LA-UR-22-21251

Approved for public release; distribution is unlimited.

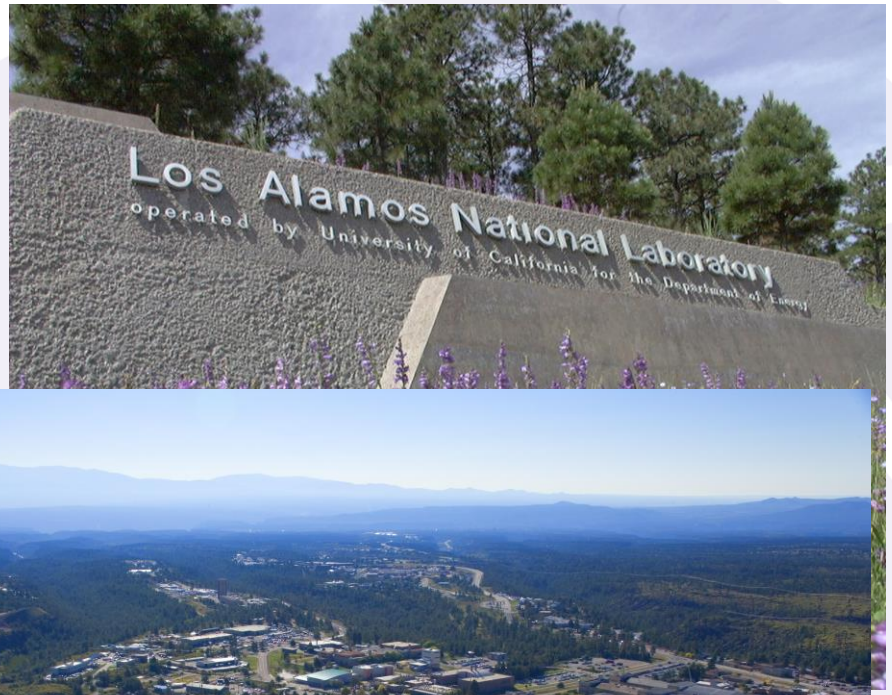
Title:	My path to becoming a DOE scientist
Author(s):	Nebgen, Benjamin Tyler
Intended for:	Presentation to students at my former high school on my career path.
Issued:	2022-02-14

My path to becoming a DOE scientist

Benjamin Nebgen
Physics and Chemistry of Materials (T-1)
Los Alamos National Laboratory (LANL)

