Welcome to MSE598DM - Spring 2022

Date and time: Tue/Thu, 11-12.30 pm (lecture)

Location: 2051 Sidney Lu Mech Engr Building

Instructor: André Schleife

Office hours: per request

Web:

- Links (e.g. absence form), schedule, slides, recordings: MSE598DM web site https://courses.engr.illinois.edu/mse598dm/sp2022/
- Announcements, Online discussion: CampusWire
- Report submission: GradeScope (Entry Code: JBZDVP)

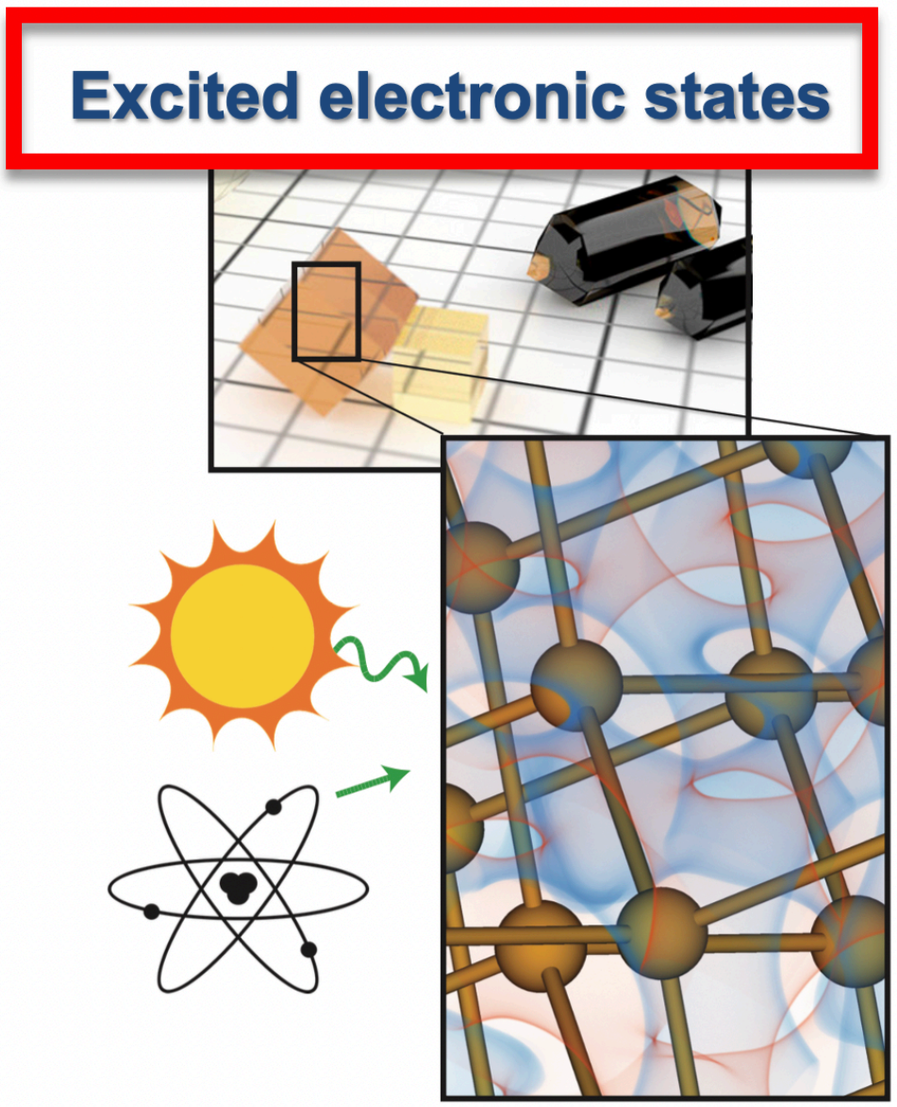
Scope and Objectives

- Introduction to the connection of materials and data science
- Specific issues regarding experimental and computational materials data
- Data acquisition and management, data curation
- Uncertainty quantification
- Applying machine learning to materials data

Logistics

- DRES information: see syllabus + make contact ASAP
- all excused absences handled through online form on the web site
- you are bound by university honor code, NO exceptions
- harassment or discrimination will **not** be tolerated
- Following University policy, all students are required to engage in appropriate behavior to protect the health and safety of the community. Students are also required to follow the campus COVID-19 protocols.
- The effectiveness of this course is dependent upon each of us to create a safe and encouraging learning environment that allows for the open exchange of ideas while also ensuring equitable opportunities and respect for all of us. Everyone is expected to help establish and maintain an environment where students, staff, and faculty can contribute without fear of personal ridicule, or intolerant or offensive language.

