

11/16/2022

- Quiz 3: Molecular Simulations
- Innovation Day
- Quantitative Structure-Property Relationships

FALL 2022 INNOVATION DAY

OVERVIEW

Innovation Day Overview

At the Kaplan Institute, we understand that practical, technological breakthroughs only come from people who are not just good at technology, but good at leadership: people who understand that influence, inspiration and human insight are as important as engineering and computer science and clean rooms; people who are looking to drive positive change, both in their communities and in the world, and see technology as the means.

The Innovation Day presentation is in effect the final exam for IPRO projects. The presentations demonstrate the entire development process requiring teams to assemble all work done over the course of the semester and present that work to the partners in person.

Innovation Day Project Submission

In order for us to be able to develop exhibit materials as well as distribute content with our partners, all teams must submit their project deliverables by **November 30**. The deliverables may include the following:

Innovation Day Deliverables

1. Presentation Slide Deck
2. Research Deck and/ or Written Report
3. Supporting Media/ Documentation

(Poster, Videos/ Animations/ Renderings/ Documentation of Prototypes)

Please submit all relevant project materials using the following the link **below**:

- [Team Submission](#)

Innovation Day Schedule

Innovation Day: Friday, Dec. 2nd

8:00 - 9:00 AM
Team setup

9:30 - 12:30 PM
Doors open/ Judging begins

12:30 - 1:30 PM
Judges' deliberation & lunch

1:30 PM -2:00 PM
Recognition ceremony

Innovation Day Judging Tracks

- Sustainable Cities
- Community and Social Innovation
- Sports and Technology
- Competitions
- Research

Judging Rubric

COMMITMENT TO POSITIVE COMMUNITY CHANGE	Did the team identify and analyze a contemporary issue and problem? Did the team address and compare different perspectives, both within and across cultures?
CRITICAL AND INNOVATIVE THINKING	Did the team appropriately employ multiple quantitative and qualitative methods of analysis and evaluation? Did the team employ the best available technology to achieve the solution(s)?
PROFESSIONAL AND ETHICAL COLLABORATIONS	Did the team members successfully work with others within disciplines and cultures? Did the team identify and discuss ethical issues?
EFFECTIVE COMMUNICATION	Did the team speak and write appropriately within and across disciplines and cultures? Did the students present their project in clear, concise, and logical form both verbally and through visual/graphic supporting material? Did the team clearly establish an objective and cohesively support it?

[Click here for the evaluation form](#)

Exhibition Space

Each team will have approximately 2' x 3' of table space with access to power.

Your team needs to be able to stand out.
Build prototypes!!!

Bring your own displays (computer monitors or televisions) for more visuals.

Please have your students fill out [this form](#) for special requests regarding equipment/space needs.

Poster Guidelines & Best Practices

- Design all graphics for 24" x 36" layout. Do **NOT** scale up from a smaller page size
- Use no less than 24pt font
- Print a black and white full size version to mockup, then adjust image sizes and fonts as needed
- Check all spelling BEFORE you print
- Send files to the Post Office Mail Center at MTCC

Poster Printing

The IPRO office is offering vouchers for teams to print 24" x 36" posters that can be mounted to foam core.

- Please visit the Kaplan Welcome Desk or the IPRO Help Desk for a voucher to print your poster at the MTCC Post Office (2 vouchers/team).
- Vouchers will become available from **November 9th onwards**.
- Foam core will be available at the Idea Shop from **the week of November 14th**.

Event Deadlines & Requests

- Teams should fill out [this request form](#) by **Friday, November 25** for any special requests for Innovation Day. We cannot honor any requests made after that date.
- Teams are required to submit their project deliverables by **Wednesday November 30th [here](#)**.
- Teams must have their project space set up by 9 AM on **Friday, December 2nd**.

Prepping For Innovation Day

Make A Plan

Envision the experience you wish to deliver, what is the sequence of movements, and set goals for that.

Visualize

Imagine the exhibition space, then sketch out how you plan to set up your table. How will you display your visuals, prototypes etc.

Practice

What is the story you want to tell, how do you want the audience to feel and react. Presentations need to be 3-5 minutes.

