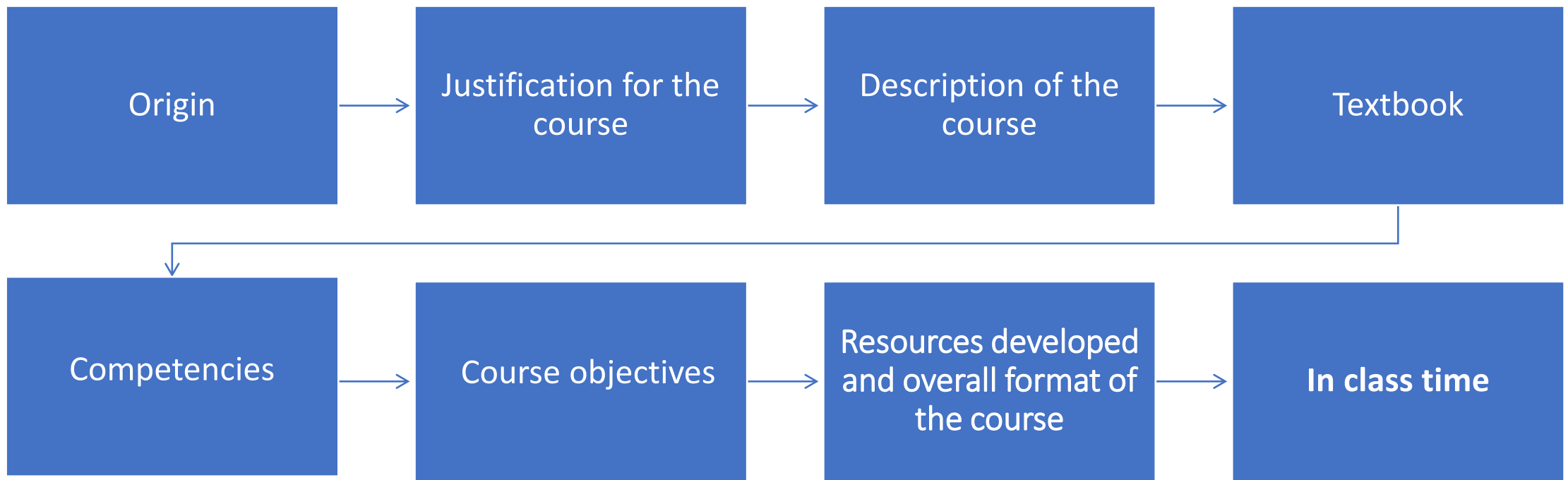




## Computational and Data Science Curriculum Exchange

- The C2Exchange is an NSF-funded pilot project exploring how to create a scalable network of institutions that can collectively offer CDS minors, concentrations, or certificates with minimal investment. Participating institutions are leading the development of one course and providing assistance to other institutions offering the course.
- Year 1: September 2018 – August 2019
  - Prepared Introduction to Modeling & Simulation and Introduction to Computational Chemistry and Molecular Modeling for blended delivery.
- Year 2: September 2019 – August 2020
  - Offered Introduction to Modeling & Simulation and at University of Puerto Rico at Mayaguez as an undergraduate course and at Southern University A & M as an upper-level special topics course
  - Offered Introduction to Computational Chemistry and Molecular Modeling at Clark Atlanta and Bethune Cookman University incorporated modules into a Physical Chemistry course
  - Prepared Computational Linear Algebra and Transdisciplinary Visualization for blended delivery.
  - Drafted a Memorandum of Understanding for C2Exchange membership.
  - Evaluation collected data and feedback from participating faculty. Sharing expertise and access to computational resources via XSEDE were identified a highly valuable. Participants found value significant value in participating.
  - Unexpected outcome – participating faculty assisted their campuses with the shift to online Spring 2020 in response to COVID-19.
  - Lesson learned - How institutions incorporate courses varies to ensure the courses are offered for credit. This has included initially offering as special topics, using an existing course, or only using selected modules as a pathway to adding the course to the catalogue.
- Year 3: September 2020 – August 2021
  - Offer all four courses and complete the evaluation.
  - Complete the development of the Memorandum of Understanding and governance structure for expansion to additional institutions.