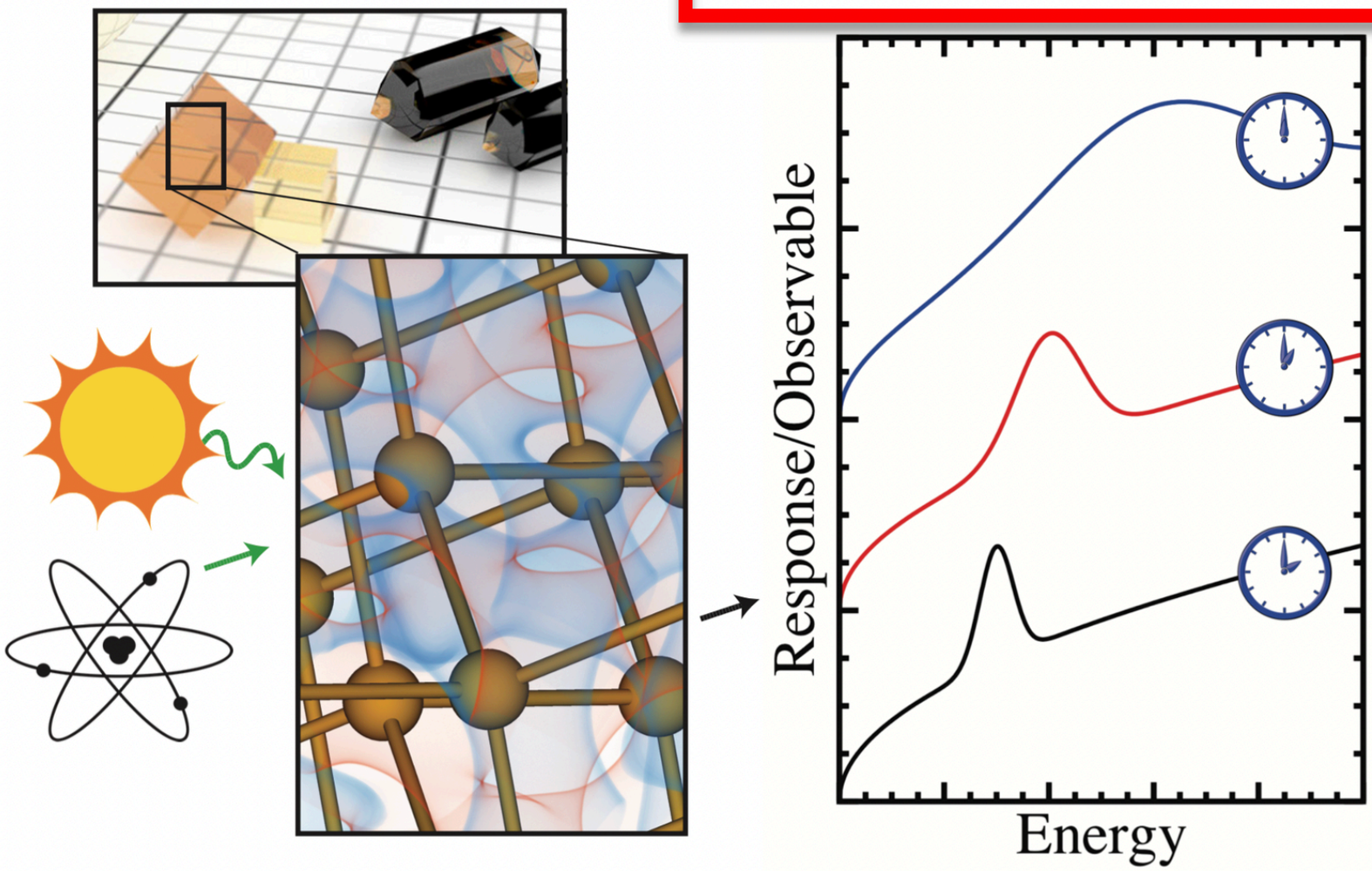
Introductions



Introductions

Excited electronic states

Femto-second dynamics



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