2/17/2022

Los Alamos National Laboratory



Office of Science Laboratories

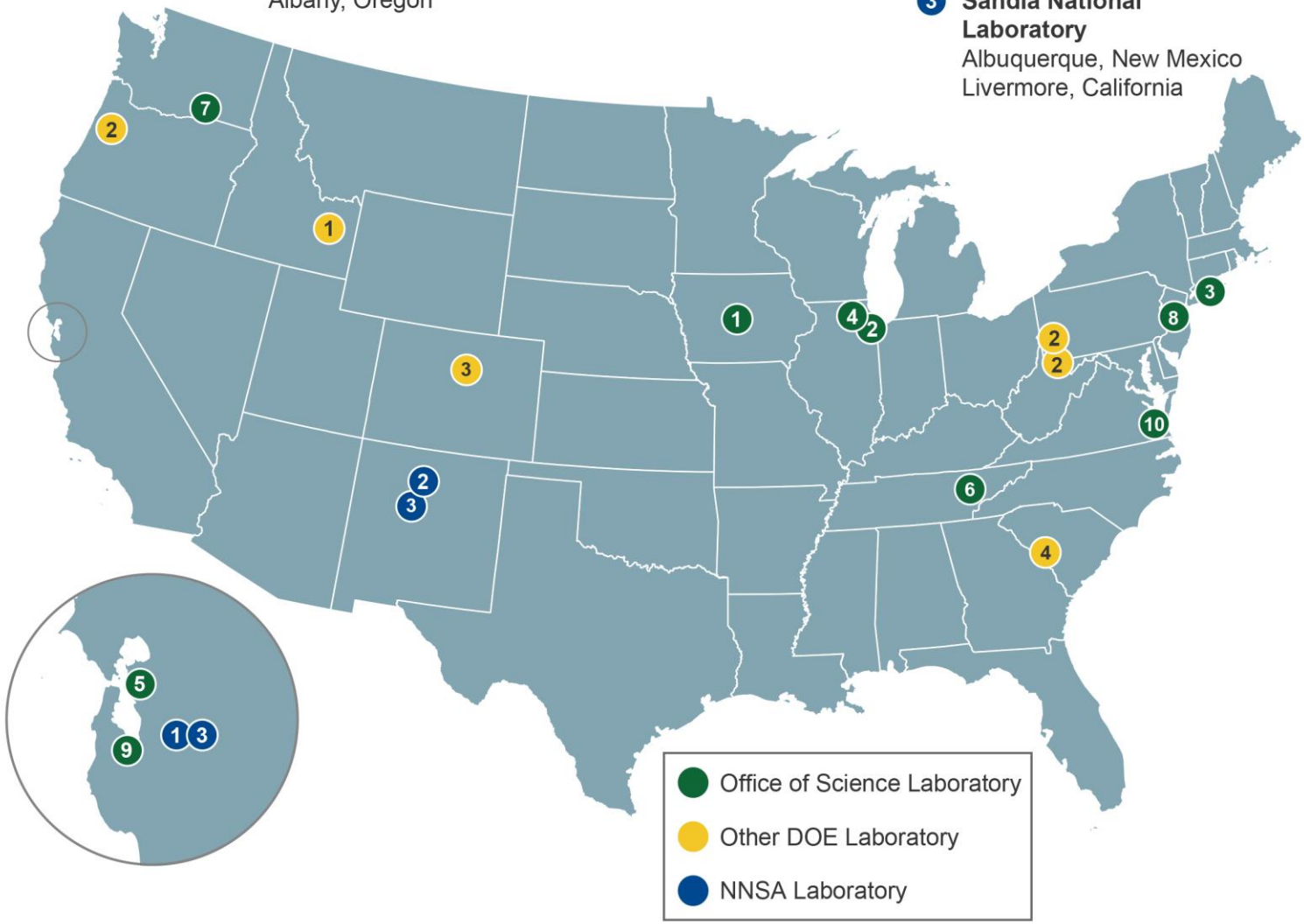
1. **Ames Laboratory**
   Ames, Iowa
2. **Argonne National Laboratory**
   Argonne, Illinois
3. **Brookhaven National Laboratory**
   Upton, New York
4. **Fermi National Accelerator Laboratory**
   Batavia, Illinois
5. **Lawrence Berkeley National Laboratory**
   Berkeley, California
6. **Oak Ridge National Laboratory**
   Oak Ridge, Tennessee
7. **Pacific Northwest National Laboratory**
   Richland, Washington
8. **Princeton Plasma Physics Laboratory**
   Princeton, New Jersey
9. **SLAC National Accelerator Laboratory**
   Menlo Park, California
10. **Thomas Jefferson National Accelerator Facility**
    Newport News, Virginia

Other DOE Laboratories

1. **Idaho National Laboratory**
   Idaho Falls, Idaho
2. **National Energy Technology Laboratory**
   Morgantown, West Virginia
   Pittsburgh, Pennsylvania
   Albany, Oregon
3. **National Renewable Energy Laboratory**
   Golden, Colorado
4. **Savannah River National Laboratory**
   Aiken, South Carolina