# Experiences creating and implementing an introductory course in modeling, simulation, and computation.





# Identifying Opportunities and Needs for Science Gateways in Education at Minority Serving Institutions

**Dr. Dinadayalane Tandabany (Dina)**

**Associate Professor of Chemistry**

**XSEDE Campus Champion**

**Clark Atlanta University**

**Atlanta, GA**

**Acknowledgements: NSF Grants 1623287; 1829717**



**Presentation to Bird of Feathers session at PEARC20 conference on July 28, 2020**

# Supercomputers & Current Research

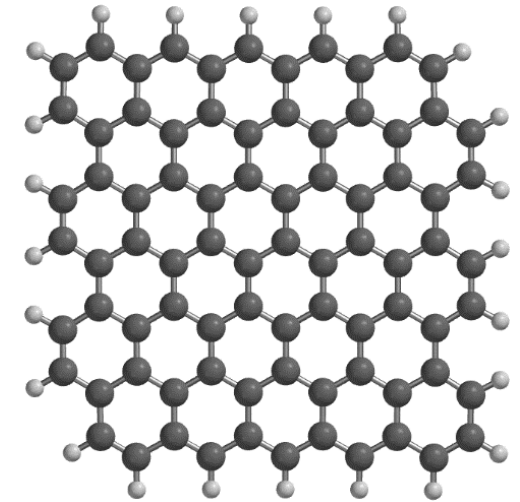
## XSEDE (Extreme Science and Engineering Discovery Environment)

- **Bridges** – Pittsburgh Supercomputing Center (PSC)
  - Petascale resource for empowering diverse communities by bringing together HPC, AI and Big Data
  - Regular, Large, and Extreme Shared Memory nodes – 128GB, 3TB, and 12TB memory
  - GPU nodes – Tesla K80 and P100 GPUs, 128GB RAM each
- **Comet** – San Diego Supercomputer Center (SDSC)
  - Standard Compute nodes – 128 GB memory and 24 cores
  - Large Memory nodes – 1.5 TB memory and 64 cores
  - GPU nodes - NVIDIA K80 and P100 GPUs



## Current Research

- DFT and QM Modeling of Nanomaterials
- Machine Learning



## My Research Group

- 5 Graduate Students (Ph.D. and M.S.)
- 3-4 Undergraduate Students

**XSEDE resources are used by other research groups**

- **Three** other research groups use XSEDE supercomputers

**Physics** – 2 faculty and **Chemistry** – 1 faculty

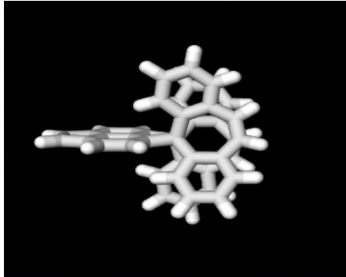
- Web Portal Interface & Desktop Client
- Simplifies access to HPC resources on behalf of a wide variety of research communities and broad Science and Engineering domains
- In operation since 2005, serves more than 600 scientists and students under 320 projects
- **Easy job submission and project file management**
- Built in molecular editors and input file creation – Desktop Client
- **Student experience:**
  - Easily accessible – **one stop dashboard** to handle multiple applications, projects, allocations, and compute resources – Highly Recommended

- SEAGrid Data Catalog
  - Easy viewing of initial job collection, summary, metadata, and visualization

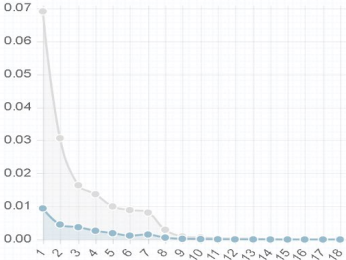
SEAGrid Data Catalog Search Directory Browser

*N.B: This data is automatically extracted using set of configured parser and may contain errors. Please report any issues in the issue tracker*

Calculation	
Package	Gaussian 09, Revision E.01
Calculation Type	F0pt; Freq
Methods	RB3LYP; RB3LYP
Basis Set	6-31G(d,p)
Number of Basis Functions	760
Number of Molecular Orbitals in the Calculation	760
Keywords	# RB3LYP/6-31G(d,p) GFInput GFPrint lop(6/7=3) Opt Freq; #NGeom=AllCheck Guess=TCheck SCRF=Check Test GenChk RB3LYP/6-31G(d,p) Freq
Job Status	CalcDone
Calculated Properties	
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Dipole (debye)	-0.0328227,-0.1402467,0.0158595
HF (au)	-1616.0971637
Homos	138
Homo Eigenvalue (ev)	-5.340506429913
Homo Eigenvalues (ev)	Homo - 1 : -5.3832283044415, Homo - 2 : -5.78514046163, Homo - 3 : -5.8621486813215, Homo - 4 : -6.3320893011349995, Homo - 5 : -6.3739948341120005, Homo - 6 : -6.556311113946999, Homo - 7 : -6.667333564951, Homo - 8 : -6.744613898493, Homo - 9 : -6.965570345099,



Final Molecular Structure



Gradient vs Iteration