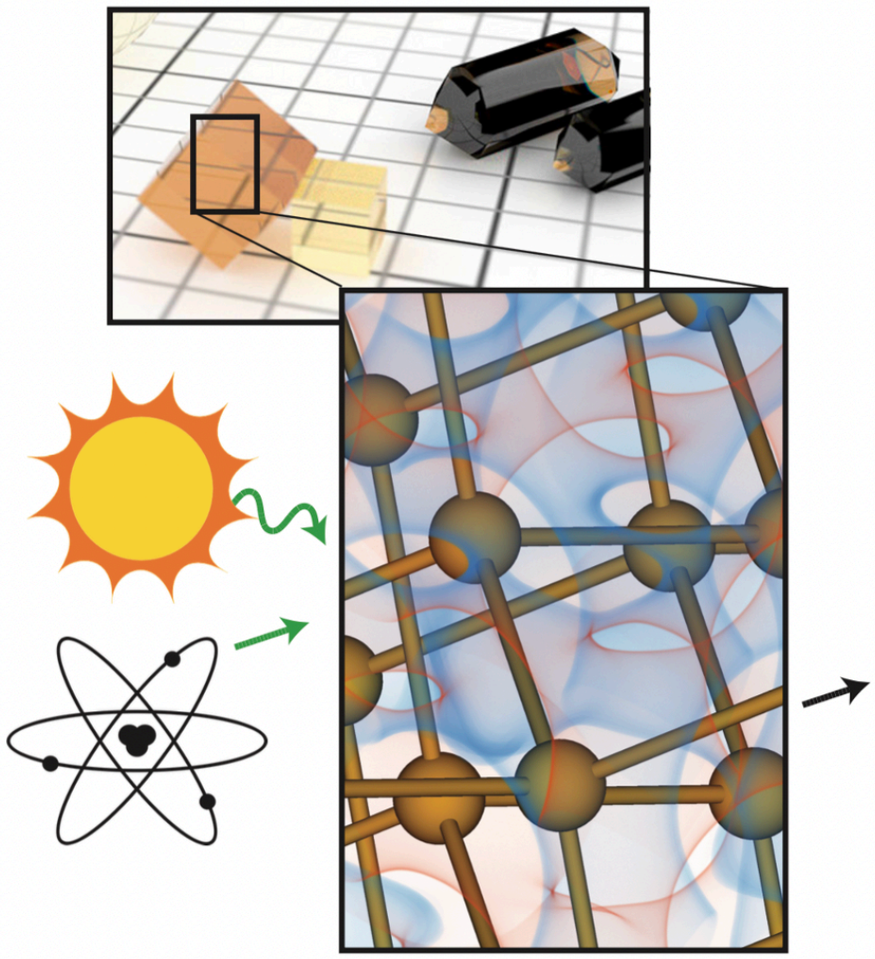
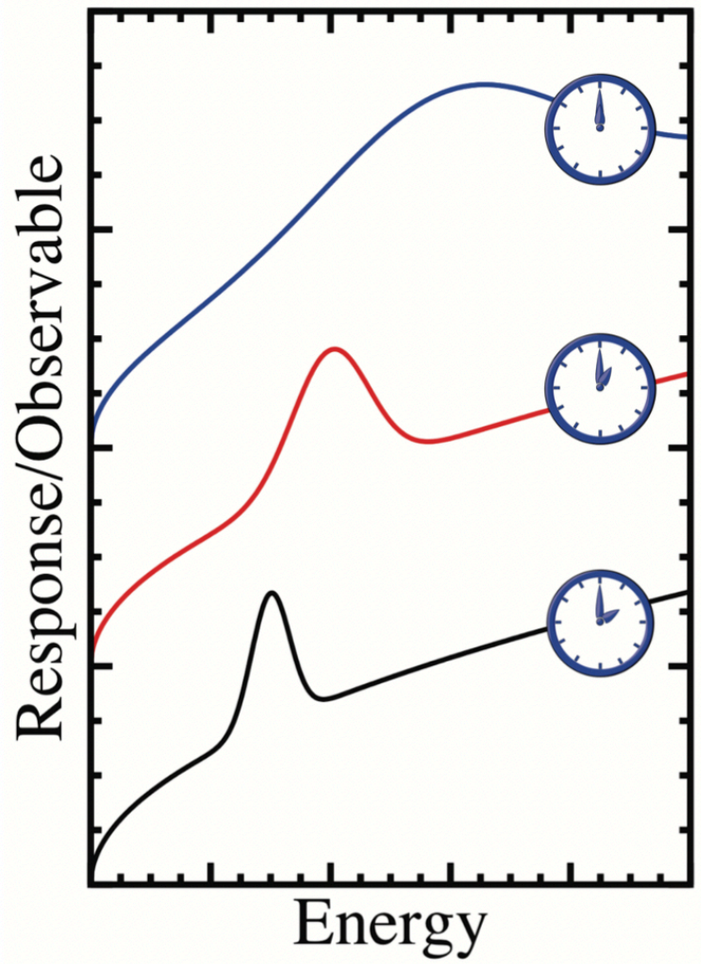
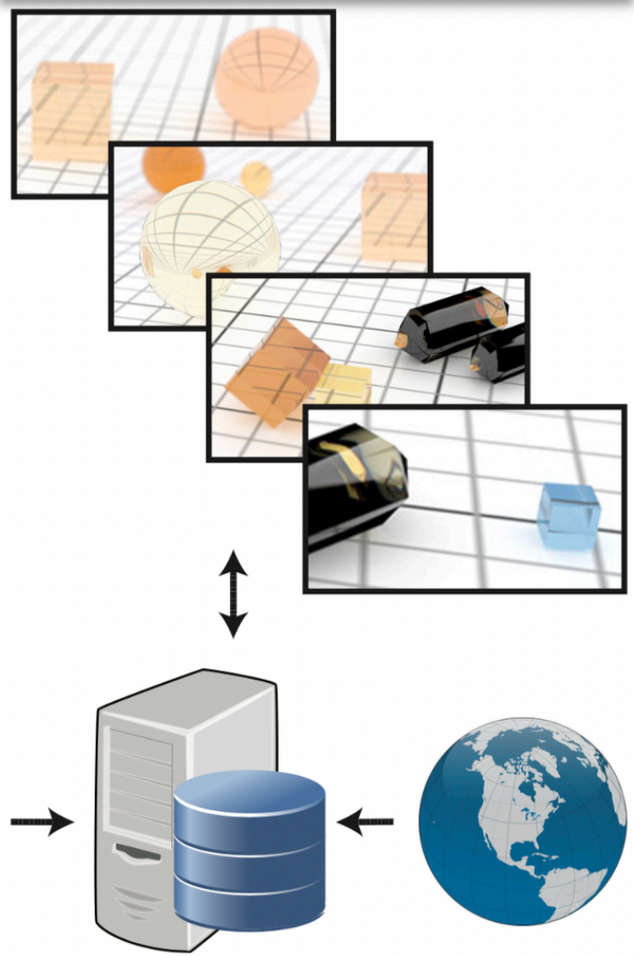
Excited electronic states