Work With Your Professors

Professors can help determine ways to best portray your work

Divide & Conquer

Everyone on the team needs to contribute, work to each others strengths.

Using Video & Multimedia

- Video & media is a great medium to tell your story and illicit emotion
- Remember audio will be hard to hear on Innovation Day
- Videos & animations can effectively demonstrate functions of your concept

**Videos/ Media is not required for
Innovation Day*

Resources

IPRO Office Resources

Supplies and Purchasing

1. <https://ideashop.iit.edu/portal/>
2. <https://ipro.iit.edu/class-resources/>

Software on Campus

1. <https://ots.iit.edu/classrooms-labs/lab-software>
2. https://wiki.ideashop.iit.edu/index.php?title=Computer_Software

Visual Assets

Icons

- The Noun Project: <https://thenounproject.com>
- Font Awesome: <https://fontawesome.com/icons?d=gallery>
- Dryicons: <http://dryicons.com/free-icons/>
- FREEBIESBUG: <http://freebiesbug.com/psd-freebies/icons/>

Free Imagery - Photography

- UNSPLASH: <https://unsplash.com>
- PixaBay: <https://pixabay.com>
- Free Images: <http://www.freeimages.com>
- PEXELS: <https://www.pexels.com>
- PICJUMBO: <https://picjumbo.com>
- PixaBay: <https://pixabay.com>

Visual Assets

Video Clips (Free - select ones on sites)

- <https://www.wedistill.io/>
- <https://coverr.co/>
- <https://www.pexels.com/>
- <https://pixabay.com/>
- <https://www.videvo.net/>
- <https://www.videezy.com/>
- <https://www.vidsplay.com/>
- <https://mazwai.com/>

More generic, aerial & drone shots:

- <https://www.lifeofvids.com/>
- <https://dareful.com/>
- <https://www.splitshire.com/>

