SONOMA STATE UNIVERSITY | School of Science and Technology

Chem Compute Science Gateway for Undergraduates

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About Sonoma State University

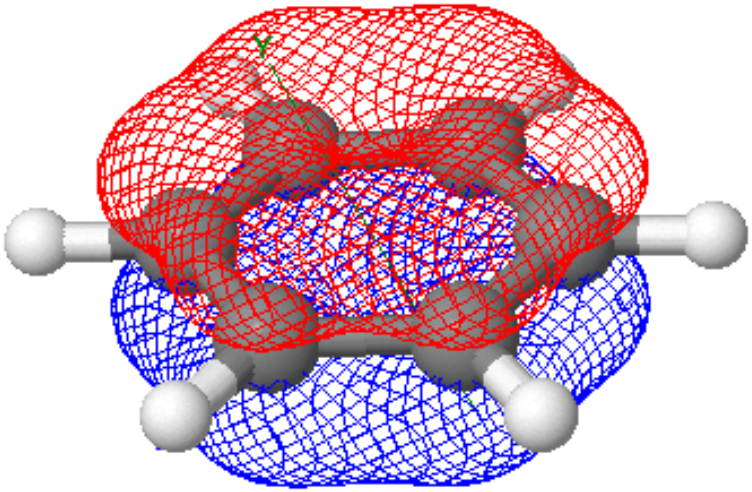
- One of 23 California State Universities

- PUI (Primarily Undergraduate University)
- 9,000 Undergraduate, 800 Graduate Students

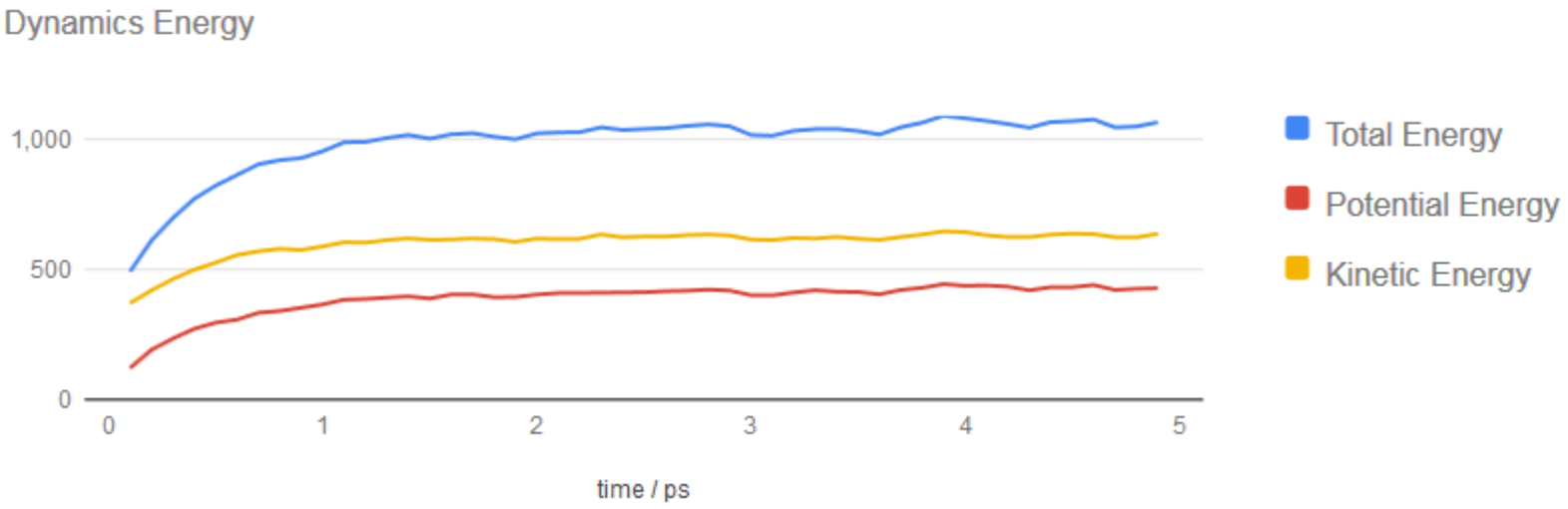
- Little / no resources for computational chemistry