Femto-second dynamics



Materials selection



Introductions

Aboutaleb, Sohaila Mostafa Gamaleldin
Bean, Chris
Brandvold, Ally
Celebi, Orcun Koray
Chee, Gwendolyn Jin Yi
Desilva, Charith Ravana
Ellis-Mohr, Austin Russell
Foiles, Dreycen
Furlanetto Ferrari, Paolo
Han, Joon Su
He, Jimmy
Hwang, Kelly
Khodakarami, Siavash
Krishnan, Siddharth
Lee, Yi-Ting
Lo, Tzu-Hsiang
Nahid, Shahriar Muhammad
Ni, Hsu-Chih
Nolan, Gillian Margaret
Pak, Angela Areum
Palmer, Dan
Paranjape, Salil
Sin, Phillip Hyun
Wonner, Sara Katlyn
Xie, Dajie
Xu, Rui Hua Jeff
Yardas, Olek
Yin, Kaijun
Zhang, Zhixin

- What is your background (Stats, MatSE, Phys, MechSE, …)?
- PhD/MS/other?
- What is your current research on?
- Programming experience?
- Any specific topic requests?

- ML, - data sci ⟷ classical sims (FEM)
- soft/bio/polymers
- nuclear cross section data

Computational Methods: What? Why?

Theory:

- Newtonian Mechanics
- Maxwell Equations
- Thermodynamics
- Statistics
- Quantum Mechanics

Experiment

Computational Methods: What? Why?

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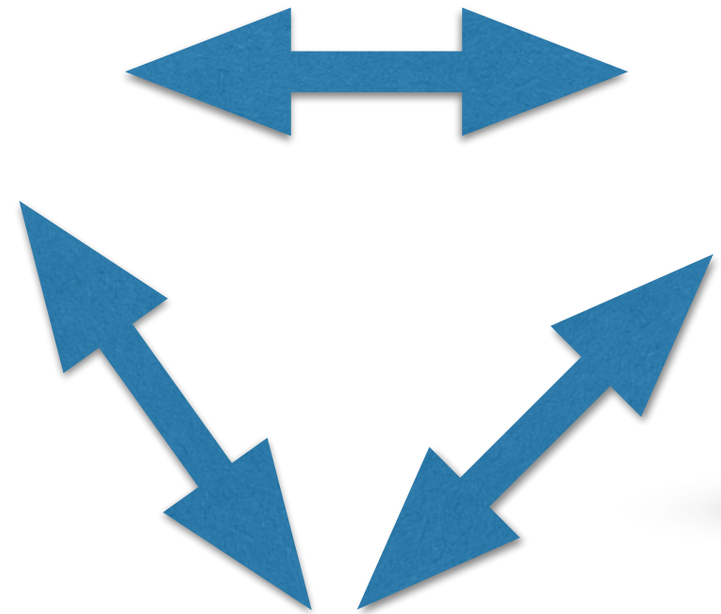
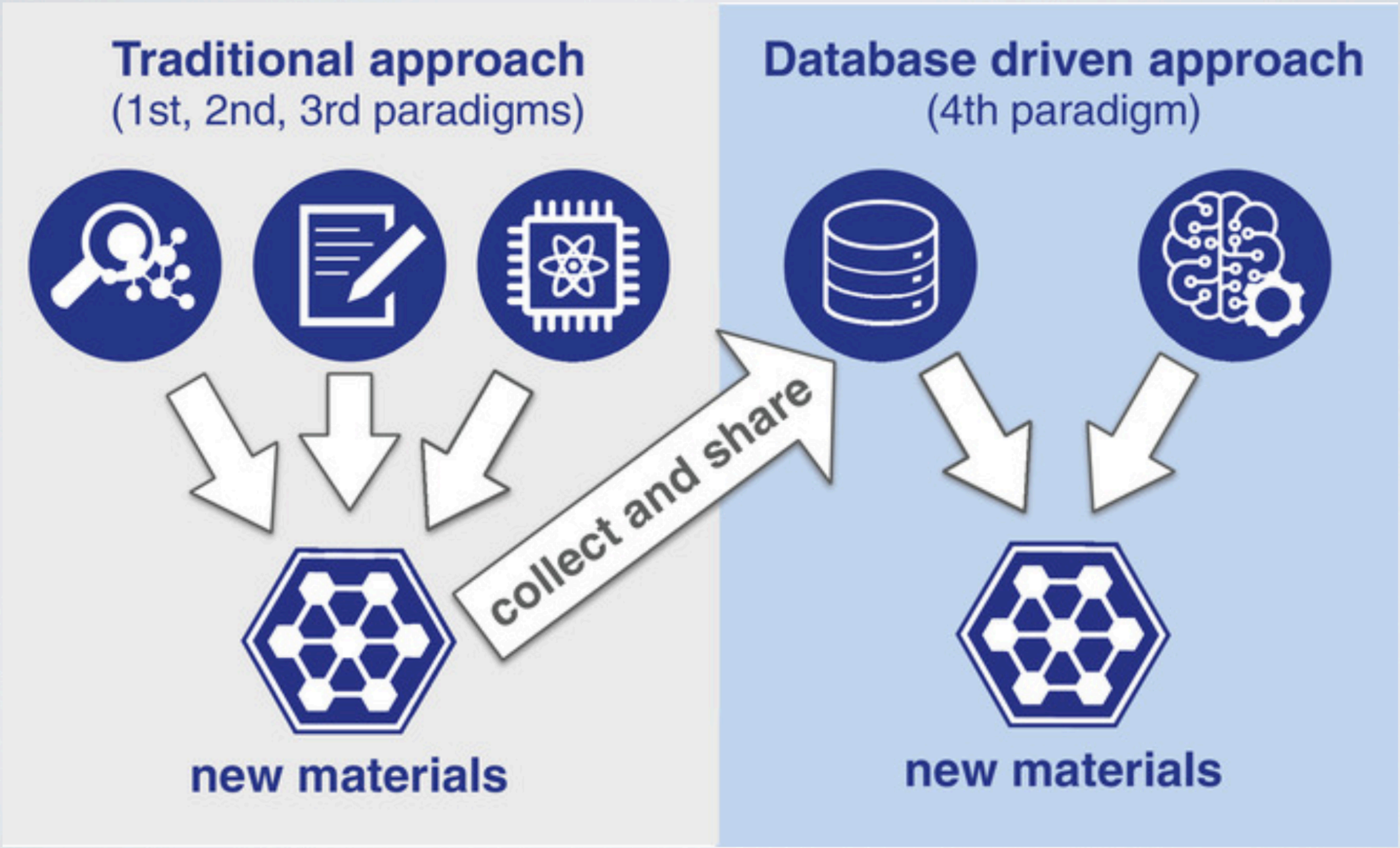