Interaction Design Tools

Figma: <https://www.figma.com/>

Figma for beginners: <https://www.youtube.com/watch?v=Saz6S1svYns>

Sketch: <https://www.sketch.com/>

A guide to sketch basic: <https://www.youtube.com/watch?v=qywB0JHQeC4>

Mockplus: <https://www.mockplus.com/>

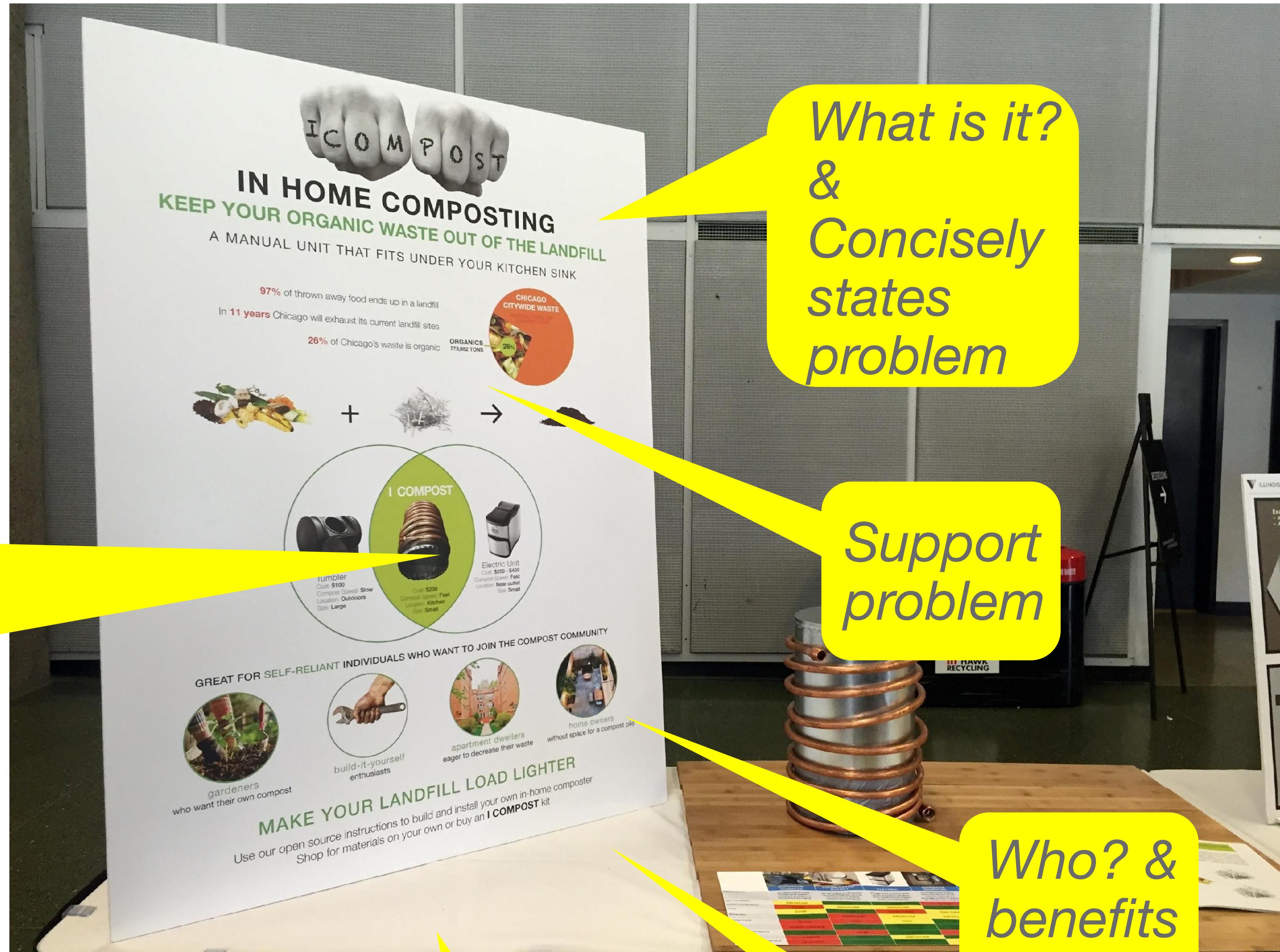
Mockplus Tutorial: <https://www.youtube.com/watch?v=LGZDZ-L0ejo>

