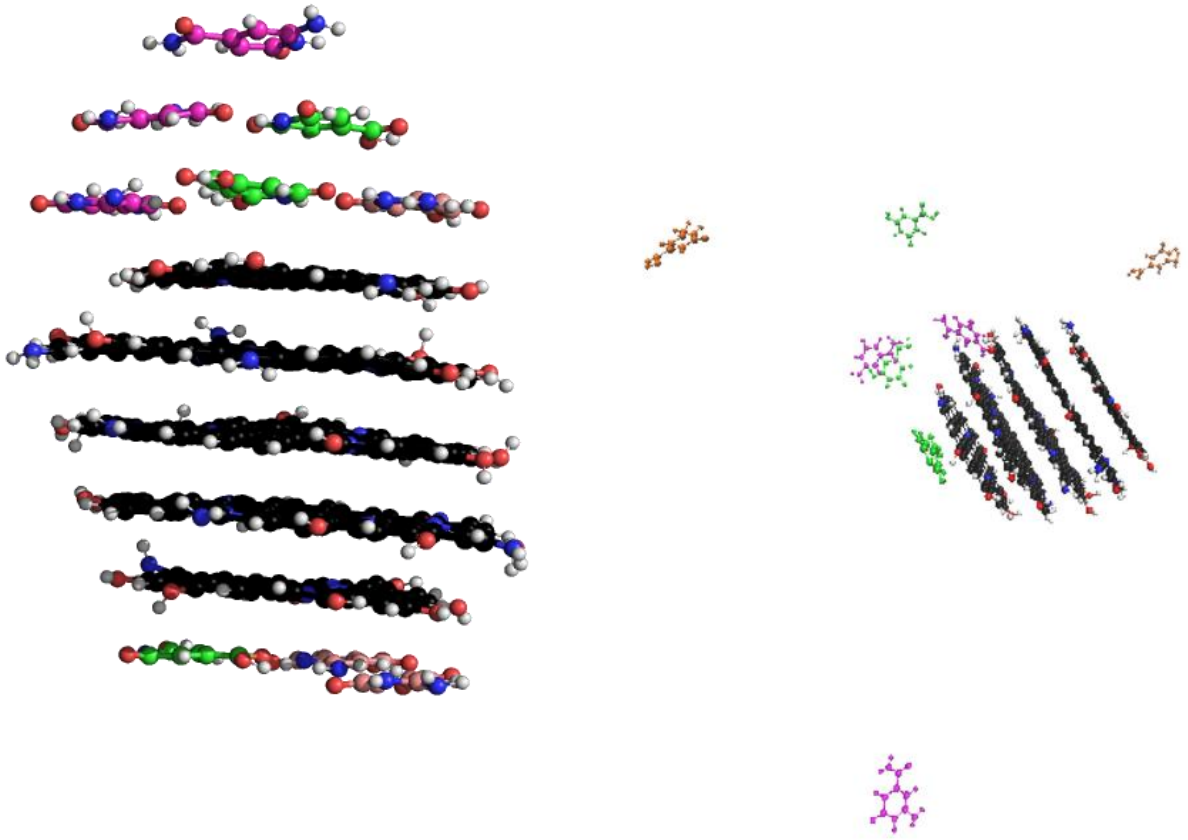



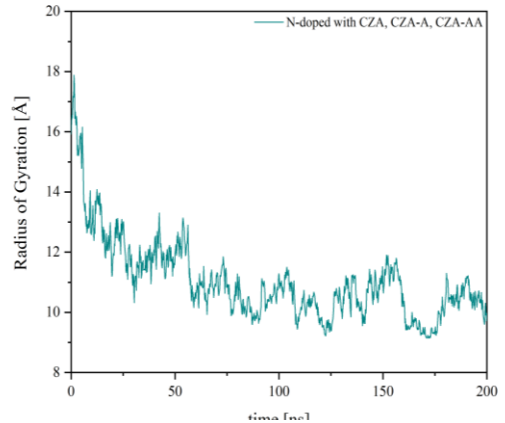

Water model: SPCE
$\Delta t$ : 2 $fs$
Time : 200 ns
FF : GAFF

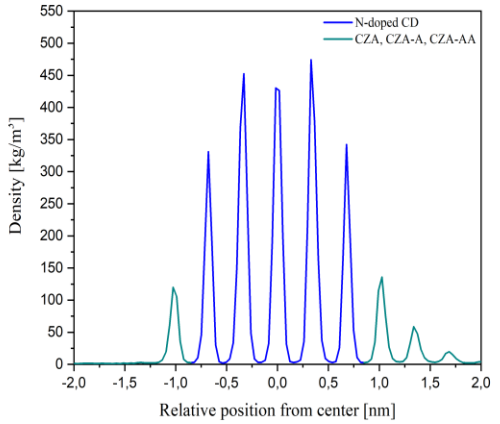
# Graphitc N-doped Carbon Dot: N-doped CD