Experiment

Computer Experiments/Simulations

e.g. Blue Waters @ UIUC

Data-driven design as 4th paradigm



Advanced Science, Volume: 6, Issue: 21, First published: 01 September 2019, DOI: (10.1002/advs.201900808)

Group work

F	Bean, Chris	Nolan, Gillian Margaret	Furlanetto Ferrari, Paolo	Palmer, Dan	Paranjape, Salil	Xie, Dajie
M	Yardas, Olek	Zhang, Zhixin	Nahid, Shahriar Muhammad	Yin, Kaijun	Brandvold, Ally	Khodakarami, Siavash
P	Lee, Yi-Ting	Foiles, Dreycen	Celebi, Orcun Koray	Han, Joon Su	Bipasha, Ferdaushi Alam	Pak, Angela Areum
S	Aboutaleb, Sohaila Mostafa Gamaleldin	Wonner, Sara Katlyn	Ellis-Mohr, Austin Russell	Chee, Gwendolyn Jin Yi	Paranjape, Salil	Xu, Rui Hua Jeff
D	Lo, Tzu-Hsiang	Ni, Hsu-Chih	He, Jimmy	Desilva, Charith Ravana	Krishnan, Siddharth	Sin, Phillip Hyun
D						Hwang, Kelly

- **Group roles:**

  Facilitator: Make sure that the goals are all achieved
  Moderator: Make sure that everyone's ideas are heard, finds resolutions to disagreements.
  Presenter: Will report experience or conclusion to the rest of class
  Scribe: Screen share the response document so you can work on it collaboratively.
  Devil's advocate: Quality control—does the argument make sense?

- Work on it together, but make sure to turn in your own work

Group work (15+5 mins)

- **How do you think data can be used to solve problems in materials?**
- **1 paragraph or a few bullet points**

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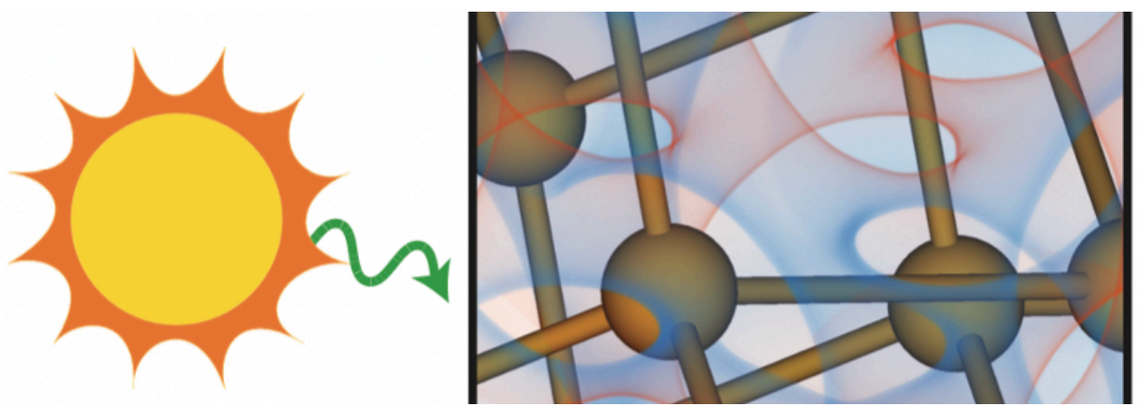
Solar Cells