Gateway for Computational Chemistry

Chemcompute.org



- GAMESS (Quantum)
- TINKER (MD)

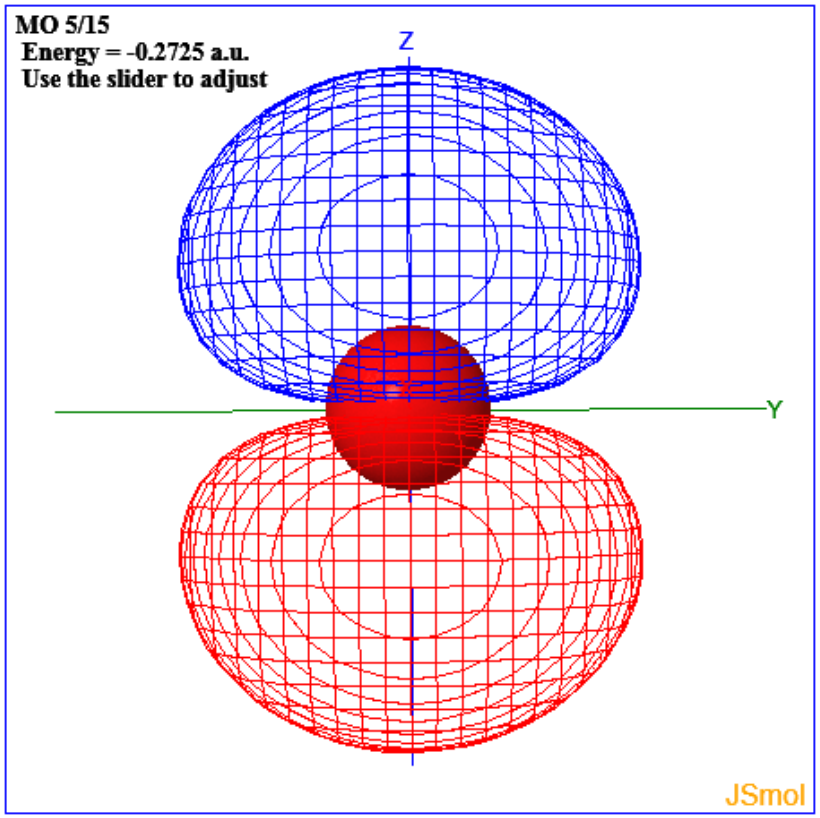


Why a Gateway?

- Solves barriers for computational chemistry
- Accessible from anywhere
  - Personal device in lecture
  - Dorm room (Run jobs before lab!)
  - Other countries
- Familiar to Students
- Easy for Faculty (embedded instructions)

Students respond to visualizations, not equations

$$\psi = \frac{1}{\sqrt{2\pi}} e^{i\phi} \frac{\sqrt{3}}{2} \sin\vartheta \frac{1}{2\sqrt{6}a_o^{3/2}} \frac{r}{a_o} e^{\frac{-r}{2a_o}}$$