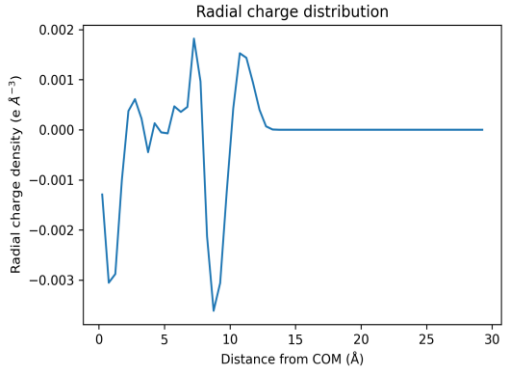
$d_l \approx 0.34\ nm$

$u \approx 0.06\ nm$





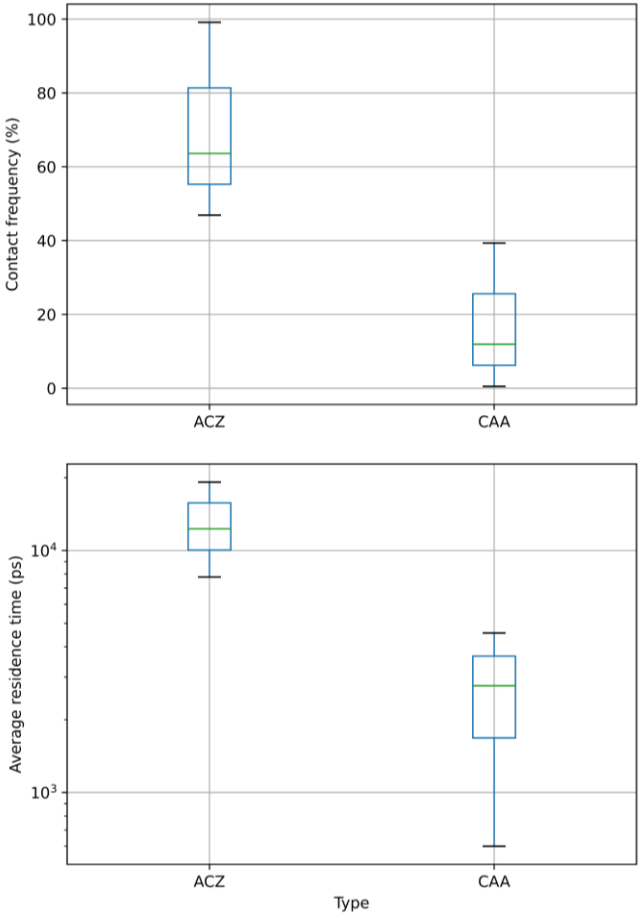



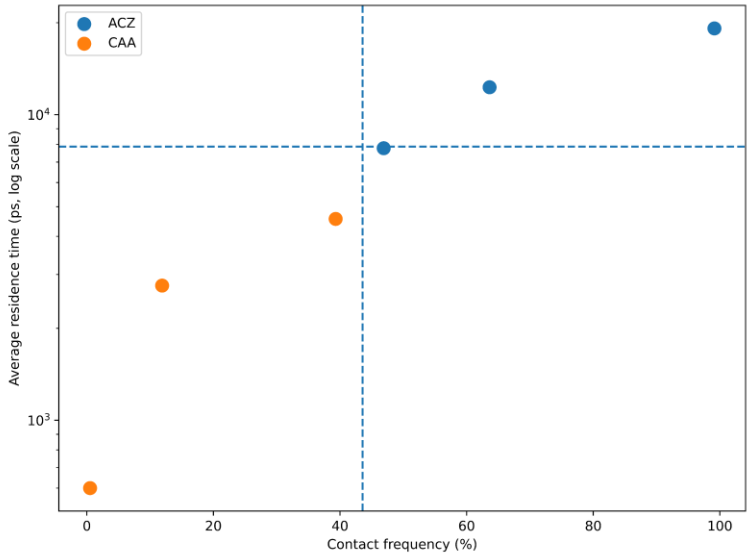




Water model: SPCE
$\Delta t$ : 2 $fs$
Time : 200 ns
FF : GAFF

jupyter

# Work in progress: Molecular Fluorophores – CD affinity

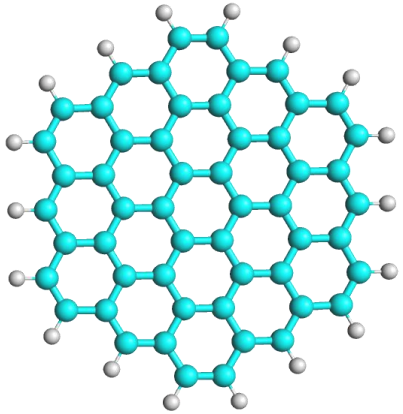


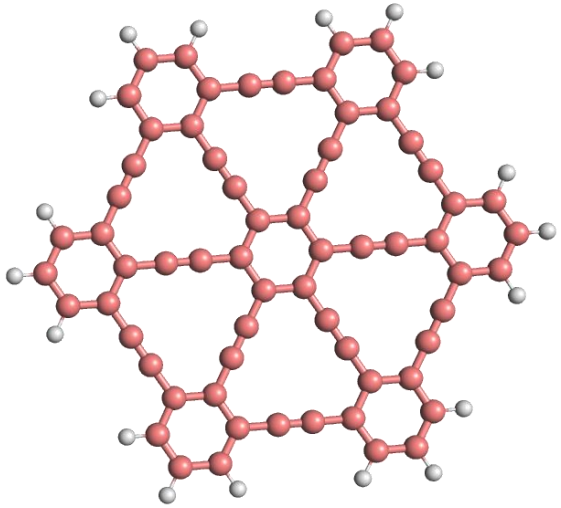

In the competitive adsorption simulation, the Kruskal–Wallis test indicated a statistically significant difference in residence time between ACZ (CZA-A) and CAA (CZA-AA) ($p = 0.049$), suggesting different adsorption persistence under competitive conditions.