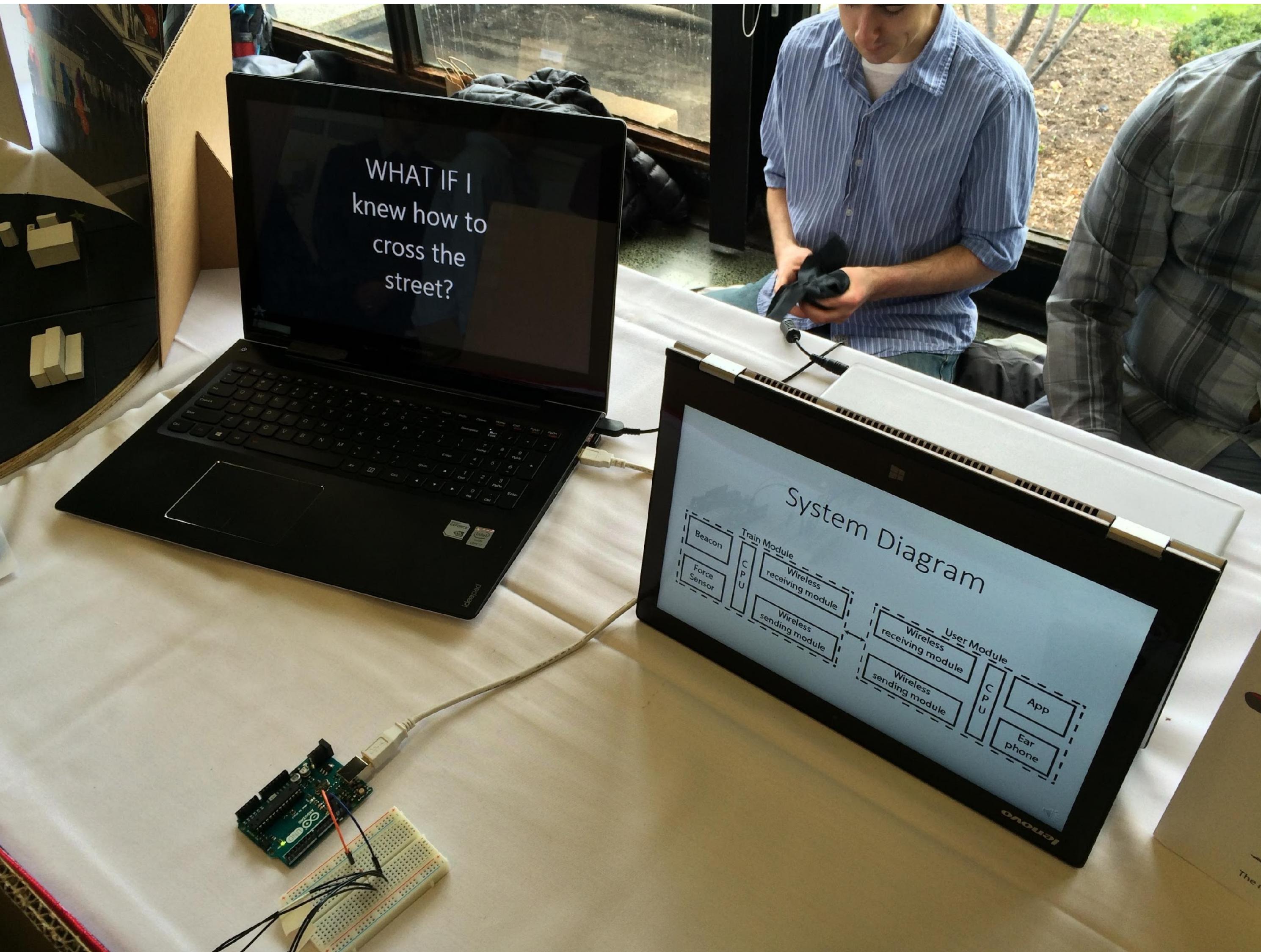
Adobe XD (can use from Idea Shop at Kaplan: [Ideashop Link](#))

Top ten things to know when getting started with Adobe XD: <https://www.youtube.com/watch?v=JtI6YpmPGI>