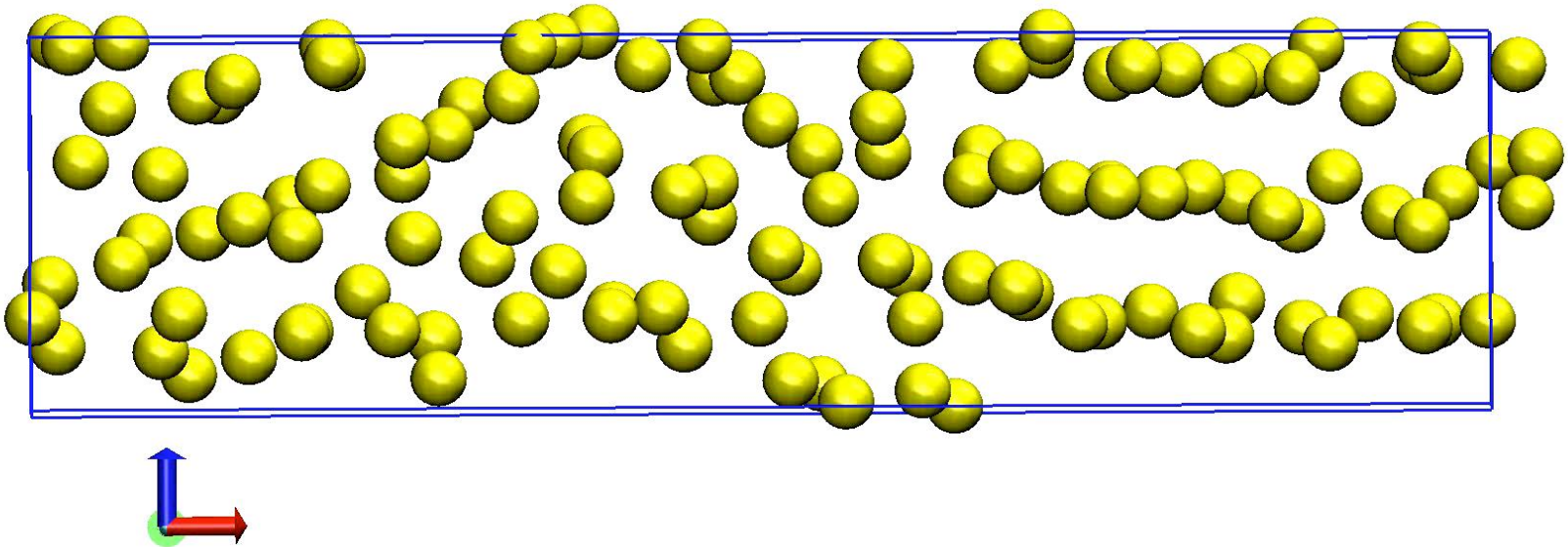
NNSA Laboratories

1. **Lawrence Livermore National Laboratory**
   Livermore, California
2. **Los Alamos National Laboratory**
   Los Alamos, New Mexico
3. **Sandia National Laboratory**
   Albuquerque, New Mexico
   Livermore, California

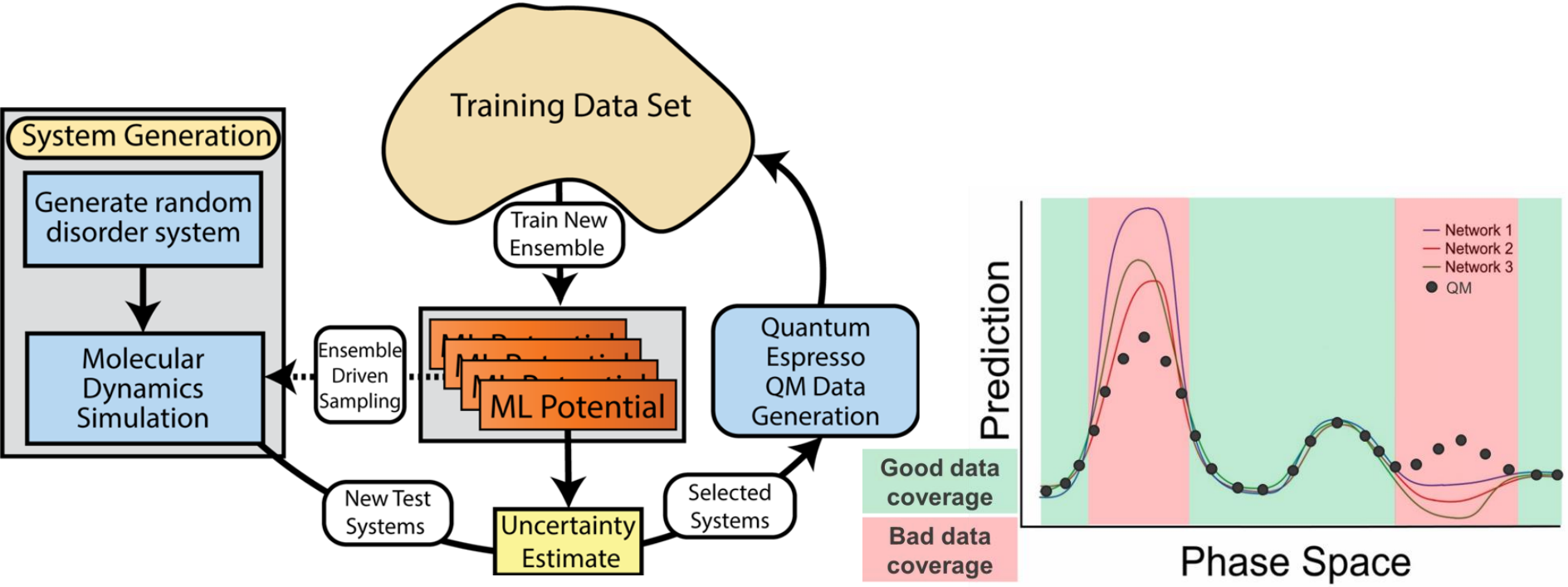


Atom motion controls chemical and material properties

- My job lies at the intersection of Chemistry, Physics, Mathematics, and Computer Science.
- Atomic motion is (mostly) classical, not quantum.
- $E(x_1, y_1, z_1, \ldots, x_n, y_n z_n)$: System energy as a function of nuclear configuration.
- $F = -\nabla E$: Force is the derivative of energy.
- $F = m\,a$: Use Newton's equations to propagate atom positions.
- E depends on how electrons move around atoms.
  - This requires solving Schrödinger equation: $O(N^3)$
  - Alternative: classical force fields
  - New Alternative: machine learning