# Exploration of Graphene–Graphyne Hybrid Structures

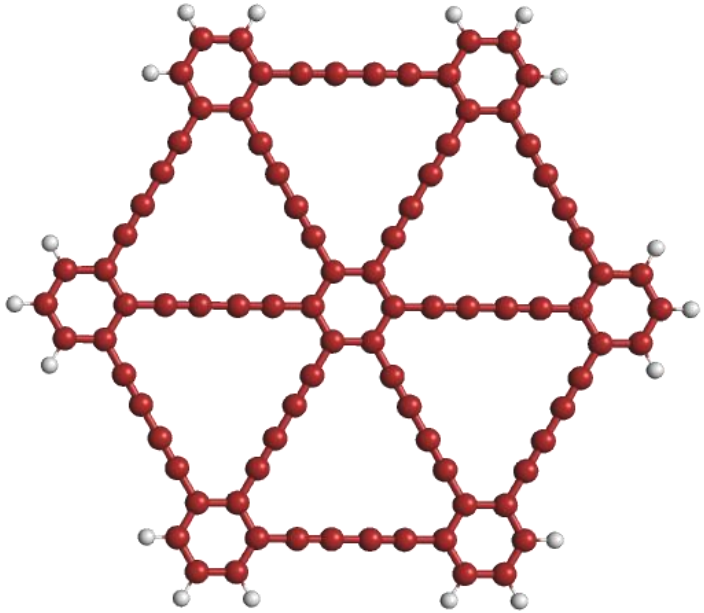
# Structures



Circumcoronene
$gG2 \sim 1,35\ nm$

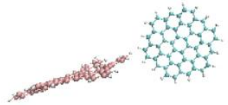


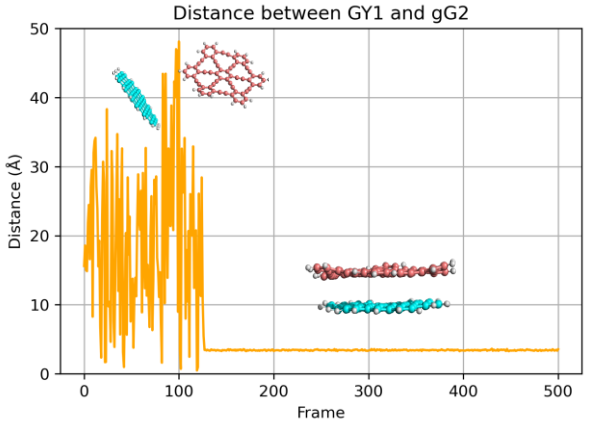
Graphyne
$GY1 \sim 1,9\ nm$

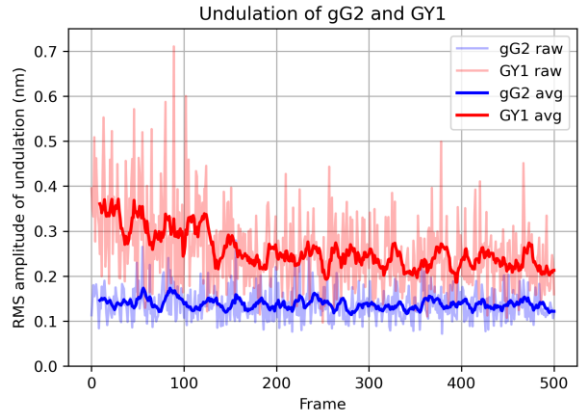


Graphdiyne
$GDY \sim 2,4\ nm$

# Simulations



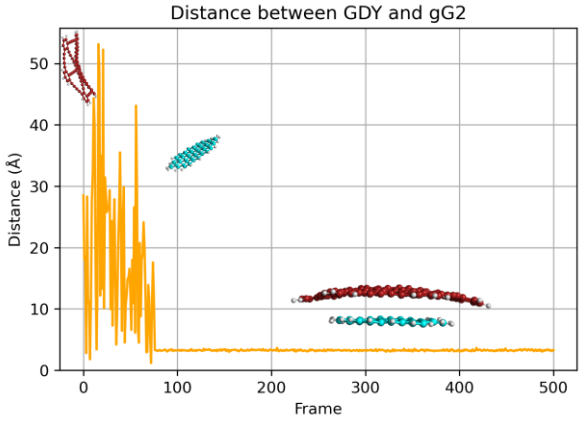


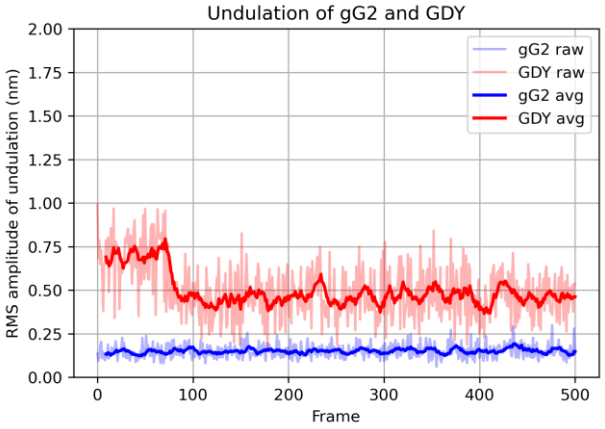




Water model: SPCE
$\Delta t$ : 2 $fs$
Time : 100 ns
FF : GAFF

## gG2 with GY1



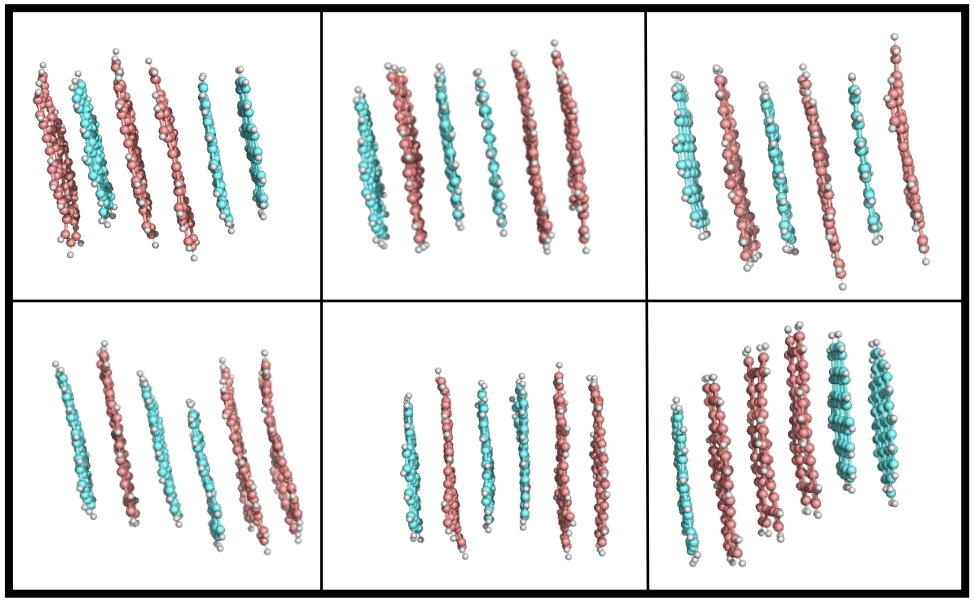


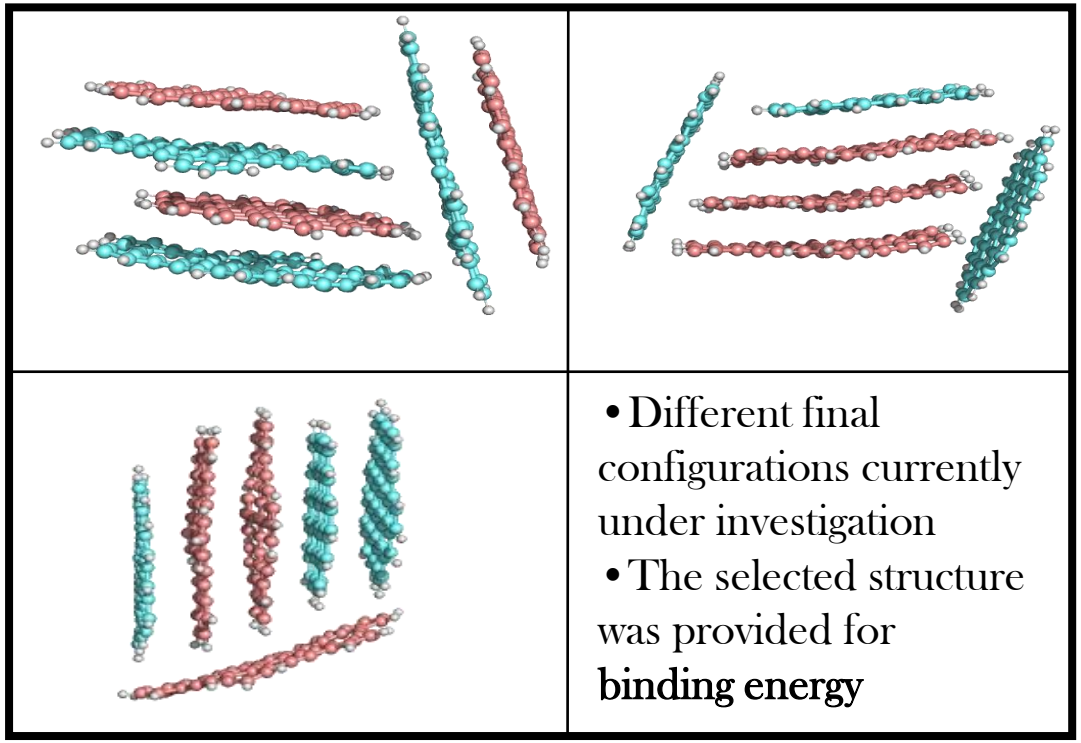