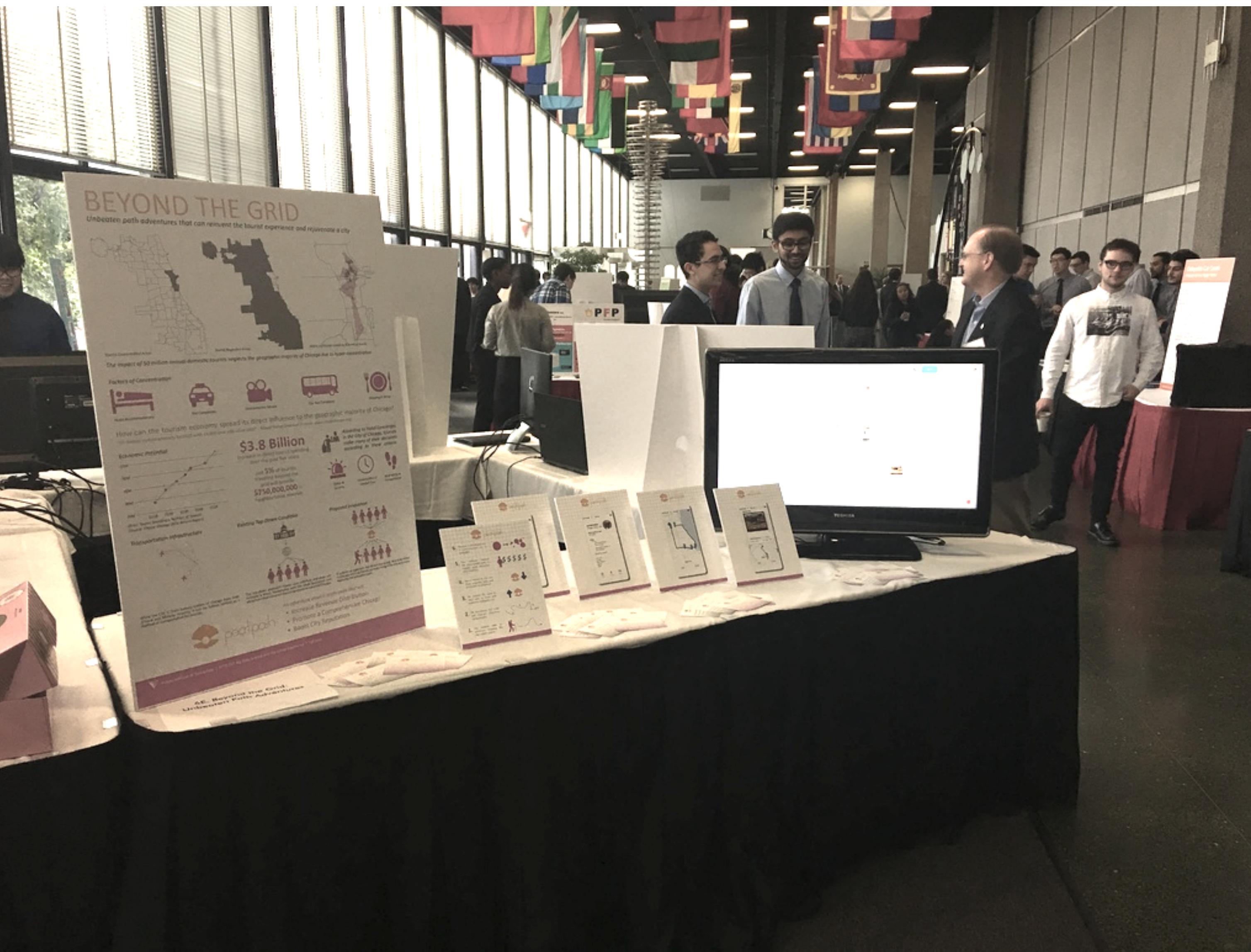
Examples for Innovation Day