Gateway Usage

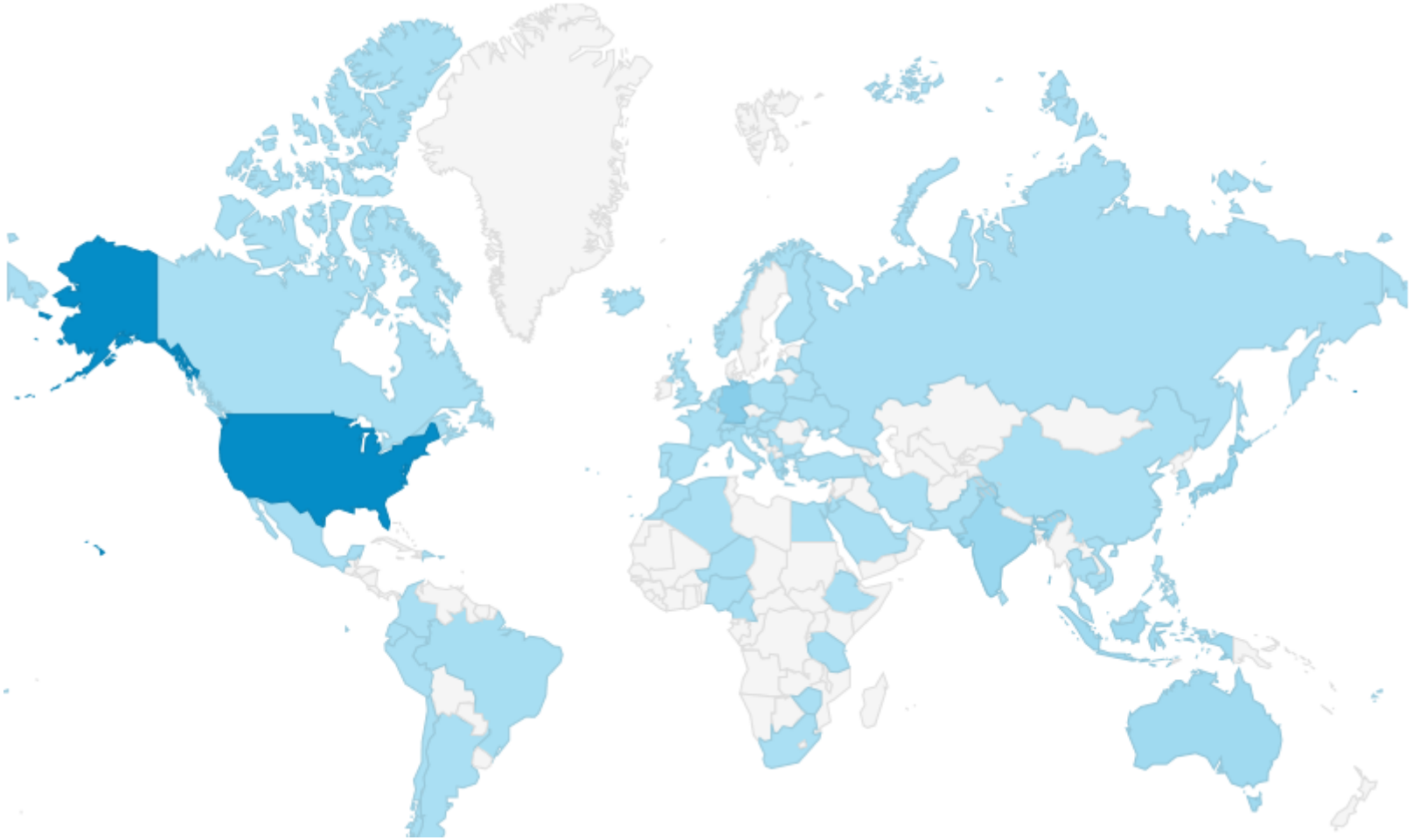
Heaviest usage in late Fall, late Spring

Most jobs run during class time

small, fast jobs: 1 core, 5 – 10 minutes

Minority usage for research (full node)

25,000 Jobs since Fall 2016



Web Framework

- Django (1.10) / Python 3

- Celery (async python task queue)
- RabbitMQ (message queue)