Active learning allows rapid model construction

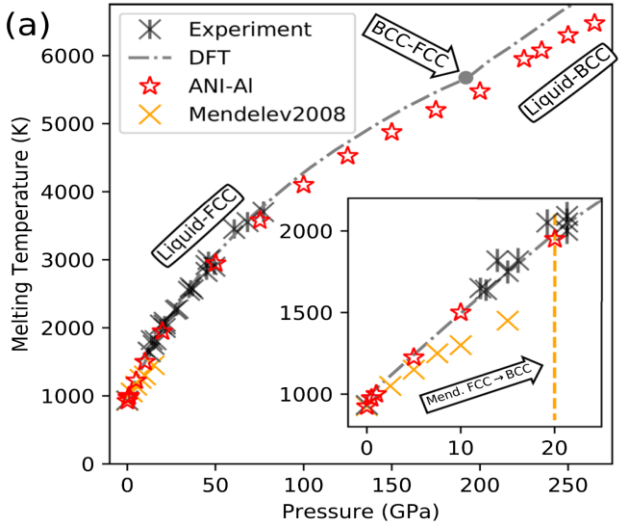


An Active Learning system was developed for the automated exploration of phase space. This system builds a training dataset for a Machine Learned interatomic potential with little to no human intervention.

Using the dataset produced above, a Machine Learned interatomic potential for Aluminum was developed that closely matches experimental properties (right).

Applications using large compute resources

- Use large clusters (Summit 27,648 V100 GPUs) to generate dataset for machine learning.
- Perform large scale dynamics simulations.



Summit (ORNL)

Los Alamos NATIONAL LABORATORY

Travel: Absolutely!

- Encouraged/required to attend 2-3 conferences per year:
  - Telluride, CO
  - Kauai, HA
  - Boston, MA
  - Chicago, IL
- Travel to other DOE locations
  - Argonne National Laboratory
  - Nevada National Security Site
  - Pacific Northwest National Laboratory
  - Lawrence Livermore National Laboratory

Advanced Photon Source
Argonne National Laboratory

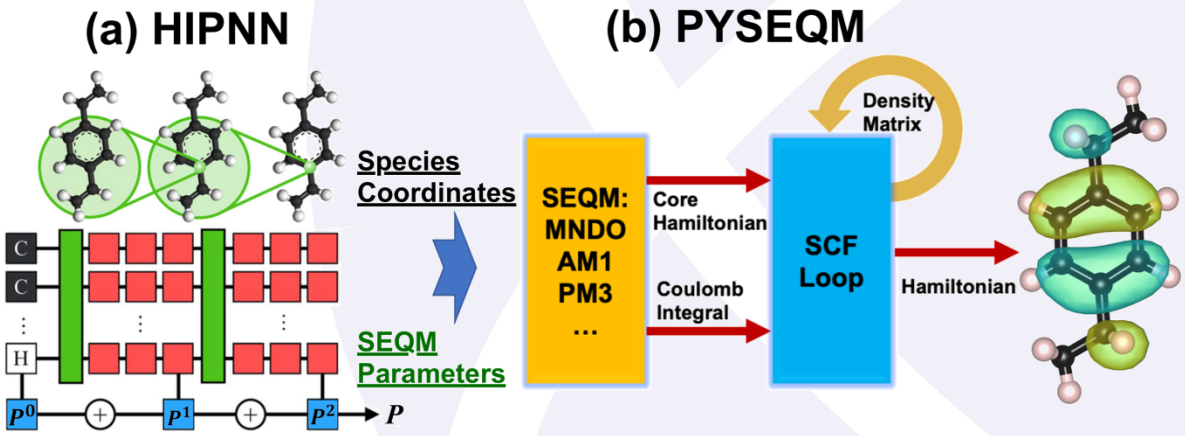
Sedan Crater
Nevada National Security Site

Typical Workday/Workweek

- Work schedule: 9/80
  - Mon-Thurs: 9-hour day
  - Friday: alternating between 8-hour day and day off
- Meetings (2-3 hours per day)
  - Students
  - Post Docs
  - Project meetings
- Proposal writing (1 hour per day)
  - Grant proposals
  - Resource (computer time) proposals
- Paper writing and reviewing (1 hour per day)
- Other paperwork/administrative tasks (1 hour per day)
- Actual technical work (3-4 hours per day)
  - Running simulations
  - Writing code
- Very important to work well with others.
  - Collaborative coding
  - Collaborative proposal writing
  - Managing post-docs and students.