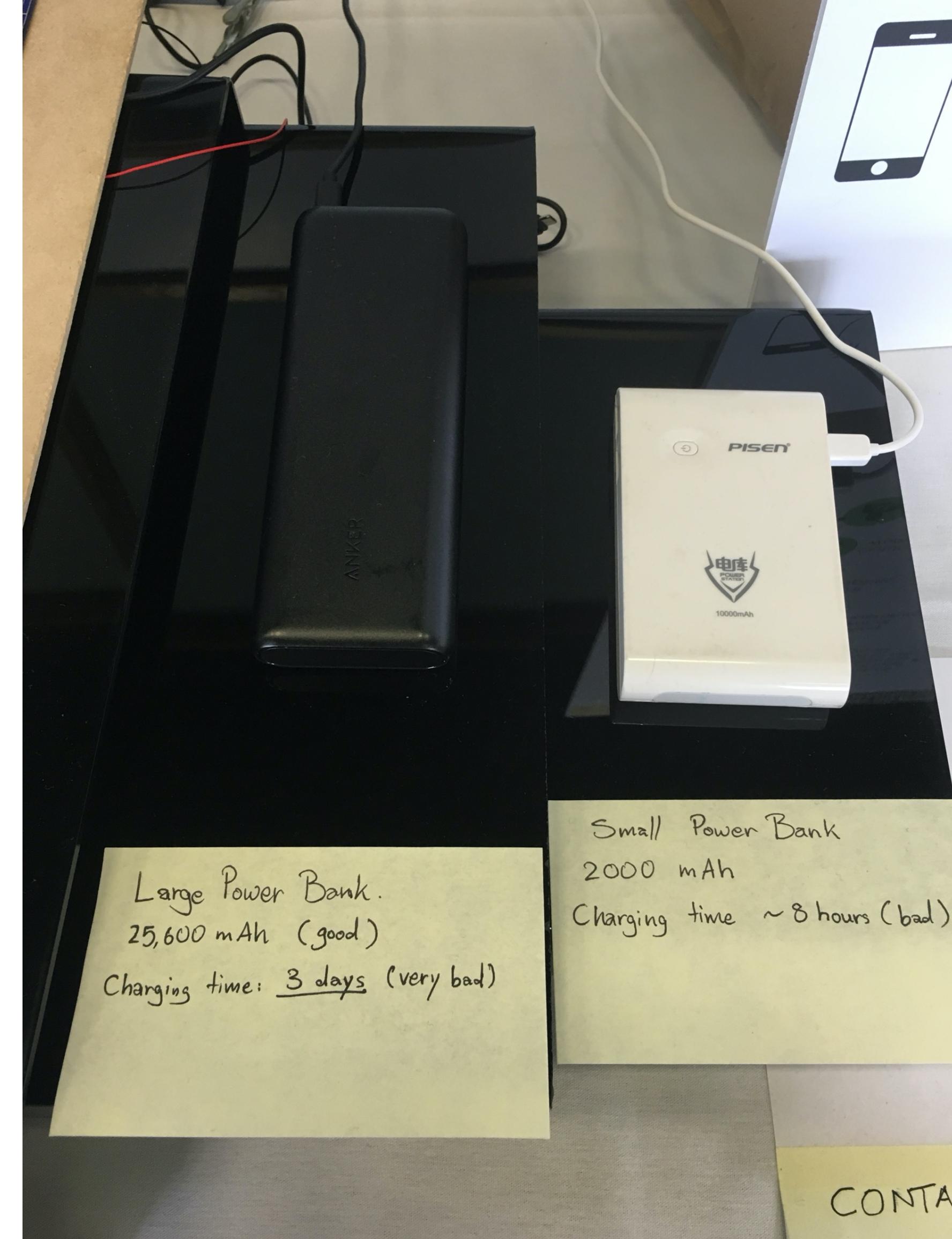
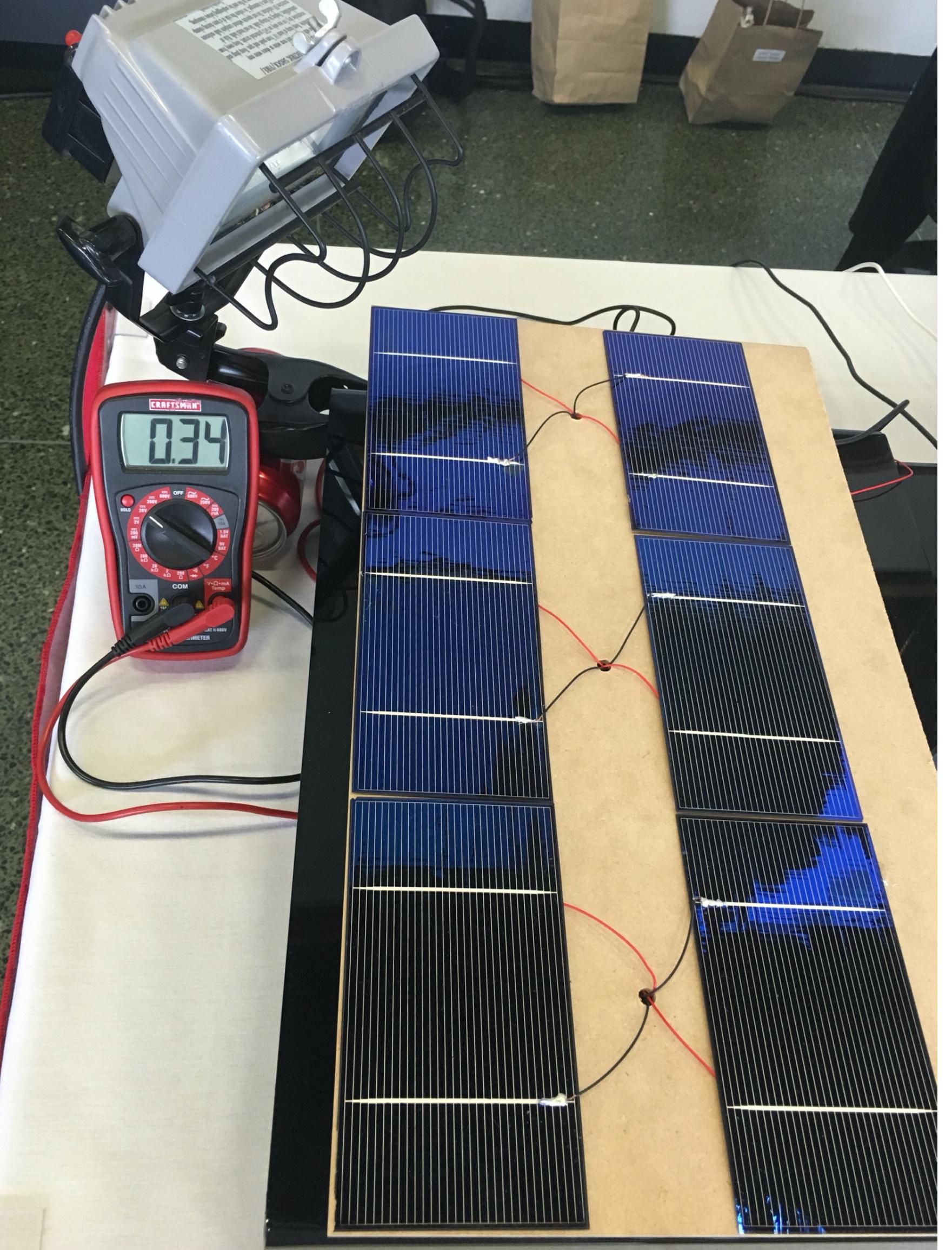
