- Mariadb

Barriers to Access at PUI

1. Hardware: XSEDE Network
   - Comet
   - Bridges

   } Long jobs / full node

   - Jetstream Short jobs / 1 core / Guest accounts

     openstack scaling 1 – 6 nodes

     Redundancy: important for scheduled labs

Barriers to Access at PUI

2. Software / Graphical Interface

- Generating input file too much for undergraduates

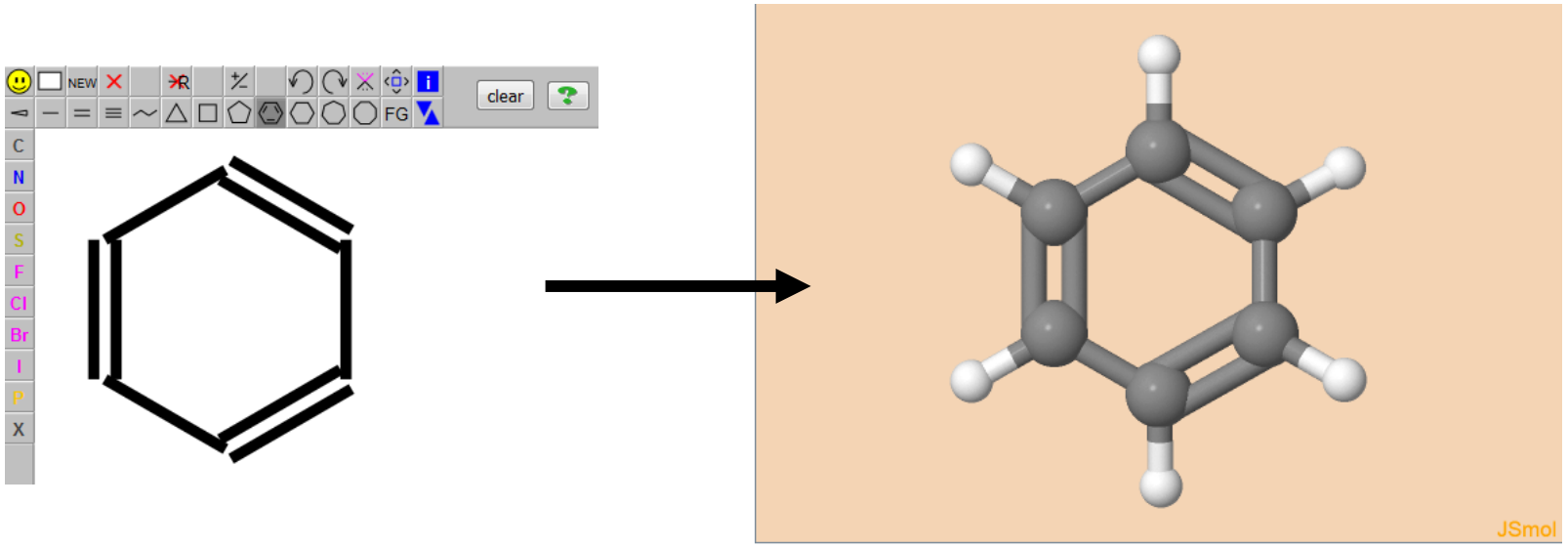
- Typical Run: Compute Molecular Orbitals for benzene (“Where are the electrons?”)

