Argonne NATIONAL LABORATORY

PSE directions & strategic initiatives

March 5, 2015

H. Weerts

PSE Open Mic series

U.S. DEPARTMENT OF ENERGY

Hope not too boring today and not too long.

Be happy to answer questions

Try to tell you "the story" ……..
Danger with telling stories…..
Being used to put kids to sleep……

PSE Open Mic

more collaboration and information-sharing,

PSE Open Mic Seminars -- 1st Thursday of month
different structure
NOT traditional seminars and colloquia
will be Argonne-centric

mostly internal speakers
not just science – all aspects of "life at Argonne"
Recycle talks given outside Argonne (invited talks, seminars, colloquia etc.)
Can have different forms -- discussions, panels, forums

Asking for volunteers….. But PSE office signs all travel…….so knows

First Open Mic: PSE's strategic plan.

what are we doing and what we plan to do, and will welcome your feedback on our future.

Strategic planning overview

Annual cycle for everything…..

~ mid April Argonne submits strategic plan to DOE

Presentation in early June

Lab status & future plans

~ early February directorates (ALDs) asked for input to above

"Strategic initiatives in/of PSE"

Asked divisions → PSE sent in a list of 14 initiatives (a lot !)

Form->

EXAMPLE

FY 16-20 strategic initiative summary: Additive Manufacturing

RESPONSIBLE ALD

Physical Sciences and Engineering

VISION

Additive manufacturing (AM) will be reimagined to provide mesoscopic control of materials synthesis while demonstrating a series of prototype devices chosen to drive sponsor interest.

STRATEGY

Additive manufacturing as currently envisioned is simply a printing and melting/sintering operation. However, the voxel size can easily be moved into the >100 nanometer size range and the print environment provides a unique synthetic environment, which can be used to control morphology and composition. Argonne's APS provides a perfect platform to interrogate each voxel and follow, for instance, time dependent crystallization. Argonne's computational ability will provide insight into the complex thermo-chemical properties of the growing environment.

WHY IS THIS IMPORTANT ?

Additive manufacturing (AM) already represents the future of applied material science due to its ability to build complete machines that are impossible to produce any other way. Worldwide AM is expected to be a $550B industry by 2025. Yet the current vision for AM is limited to sintering and melting. New instruments, techniques capable of controlling morphology (crystallinity), or to synthesize within each voxel, provide an opportunity to reinvent AM and place Argonne at the forefront of the field.

WHY ARGONNE?

1) APS provides a unique time dependent way to evaluate the printing process. 2) Computational modeling of thermal, chemical, and morphology can help define instrument properties. 3) Argonne uniquely combines applied and basic capabilities required to understand and control growth.

INITIATIVE LEADER(S) & KEY STAFF

Leaders: M. Pellin, J. Elam, L. Yacout, APS staff, computation leader
Staff: M. Demarteau, T. Prolier, L. Curtiss

PARTICIPATING ARGONNE ORGANIZATIONS

MSD, HEP, NE, ES, APS, JCESR

KEY OUTSIDE COLLABORATORS

Northwestern U, UC, UIUC, NASA, DMDII (Goose Island)

POTENTIAL SPONSORS & ANNUAL INCOME

LDRD, DARPA, NASA, NNSA, DOE (BES, NE, EERE); Funding potential $30 M + broadly enhanced funding across the lab arising from the ability to prototype as part of any proposal.

PROJECT GOALS FOR FY 2016 (LAB AGENDA)

- **Develop a multi-year plan for establishing a strong basic, applied, analytical, and computational program needed to establish Argonne as a key AM center**
- **Prototype two channel plate detectors- one for neutron and one for photon detection.**
- **Prototype nuclear fuel structures for both enhanced thermal conduction and enhanced accident tolerance (beginning with non-radioactive surrogates).**
- **Build unique single crystal structures, build materials with single-size, potentially-oriented crystallites.**
- **Establish relationships with AM instrument manufacturers .**

PROJECT GOALS BY FY 2020 (FOR STRAT PLAN)

1) Establish a new technology portfolio that can be transferred to both AM instrument manufacturers and detector manufacturers. 2) Use prototypes and new technology to build sponsored programs with NE, NASA, DARPA, NNSA, etc.

