

Liu Group Database Website Plans

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Link to this Google Doc (“Liu Group Database Website Plans”):

https://docs.google.com/document/d/18N7HasQ_jVM7JYmAk5Ua3-3R2ZhmTneQYEx8KQuaTw4/edit?usp=sharing

Instructions To Set Up Local Build From GitHub

For /aidamwebsite:

- connect to aidamwebsite repo using github (whatever your method) to run locally
- open the local repo folder in your IDE

1. TO ONLY CONNECT TO TW CSS WITHOUT DATABASE CONNECTION AND UPDATE TW CSS CONTINUALLY:

Tailwind Commands

```
npx tailwindcss -o ./dist/output.css --watch
```

send that in website directory to terminal and it will constantly update the css

after you install it the first time you can just run

```
browser-sync start --server --files "**/*.*"
```

2. TO CONNECT TO DB AND LAUNCH WEBSITE:

in one terminal: `node connect_to_db.js`

in new terminal: `browser-sync start --server --files "**/*.*"`

For /research and /research-app:

Max Github setup instructions:

Bruce: necessary packages for github

1. Python (python.exe): [Download Python | Python.org](https://www.python.org/downloads/)

2. Pandas: `python -m pip install pandas`

3. Matplotlib: `python -m pip install matplotlib`

- connect to research repo using github (whatever your method)
- then in a separate folder, connect to research-app repo
- then put research-app repo in original research repo folder
- then open a terminal and cd into research-app
 - `cd research-app`
 - `npm i`
 - `npm run dev`
- then open a new terminal window and cd into research-backend
 - `cd research-backend`
 - `npm i`
 - `npm install -g nodemon`

- nodemon server.js or node server.js or nodemon.cmd server.js or node server.js
- then go back to research-app and click local host link. Should launch website in your browser
- helpful link:
<https://thinkster.io/tutorials/node-json-api/initializing-a-starter-node-project>

Future Plan

Focus

- Ashley - continue to test breakpoints for CSS adjustments on different screen sizes
- Ashley - add pictures for three tools on home page
- Ashley - look through Preline (tailwind) to add pre-coded Tailwind to make site look better
- Max - Make interface for xyz file generation
 - add two options - one to only count and one to save files
- Max - Get GitHub Pages to use database API for live site or host somewhere else
- Justin - save generated files to database
- Justin - make it easier to send xyz and other info files to HiPerGator
- combine generation project and main website

GitHub Repository

Link to current GitHub repository:

<https://github.com/Liu-Group-UF/adaimwebsite/tree/ashleySeptUpdate>

<https://github.com/Liu-Group-UF/research>

<https://github.com/Liu-Group-UF/research-app>

Note: /website is archived and no longer current

Link to live site (GitHub Pages):

CURRENTLY DISCONTINUED

RUN LOCALLY USING COMMAND LINE NOW

<https://research-database.github.io/website/>

Visualization Progress

JSmol DISCONTINUED (Ashley)

- <https://www.youtube.com/watch?v=slr-aeRCXPI>
- ^ tutorial that shows how to insert JSmol window into webpage, uses 1AHO protein from <https://www.rcsb.org/structure/1AHO>
- [Jmol: an open-source Java viewer for chemical structures in 3D](#)
- https://books.google.com/books?id=59kQFyfsJMC&pg=PA13&source=gbp_toc_r&cad=3#v=onepage&q&f=false
- [Jmol wiki](#)
- <https://jmol.sourceforge.net/demo/jssample0.html>

3Dmol DISCONTINUED (Ashley)

- link to example molecules is active on website
- currently working on using data from database to visualize molecules with 3Dmol
- [3Dmol.js Documentation Embedding a 3Dmol Viewer](#)
- [3Dmol.js Documentation Home](#)
- [molSimplify Lite](#)
- [3Dmol.js FAQ](#)
- [8FLT](#)
- [1AHO](#)
- discontinued; see ChemDoodle

ChemDoodle (Liu, Ashley)

- Initiated
- [ChemDoodle 3D | Molecular Modeling and Graphics Software](#)
- search visualized
- file upload (xyz) visualized (9/14/23 Ashley)
- Ashley - work on using ChemDoodle molecule visualizer to visualize molecules (completed September)