Water model: SPCE
$\Delta t$ : 2 $fs$
Time : 100 ns
FF : GAFF

## gG2 with GDY

# Multiple layers of Graphyne and Circumcoronene



Performed **10 replicas** of the simulations with **3 graphyne molecules and 3 circumcoronene molecules.**



Water box : 7 x 7 x 7 nm
Water model: SPCE
$\Delta t$ : 2 $fs$
Time : 200 ns
FF : GAFF

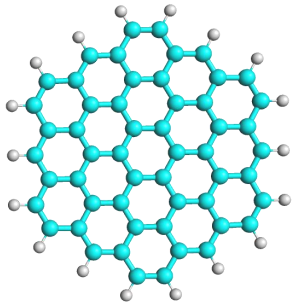
- Different final configurations currently under investigation
- The selected structure was provided for **binding energy**

# Computational details

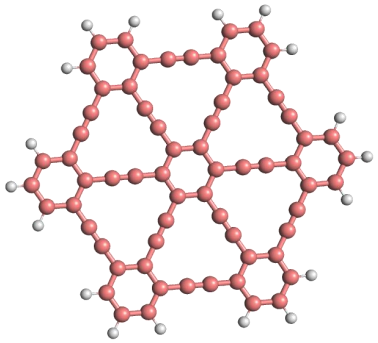