Generate Input File

Draw molecule

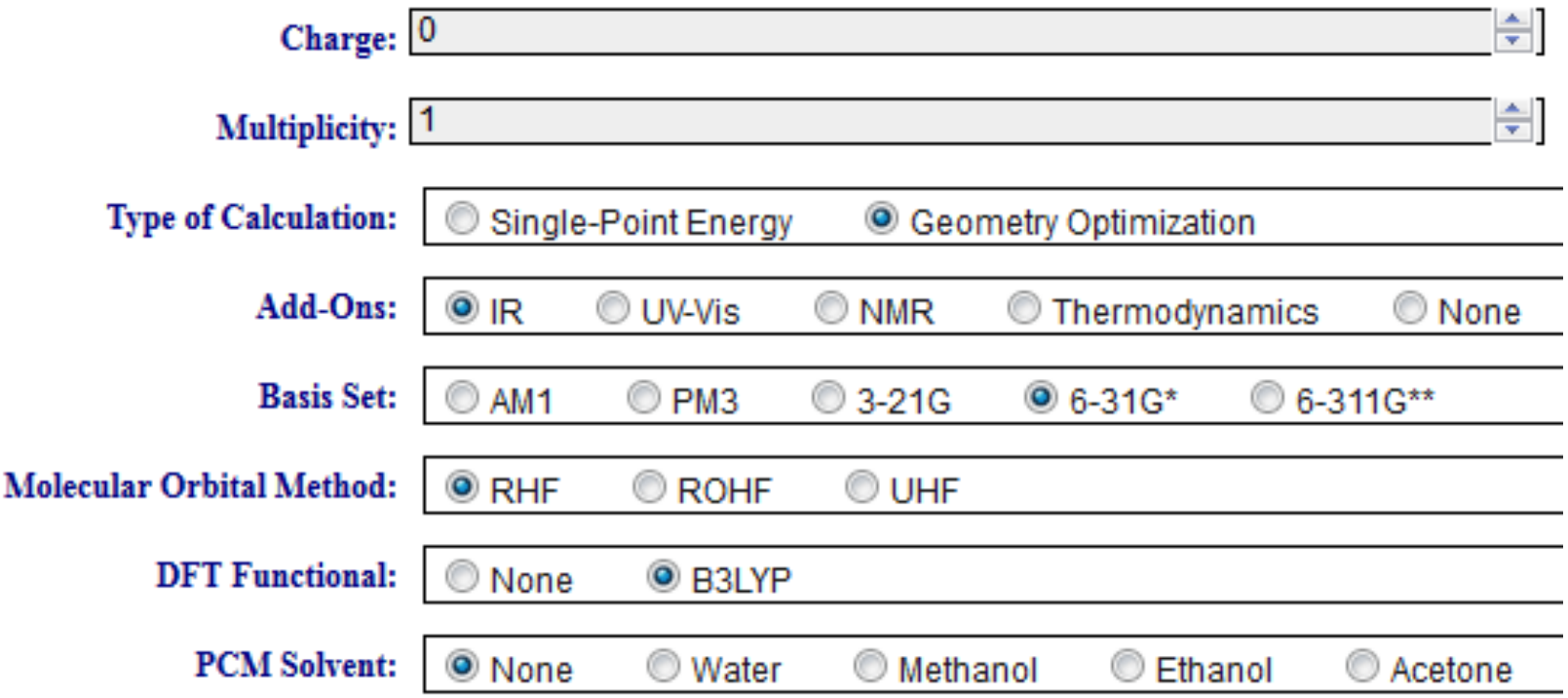
Search database for molecule (PubChem – NIH)

Transfer 2D to 3D



(JSME / DIY molecules / JSmol)

Generate Input File (Work in progress)



(CH5M3D)

Submit Job to Server

Airavata (Python 3 via Thrift)

- Lots of support from team
- Supports many queues
- Just need to write python API calls

- No allocation model
- No intermediate output

Submit Job to Server

SSH

- Fast
- Intermediate output (rsync)

- Write everything yourself
- Multiplexing

Submit Job to Server

Keeping track of jobs:

- Mariadb

- Celery (squeue)
- RabbitMQ (messages for SSH job completion)

- Allocations handled internally in user database

Output

- Undergraduates don’t like to wait
- Resubmit jobs if it takes too long

- Don’t like to read output files

Intermediate Output

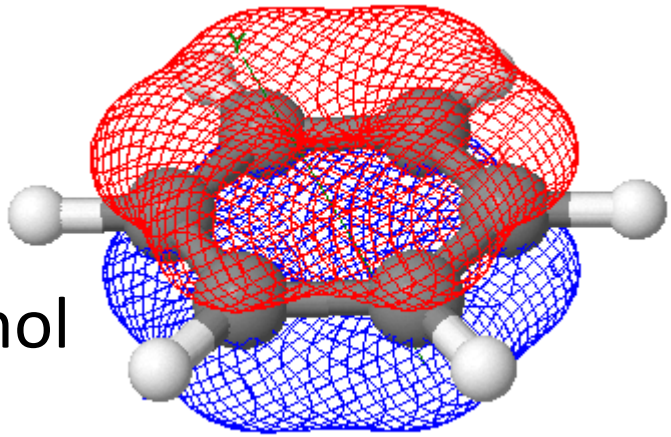
Easiest solution: Helper script on compute node