Python/Upload to Database Progress

- currently planning how this will look and how to do it
- Max - work on using Python files to upload data to database through website (completed August)
- currently making interface for molecule generation

Front-End Progress

- switched from CSS to Tailwind CSS
- in process of converting CSS to Tailwind
- in process of integrating files to make the CSS cohesive
- [Tailwind CSS Progress | Preline UI, crafted with Tailwind CSS](#)
- [Tailwind CSS - Rapidly build modern websites without ever leaving your HTML.](#)

Tailwind Notes

Oct13

the % width files and % height files aren't in output.css

h-1/4, w-2/12, ect

the rem widths like h-8 do work though

the bg-color class doesn't work. I checked it and it seems like it should work though; it is in the stylesheet.

get tailwind command to run it

Oct26

Tailwind Commands

`npx tailwindcss -o ./dist/output.css --watch`

send that in website directory to terminal and it will constantly update the css

after you install it the first time you can just run

`browser-sync start --server --files "**/*.*"`

`node connect_to_db.js`

`start index.html`

<https://www.rapidtables.com/web/tools/window-size.html>

browser window size getter

Spring 2023 Semester Project Log

- 4/4/23 - made website plan, website design, and liu-group-database-website GitHub repository, went over database with Justin and got sample database to help with Molecule class
- 4/6/23 - shared website plan Google Doc and GitHub with Cath
- 4/10/23 - learned more about HTML, started search page, created SearchTableMolecule class in search_page.js, pushed changes to GitHub repository
- 4/11/23 - learned more about HTML, added logo image and molecules image to header and main page. Still need to learn size formatting.
- 4/16/23 - learned more about HTML, made header format better, made images format better on index.html, made table on search.html, tried to connect js file to search.html but still figuring it out; something with document.querySelector needs to be fixed
- 4/18/23 - fixed js to html connection, table now loads in values from SearchTableMolecule class objects
- 4/22/23 - set up GitHub pages so website is viewable
- 4/25/23 - downloaded Jmol and JSmol and read through website and wiki
- 4/26/23 - added Jmol and JSmol to website folder and followed tutorial to visualize a protein using .pdb file format. Changed GitHub Pages to deploy from master branch. Reorganized directories and made sure jmol had no untracked files. Added a test of jmol from jsmol folder, and is working. Updated site header (HTML and CSS) and added favicon. Changed some colors.
- 4/28/23 - visualized two molecules using 3Dmol.js. made header and image layout on main page more mobile-friendly, still working on adjusting layout to different screen sizes.

Summer 2023 Semester Project Log

- May - project meeting; introduced Tailwind, combined files
- June - project meeting
- August - project meeting
- August - Max finished GUI for molecule generation python file

Fall 2023 Semester Project Log

- 9/14/23 - Ashley finished visualization page for uploaded xyz file
- 9/15/23 - project meeting; future planning; updates
- 11/16/23 - project meeting;
 - Max has made molecule generator and added a count function to see how many molecules can be generated with the given properties. Also has made frontend for that to select the properties, then run the python script;
 - Ashley has converted index.html to tailwind css and added some frontend design features to the main page of the website. Designed two graphics in Canva. Added JS API where when you scroll, toggles classes on or off to change color or reveal an image.

Spring 2024 Semester Project Log

- 1/25/24 - Ashley mostly converted from css to tailwind css. The database page still needs to be converted to tailwind css. The header and footers are injected with javascript. Dropdown menu completed. Header completed.

RGB Image Values



light grey - rgb(145, 145, 145)

white - rgb(255, 255, 255)

gold letters - rgb(228, 187, 96)

gold ball - rgb(224, 181, 90)