- Light is absorbed by a material, creating energetic charge carriers
- These move through a circuit, which corresponds to electricity

Group work (15+5 mins)

- **What information would you want to know to tell whether Material A is better for a solar cell than Material B?**
- **1 paragraph or a few bullet points**

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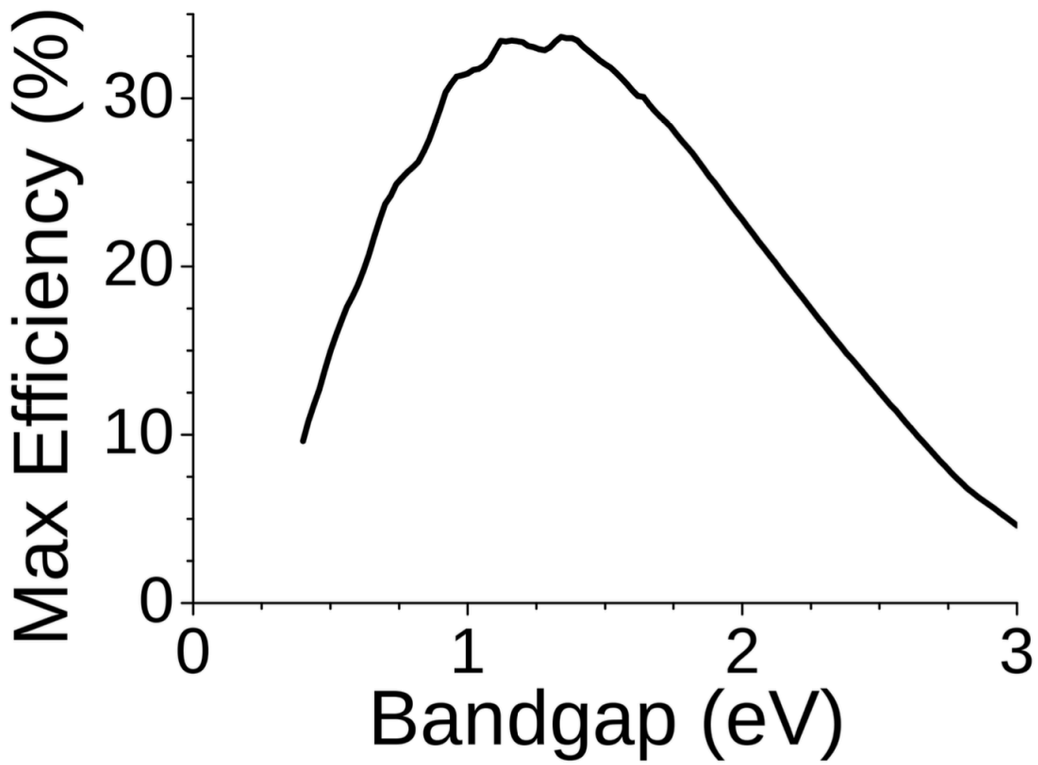
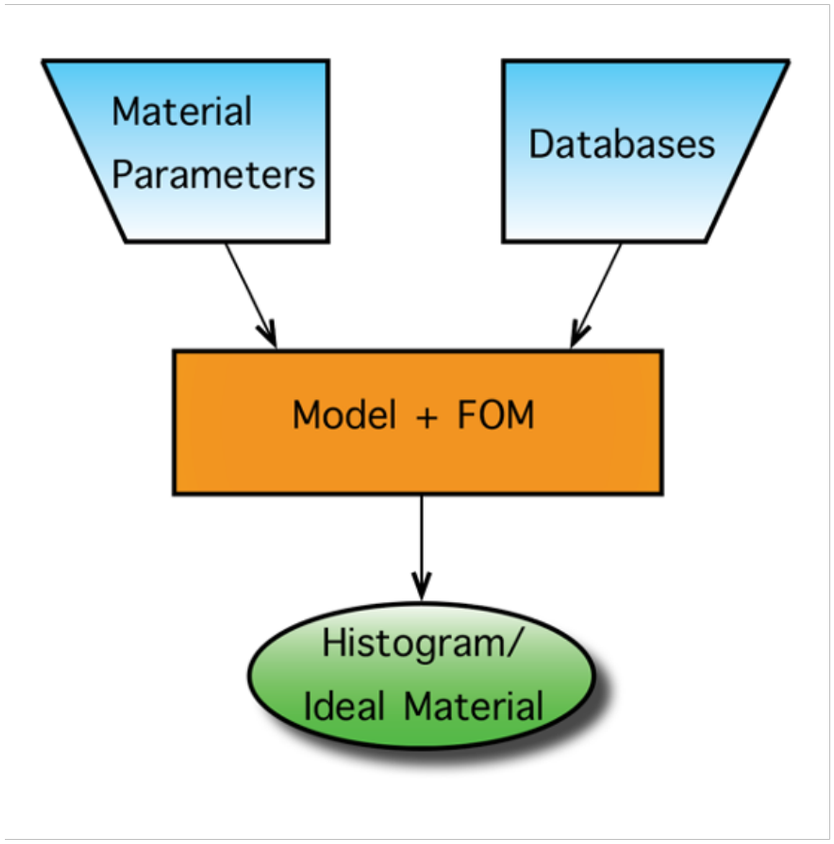
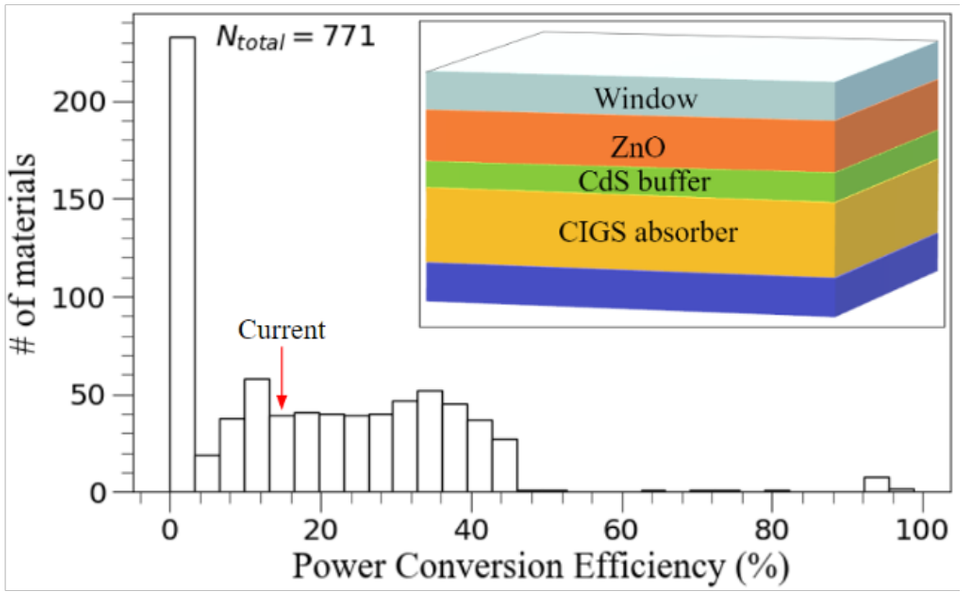