Quantitative Structure-Property Relationships

- Today's lecture is intended to help you achieve the following learning objective: Develop a model for a quantitative structure-property relationship. Describe its domain of applicability.
- QSPR Topics
 - Machine learning
 - Features/descriptors
 - Algorithms
 - Validation
 - Limitations

QSPR is an application of machine learning

- Machine learning [1]
 - “gives computers the ability to learn without being explicitly programmed” - Arthur Samuel (1959)
 - “A computer program is said to learn from experience E with respect to some task T and some performance measure P, if its performance on T, as measured by P, improves with experience E.” -Tom Mitchell (1997)
- In Quantitive Structure-Property Relationships (QSPR)
 - Experience E: chemicals
 - Task T: predicting physical property, e.g.
 - boiling point, chromatography retention times
 - activity against a biological target = QSAR
 - ADMET (absorption, distribution, metabolism, and excretion - toxicity)
 - Performance P: correlation/error in validation set/real-world applications

Features/Descriptors

- Enables chemicals to be input into machine learning models
- How would you describe a chemical in numbers that can be put into a mathematical formula?
- Features can be
 - from enumerable properties, e.g. number of a certain element, number of H bond donors/acceptors, presence/absence of an element functional group
 - based on 3D structures
 - of a chemical, e.g. surface area, radius of gyration, moments of inertia
 - of a protein-ligand complex
- <http://www.rdkit.org/docs/GettingStartedInPython.html#list-of-available-descriptors>

Algorithms

- Linear regression
 - $y = mx + b$ for simple linear regression
 - $y = m_1x_1 + m_2x_2 + \dots + b$ for multiple linear regression
 - x is projected onto a new space in partial least squares regression
- Neural networks
 - sets of nodes that transform inputs into an output
 - allows for nonlinear relationships.
- Deep learning
 - neural networks with multiple layers
 - increasingly popular and powerful with faster computers and larger datasets
- Not an exhaustive list!