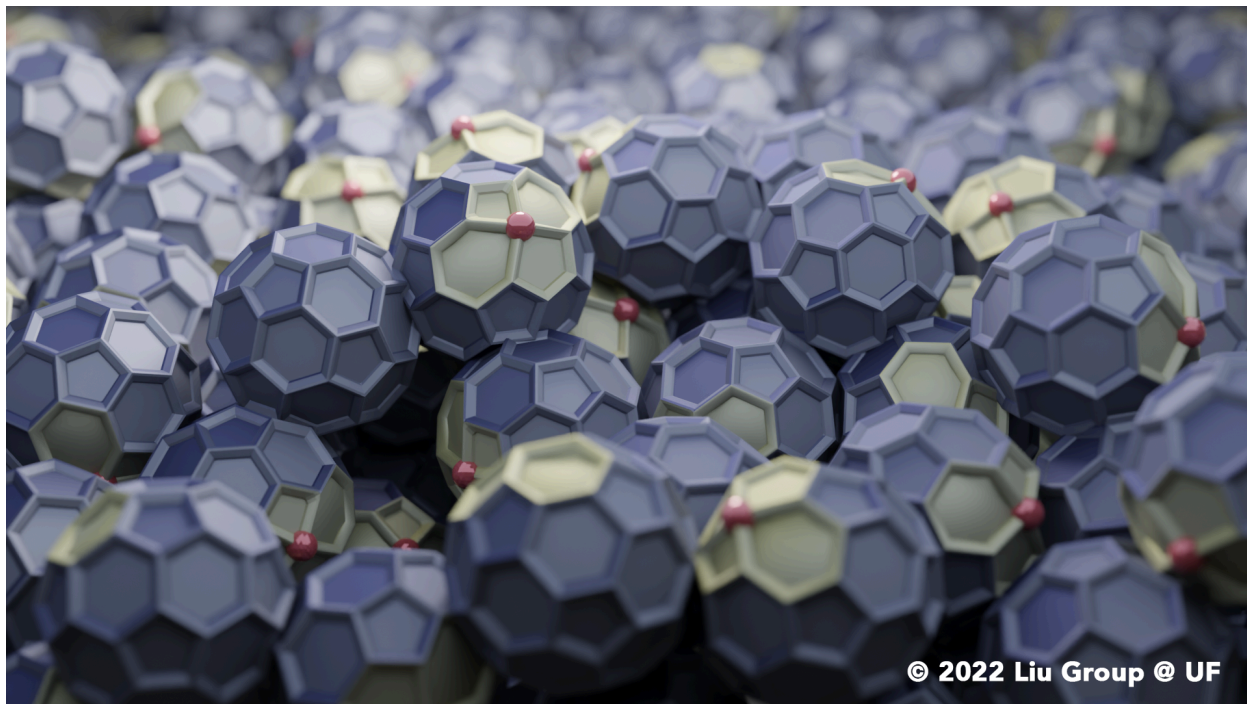
gold ball highlight - rgb(255, 252, 149)

gold ball shadow - rgb(207, 167, 82)

black - rgb(49, 49, 49)

black highlight - rgb(90, 90, 90)

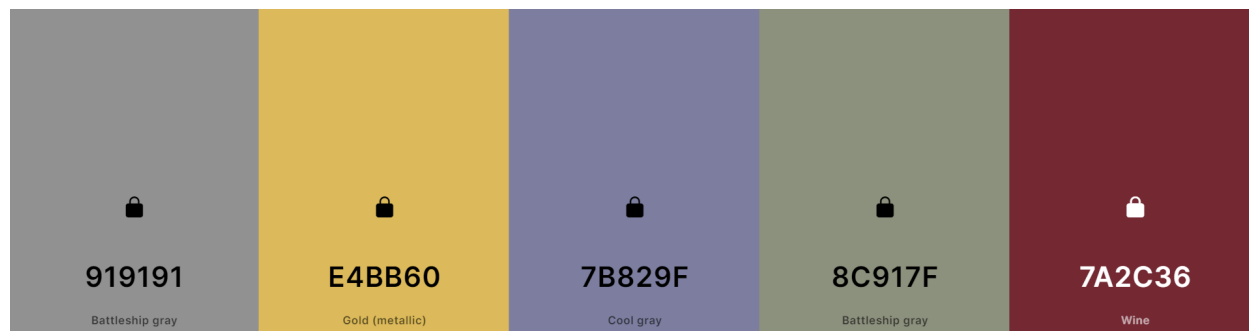
ball light black behind - rgb(108, 108, 108)