- Extract atom coordinates
- Transfer coordinates to user

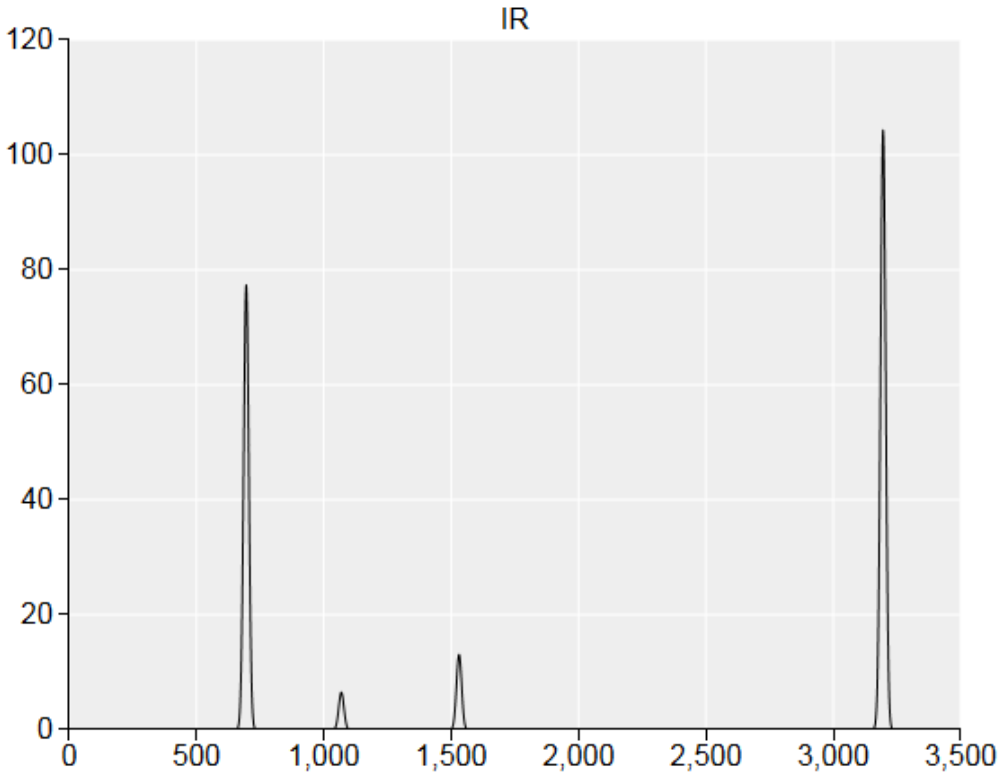
- Download full output when job is finished

Visualization of Output File

JSmol



Do More Calculations	
Dipole Moment	Bond Dipoles
Electrostatic Potential	UV-Vis
Thermo	IR