# Quantum-chemical calculations

- Software: **Gaussian 16**
- Cluster: KAROLINA
- Level of theory:
  - ✓ Geometry optimization: **B3LYP/cc-pvDZ**
  - ✓ Electrostatic potential (ESP) charges: **HF/6-31++G***, tight SCF, Merz-Kollman fit
- Resources per job: 1 CPU node (128 cores allocated), no GPU
- Parallelization: shared-memory (SMP) multithreading within a single node; no distributed (multi-node) parallelism
- Simulation time: 3 hours

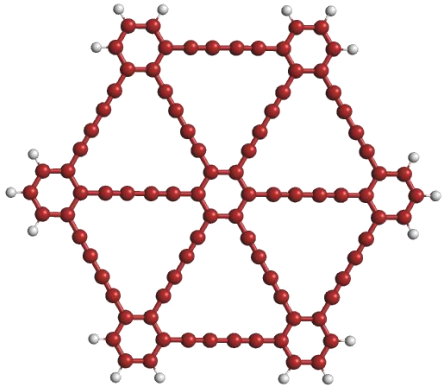
Circumcoronene
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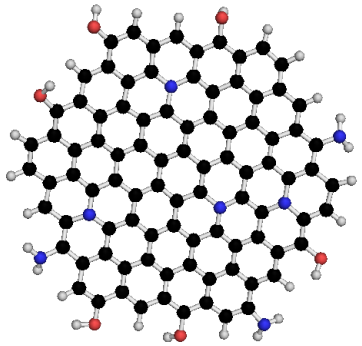