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blue - rgb(123, 130, 159)
 blue shadow - rgb(58, 64, 84)
 green - rgb(140, 145, 127)
 red - rgb(98, 44, 54)

COLOR PALLET:



light grey - rgb(145, 145, 145)
 gold letters - rgb(228, 187, 96)
 blue - rgb(123, 130, 159)
 green - rgb(140, 145, 127)
 red - rgb(122G, 44, 54)

Website Design

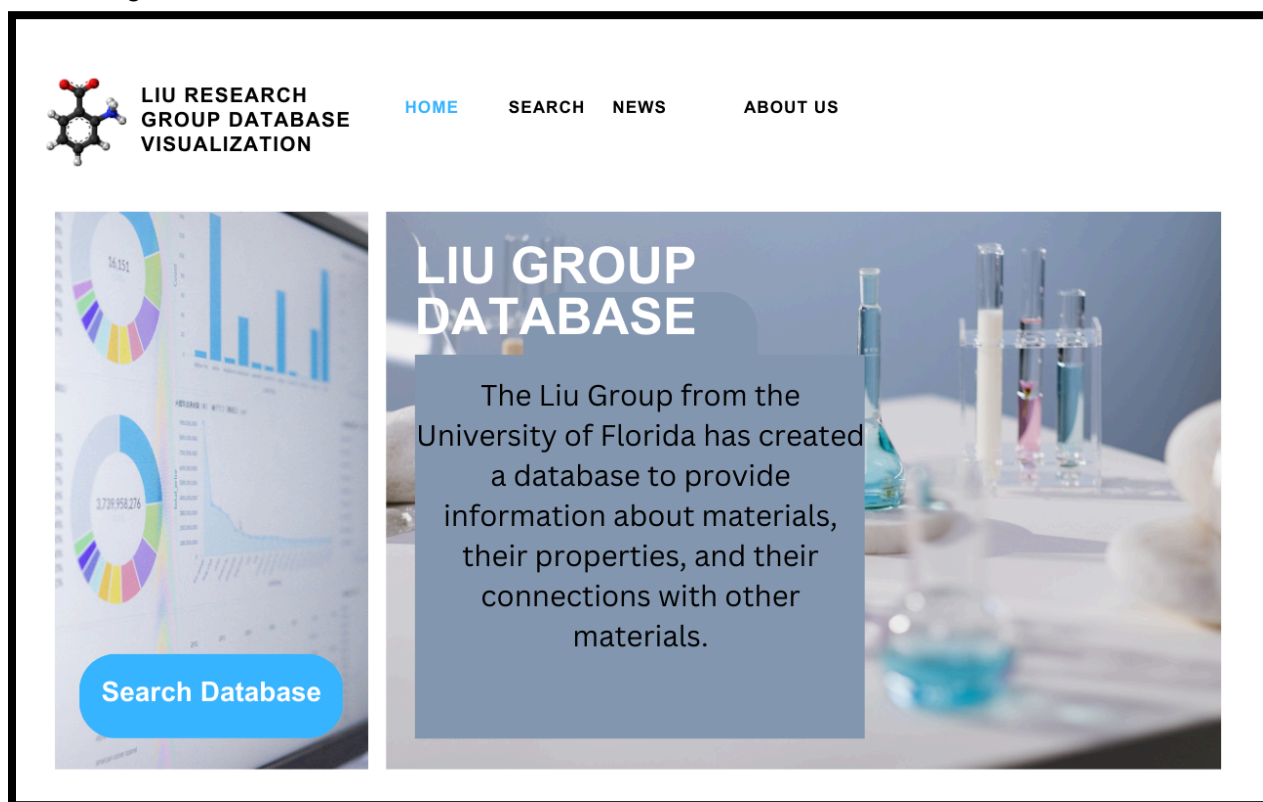
- designed on Canva
- Important Pages
 - Home page
 - Search page
 - Material page

Canva link:

https://www.canva.com/design/DAFfGiHvv44/TIAh7bHdcN3T1YiV5wT51A/view?utm_content=DAFfGiHvv44&utm_campaign=celebratory_first_publish&utm_medium=link&utm_source=celebratory_first_publish

Canva images:

Home Page



MORE INFORMATION

Paragraph with more information

sdglajsd'gj

;lsk;lsd;sldkg;

sld;g;askg

slg

dsgs

dg

g

sdg

sdg

ABOUT

Liu Research Group from UF
link to liu.chem.ufl.edu

SITE NAVIGATION

[Home](#)
[Search](#)

[News](#)
[About Us](#)

Search Page



LIU RESEARCH
GROUP DATABASE
VISUALIZATION

[HOME](#)

[SEARCH](#)

[NEWS](#)

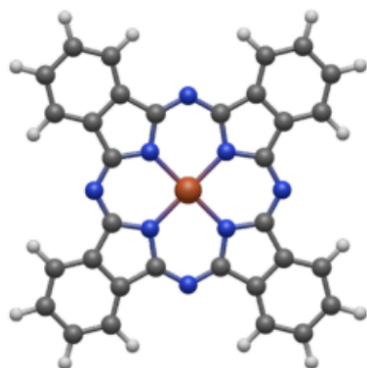
[ABOUT US](#)

Filters/Parameters

Material	Number of Atoms	Number of Vacancies



Iron(II) phthalocyanine



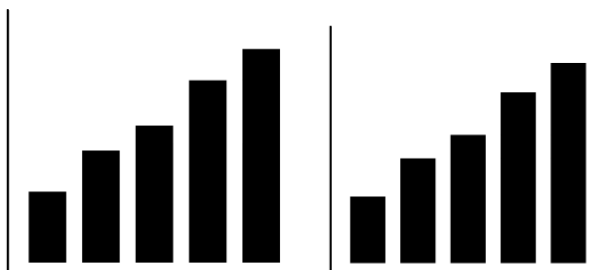
FePc

Main Properties

asjgdlksdjgksdasdgggggggggggggg

dsaklgjlsjgkdsdgggggggggggggggg

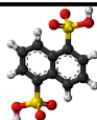
slkdjlsdjgsldagsgdddddgggggg



Subproperties/Graphs

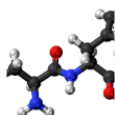
Related Materials

Filters/Parameters



Name

related properties...



Name

related properties...

Material View Page

- takes here when click on “view” in search page
- opens in new tab

Potentially Helpful Resources

Research

[Materials Project - Home](#)

[Read and Write with the Data API — MongoDB Atlas](#)

[How to connect MongoDB with ReactJS ? - GeeksforGeeks](#)

[How To Use MERN Stack: A Complete Guide | MongoDB](#)

[Liu Group Database Website Plans - Google Docs](#)

[Metal Organic Framework Database | Mofs](#)

[Jmol: an open-source Java viewer for chemical structures in 3D](#)

[How to Use Jmol to Study and Present Molecular Structures - Angel Herráez - Google Books](#)

[Jmol wiki](#)

[JSmol simple example](#)

[FileZilla - The free FTP solution](#)

[3Dmol.js Documentation Embedding a 3Dmol Viewer](#)

[3Dmol.js Documentation Home](#)

[3Dmol.js FAQ](#)

[8FLT](#)

[1AHO](#)

[mongodb - npm](#)

[ChemDoodle 3D | Molecular Modeling and Graphics Software](#)

[Tailwind CSS Progress | Preline UI, crafted with Tailwind CSS](#)

[Tailwind CSS - Rapidly build modern websites without ever leaving your HTML.](#)

[Oh My Zsh - a delightful & open source framework for Zsh](#)

[Website Research Meeting 5/27 Notes - Google Docs](#)

[Liu Group AIDAM Database](#)

[Frequently Asked Questions – UF CUR](#)

[Replace line breaks with \n](#)

[ChemDoodle Web Components | Tutorial > Loading Data](#)

[Research Visualization Notes August 31, 2023 - Google Docs](#)

[research-database/website at ashleySeptUpdate](#)

[FileReader: readAsText\(\) method - Web APIs | MDN](#)

[How to read a local text file using JavaScript? - GeeksforGeeks](#)

[Using files from web applications - Web APIs | MDN](#)

[Tailwind CSS LL Notes/Files](#)

[Cursor - The AI-first Code Editor](#)

[GitHub Desktop | Simple collaboration from your desktop](#)

[What is my browser window size](#)