Creating a browser-based version of VTAnDeM

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BACKGROUND

- DFT (Density functional theory) calculations made to get more information about the properties of materials
- Calculations made with VASP (Vienna Ab initio Simulation Package)
- Post-processing done for calculations to be useful
- VTAnDeM - The Visualization Toolkit for Analyzing Defects in Materials
  - Python based
  - Desktop application
  - Primarily used to analyze ternary and quaternary compounds
- Functions of VTAnDeM:
  - Uploading data (Element, compound, defect, DOS data)
  - Generating phase diagrams, defect diagrams, and carrier concentration diagrams
  - Generating 3D phase diagrams, with 2D projected phase diagrams in the chemical potential space
  - Generating 3D phase diagrams in composition space
  - Saving all diagrams as PNG files
  - Adjusting parameters of diagrams
- Cons of VTAnDeM:
  - No capabilities to share data w/ others
  - May not be supported by all computers
- Alternative VTAnDeM-like software would be useful if it
  - Makes sharing data easy and automatic
  - Allows anyone with access to a web browser to use it
- Idea of a browser-based version of VTAnDeM was proposed and created

METHOD

1. Obtain detailed understanding of code base
2. Explore, learn, and choose infrastructure
   1. Web frameworks (Django, Flask)
   2. Database services (MySQL, PostgreSQL, MongoDB, Neo4J)
   3. Hosting services (Heroku, Amazon AWS)
   4. Version control (Github)
3. Isolate all non-GUI code into stand-alone Python scripts that can be run without relying on any user inputs
4. Testing
5. Deployment

RESULTS

Majority of features PyQT5-based version of VTAnDeM provides have been migrated over to browser-based version of VTAnDeM (see pictures below)

Significance:
- Gives anyone with access to web-browser, the same capability to perform post-processing on DFT data as someone who has PyQT5 based version of VTAnDeM
- Encourages international scientists to share data by making it easier to share data

FUTURE WORK

- Making graphs interactive and dynamic (Ex: adding sliders to the graphs, allowing users to zoom in to all phase diagram plots, allowing users to change which elements are used to plot/create phase diagrams for compounds, etc.)
- Redeployment of updated codebase to Heroku
- Setting up AWS S3 file system storage to prevent the deletion of uploaded data (Heroku file storage is ephemeral)
- Adding authentication (to restrict website/database access to only those who have proper credentials such as an @illinois.edu email)
- More detailed testing of all functionality

REFERENCES

Michael Toriyama’s VTAnDeM Paper (Available upon request)
Youtube links about Django deployment to Heroku
https://www.youtube.com/watch?v=6DI_7Zja8Zc
https://www.youtube.com/watch?v=kBwhtEIXGII
Django documentation:
https://docs.djangoproject.com/en/3.0/

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