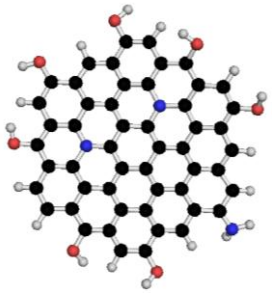
Graphyne
$GY1 \sim 1,9\ nm$



Graphdiyne
$GDY \sim 2,4\ nm$



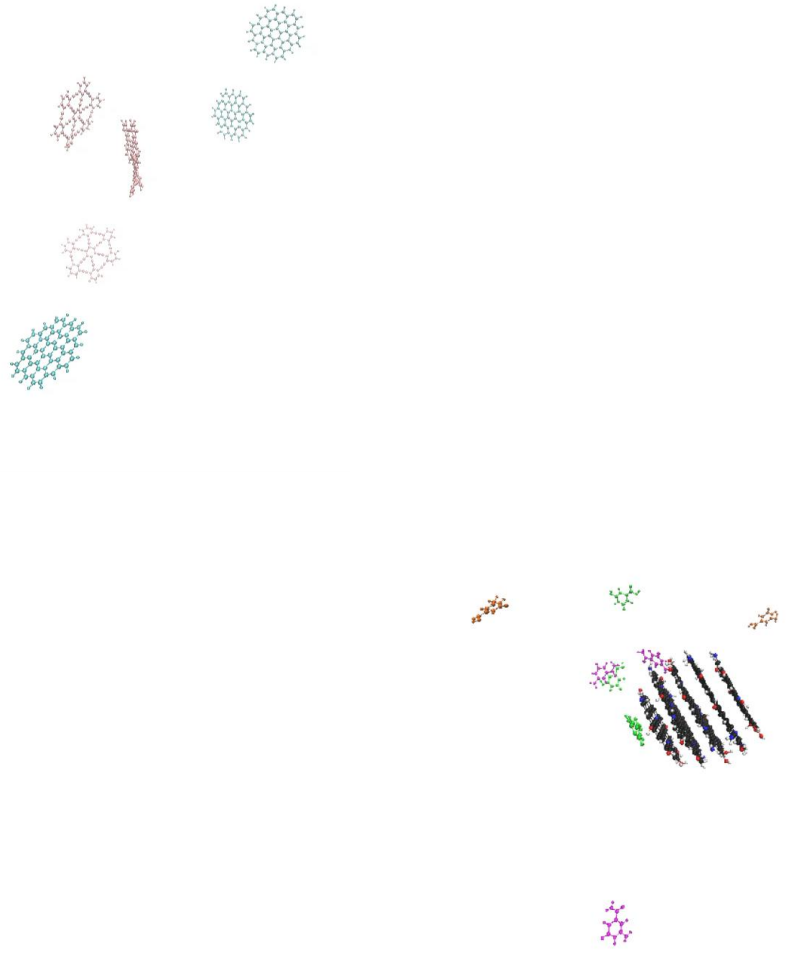




N-doped Layers

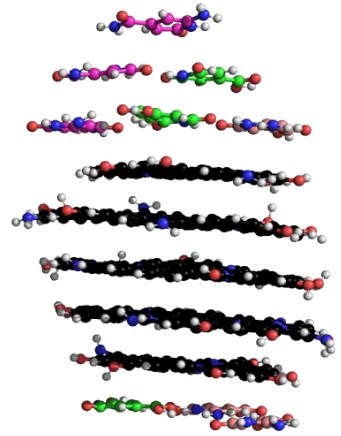
# MD simulations

- Software: GROMACS 2025.1 (mixed precision, SYCL/AdaptiveCpp GPU build)
- Cluster: LUMI , small-g partition
- Resources per job: 1 node, 1 GPU, 7 CPU cores
- Parallelization: 1 MPI rank x 7 OpenMP threads, GPU-resident run (non-bonded, most bonded interactions, PME update and constraints on the GPU)
- Simulation time: 4 hours

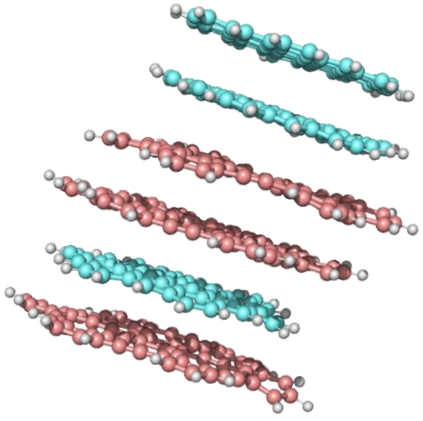


# Conclusions

- No relevant difference between N-doped and undoped CD
- N-doped CD selected as the model system
- Ongoing : CD-fluorophores interaction study



- MD simulations feasible with Graphyne and Graphdiyne
- Systems stabilize once stacking is reached
- Preferential stacking between molecule types: not yet established



# Thank you for your attention