Carrier Highlights

- Principal Investigator (leader) of a 1.6M/per year, 3 year project.
  - Focus on developing advanced machine learned interatomic potentials.
- Member of team given 2021 R&D 100 award.
  - Development of Artificial Intelligence/Tensor Factorization platform.
- Involvement in a variety of publicly available codes:
  - PYSEQM: https://github.com/lanl/PYSEQM
    - Use Pytorch to solve reduced order Hamiltonian models for electron motion in molecules
  - HIPPYNN: https://github.com/lanl/hippynn
    - Machine learned interatomic potential code
  - pyDRESCALk: https://github.com/lanl/pyDRESCALk
    - Code for tensor factorization



Diagrammatic link between HIPPYNN and PYSEQM that allows for machine learned semi-empirical quantum mechanics

Carrier Path

- High School: Rhinelander High School
  - 2002-2006
  - Yes, I had a plan. I wanted to be a Scientist that could solve problems with mathematics and simulation rather than trial and error.
  - Did it change? Not much.
- Undergraduate: Cornell University
  - Chemistry B.A. Magna Cum Laude
  - 2006-2010
- Graduate: Purdue University
  - Theoretical Chemistry Ph.D.
  - 2010-2014
  - $35-45K annual salary
- Post Doctorate: University of Southern California
  - 2015-2016
  - $40-50k annual salary
- Post Doctorate: Los Alamos National Lab
  - 2016-2018
  - $70-80K annual salary
- Staff Scientist: Los Alamos National Lab
  - 2018- current
  - $120K starting

RHINELANDER HIGH SCHOOL

Cornell University

PURDUE UNIVERSITY

USC University of Southern California

High School/College Advice

- High School Classes: AP, college if possible
- Majors I see regularly:
  - mathematics, chemistry, physics
  - engineering: chemical, mechanical, electrical, nuclear
  - Majors with a large math component are generally good
- What is the greatest barrier to success? Freedom.
  - Nobody will come after you for skipping classes/not doing homework.
  - Drugs and hobbies were major pitfalls.
  - Many drop out after Freshman year.
- You are responsible for your education! The professors do not care.
- What surprised you the most about college? I joined a fraternity.
  - AXΣ: Social/Professional chemistry fraternity.
  - Lots of fun + working together on coursework
- Different classes for majors and non-majors: Always take ‘for majors’ class.
  - Calculus (typically non-major) vs. Linear algebra + differential equations (math majors)
  - Organic chemistry for pre-meds vs. Honors organic chemistry (chemistry majors)
- Push yourself: take as many advanced classes as possible.
  - Nothing stopping you from taking graduate level courses as an undergraduate.
- Pre-requisites aren’t everything. Taking courses in the correct order can give a significant advantage.

Money Considerations

- How important do you feel scholarships are to college students? Medium
  - Money is nice.
  - Resume entry may be more valuable.
- Don’t get into lots of debt if you don’t know what you want to do.
  - Lots of programs for non-traditional (older) students.
- Community college (Nicolet) followed by larger university is a great way to save money.
- 5 year Bachelor’s/Masters programs can be very valuable.
  - People with Master’s degrees (especially engineering) make a decent amount of money.
  - Graduate school should pay you a living wage.
- If you are not getting paid after your undergraduate education, you are probably going into the wrong field.
  - Exceptions: Masters program, medical school, law school.

Pay ranges for related careers

JOB	SALRY RANGE ($)
University Professor, Ph.D.	60-100K
LANL Technologist, B.A./M.A.	85-105K
LANL Scientist, Ph.D.	120-250K
Industry, Ph.D.	60-300+K

- Working at a National Laboratory pays better than being a professor at a university
- Industry (private companies) typically pay a little more.
  - Opportunity to get paid a lot more or a little less.
- Work/Life balance is also important.

Open for questions

Photograph sources

- LANL: https://www.flickr.com/photos/losalamosnatlab/
- Advanced Photon Source:
  - https://www.anl.gov/article/argonnes-researchers-and-facilities-playing-a-key-role-in-the-fight-against-covid19
- Sedan Crater:
  - https://www.flickr.com/photos/nnsanevada/50825404881/in/album-72157717839431578/