Cclib / uvspecgen / mpld3 / d3

Suggestions for Common Errors

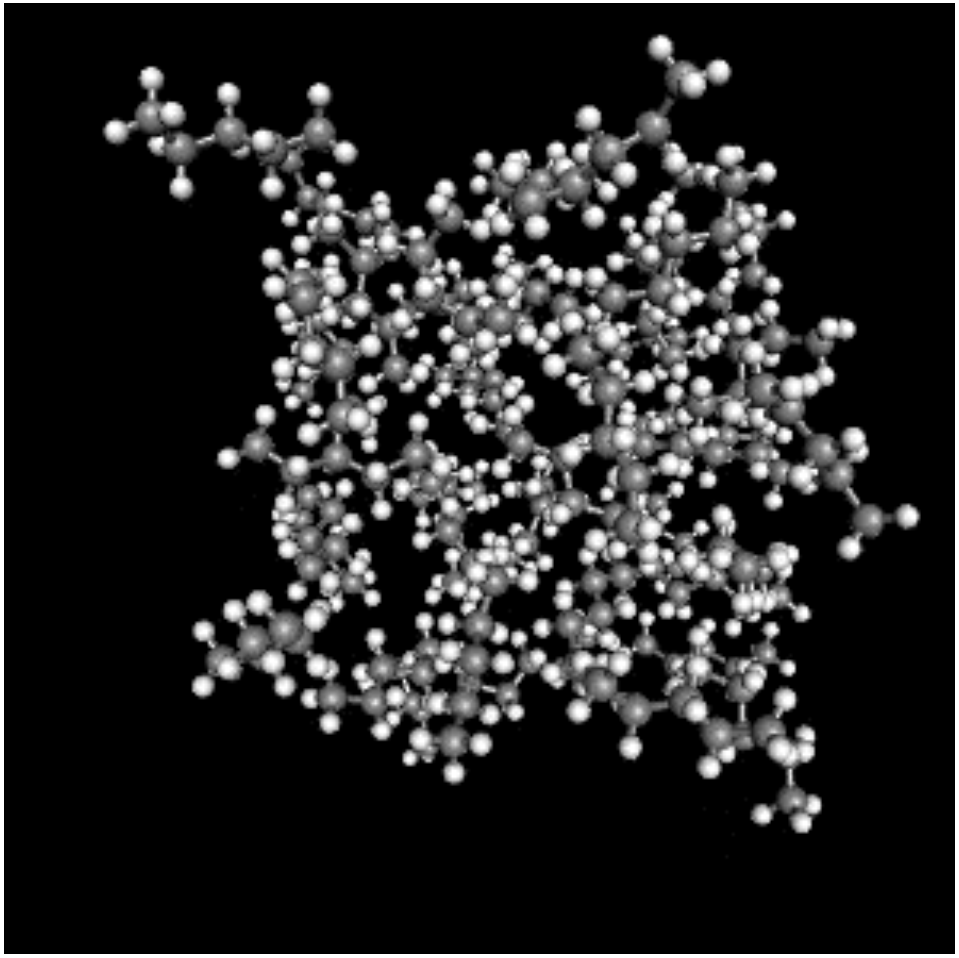
Job 025605 (Jetstream) Error

```
Your molecule's charge or spin multiplicity are not correct

Your molecule has 3 electrons.  You specified charge = 0 and spin
multiplicity = 1
You specified a singlet spin (all paired electrons), but you have an
odd number of electrons
```

Parsed by Django

Visualization of MD Output



Barriers to Access

3. Lab Exercises
   - Few web repositories
   - Instructions specific to software package / version

Chem Compute:

Built-in Experiments

On-screen Instructions

1. Enter a name for your input file, e.g. H2_lastname
2. Set Type of Calculation to: "Geometry Optimization"
3. Set Basis Set to: "6-31G*"
4. Set DFT Functional to "B3LYP"
5. Click "Create input file"
6. Click "Submit Job"

Personal Observations from Class Use

- All students completed experiments
- Students feel comfortable using a website

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- Exposes many misconceptions

Student Comments (P-Chem)

	PRE	POST
I feel confident using computers to solve chemical problems.	2.8	3.8
I felt that the computer lab assignment was engaging		4.4

	2012	2014	2015
In this course, my instructor enables me to participate actively in learning	4.6	4.6	5.0
My instructor stimulates interest in the course	4.2	4.4	4.9

Coming Soon: Use in Summer Gen Chem

Funding

- Appropriate Agency?

- XSEDE Science Gateway TG-CDA170003

- Science Gateways Community Institute
- Extended Developer Support

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