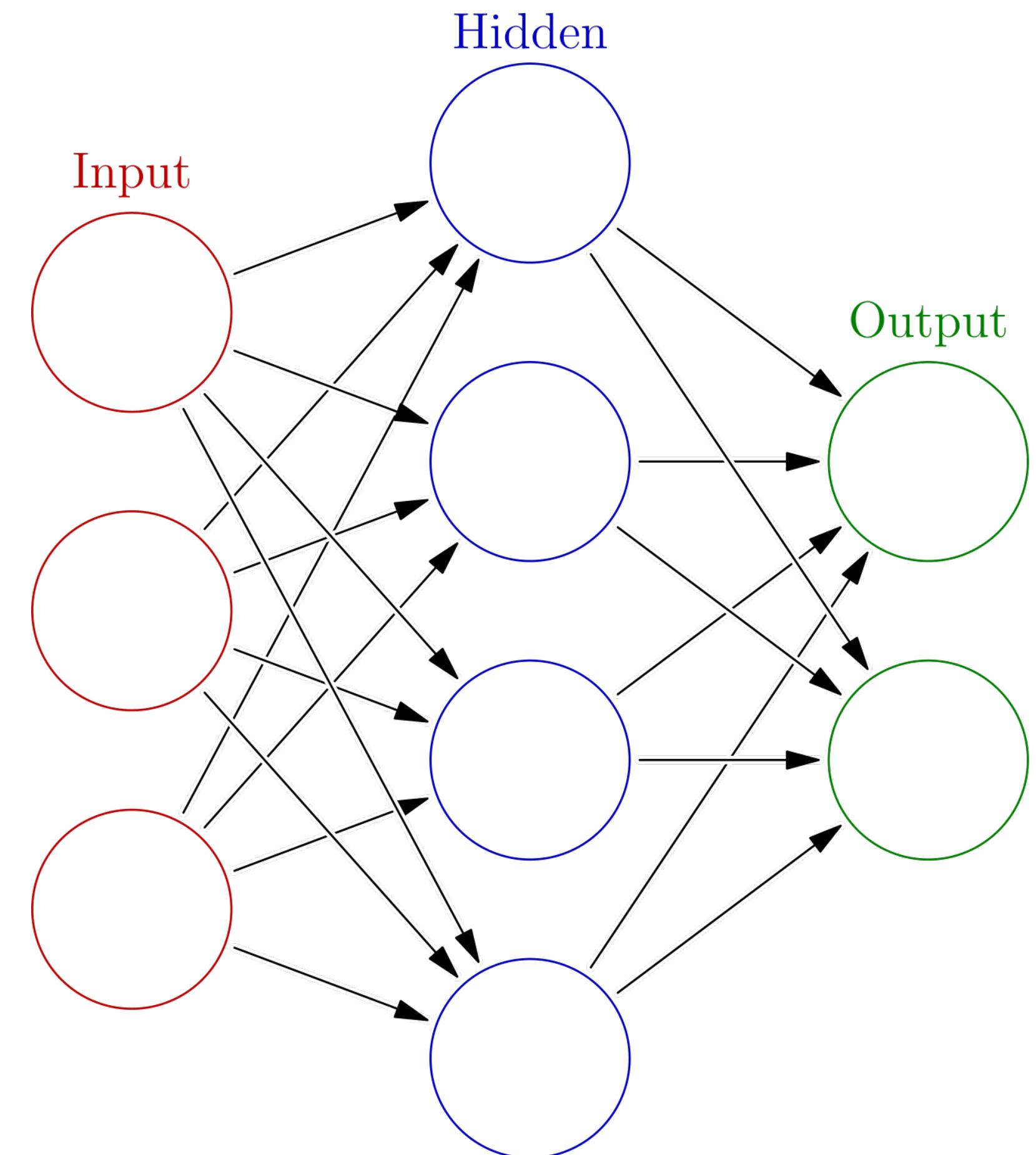


Diagram of an artificial neural network [2]

Validation

- How do you know if a model is any good?
- Data are split into training and test sets
 - Both sets should represent the same population
 - Model is built using the training set
 - Calculations on test set are compared to data

Limitations

- What do you think some limitations of QSPPR might be?
- A high-quality training set is necessary
- Models can only be applied to molecules similar to the training set
- Sometimes small changes in structure can lead to large changes in a property
 - adding a methyl can make it so that a ligand no longer fits into a binding pocket
 - in QSAR, known as an “activity cliff”

References

- [1] <https://www.geeksforgeeks.org/introduction-machine-learning/>
- [2] Downloaded from https://commons.wikimedia.org/wiki/File:Colored_neural_network.svg and reused under the [CC BY-SA 3.0](#) license