- Shockley-Queisser limit
- Theoretical maximum from detailed balance

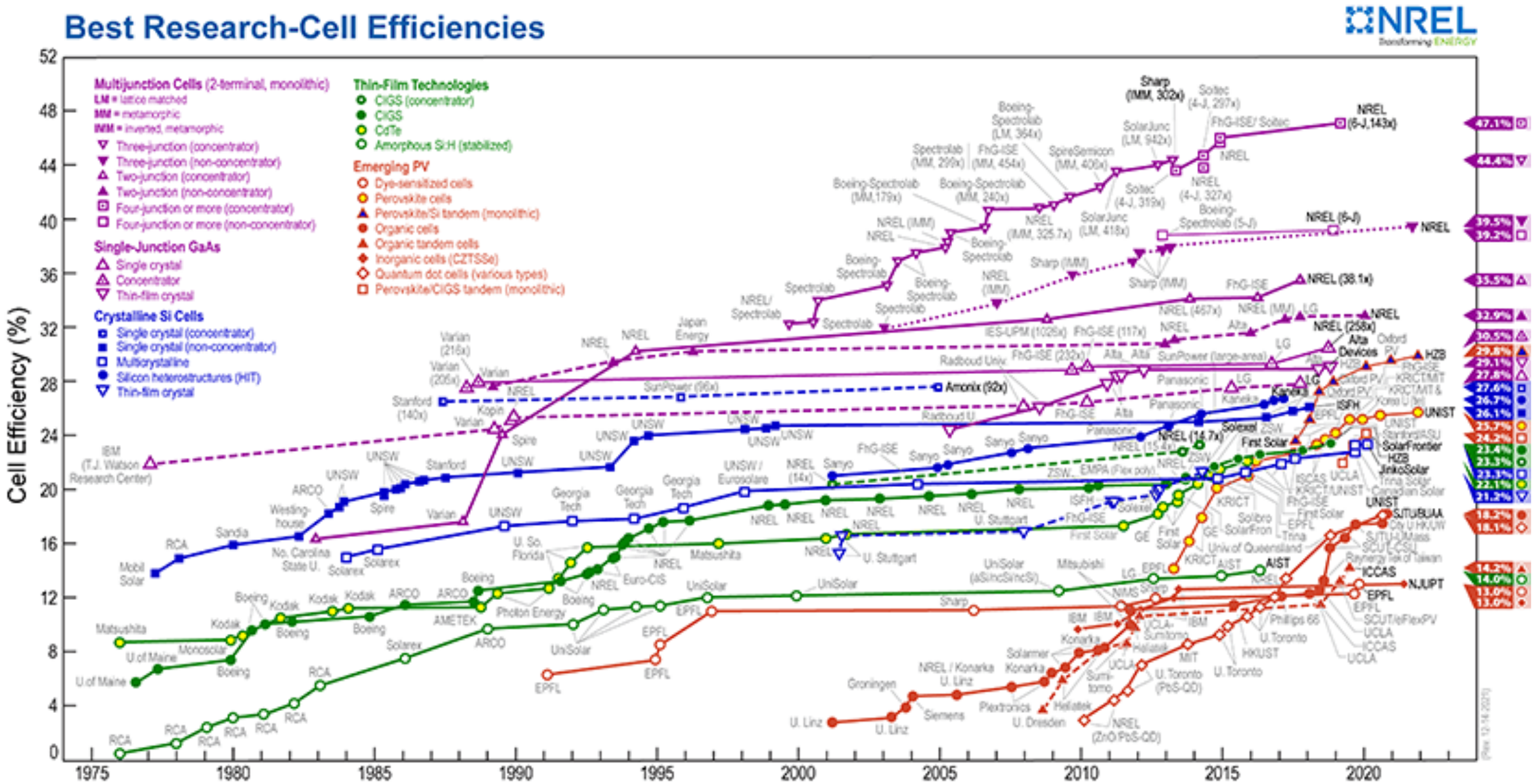
Materials and Data





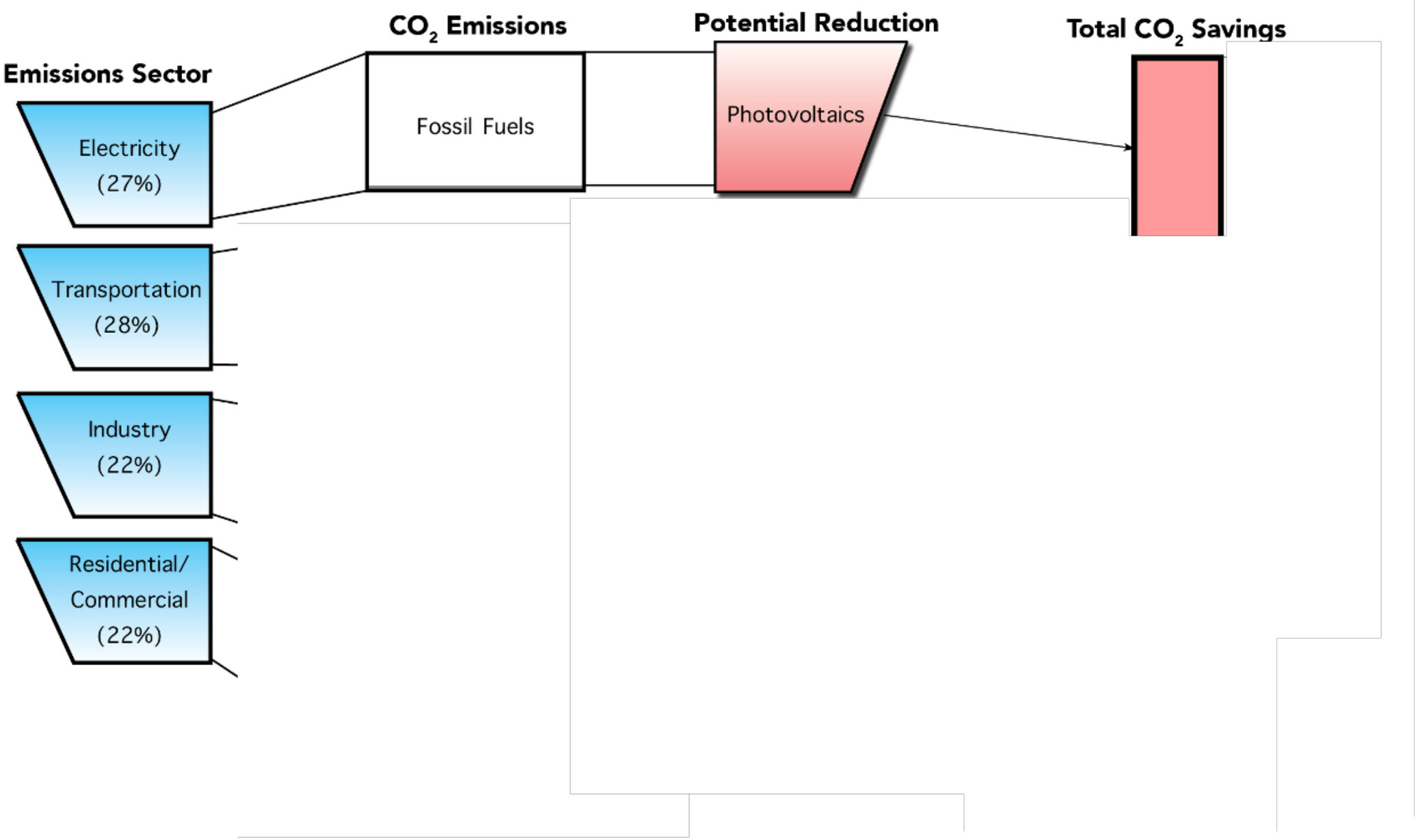
- This gives a range of what can be achieved within a specific model/paradigm
- Different paradigm needed to go beyond (Interesting for Materials Science!)

Materials and Data



- Takes all practicalities into account;
- Challenging experimentation

Materials and Data



Materials and Data