List provided by PSE:

As usual under time pressure

1. Institute for Molecular Engineering (IME)
2. National Brain Observatory (NBO)
3. Argonne Strategic Center for Energy Storage (ASCES)
4. Development of a Multi-User Upgrade of ATLAS
5. Silicon Tracking for LHC Phase II Upgrade
6. Center for Atom Trap Trace Analysis of Noble Gas Radionuclides
7. Novel devices and Applied Materials
8. Computational Chemistry and Materials
9. Integrated Imaging
10. Materials and Molecular Design and Discovery
11. Materials for Energy
12. Additive Manufacturing
13. Bio-inspired Hybrid Materials for Energy
14. Integrated Approach to Develop and Optimize Fuel Chemistry

List and each item with a page description → confusion

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Possible ingredients for lab strategic plan exists

Need to mold them into "lab plan"

In process

Need to have a story /vision that goes "14 initiatives"

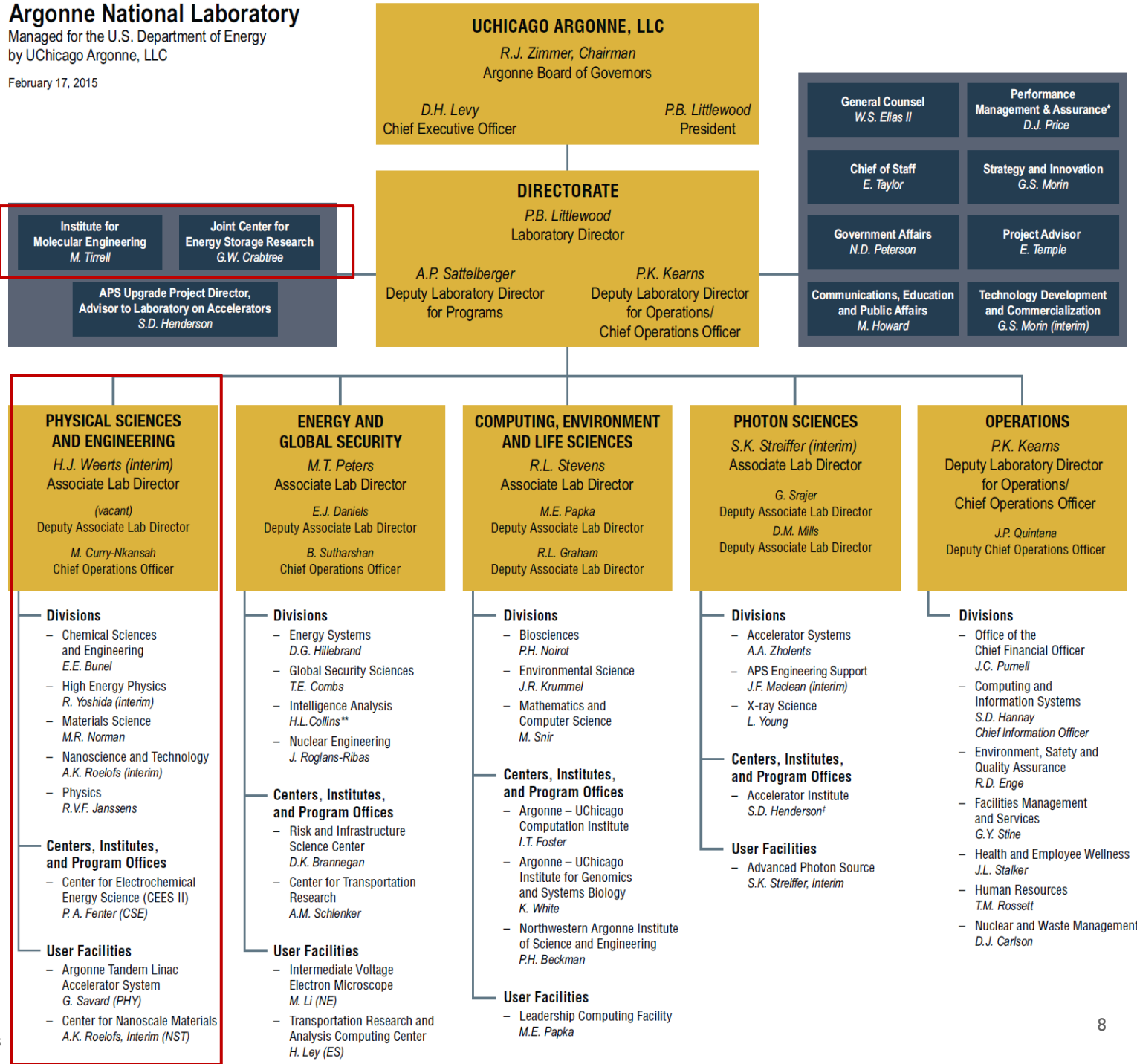
At high level

Take step back, PSE, what/who are we inside lab

Physical Sciences & Engineering – put in perspective

JCESR & IME

Physical Sciences & Engineering (PSE)



Argonne's framework

View from lab director

Discovery science

that redefines understanding of physical, mathematical and biological phenomena

~ $180M

~ PSE

Energy

technologies for energy storage, electricity generation, and transportation markets

~ $125M

~ PSE

Security

and resilience of infrastructure, sustainability, energy systems, and the environment

~ $180M

Scientific facilities

and unique tools for computation and experiment

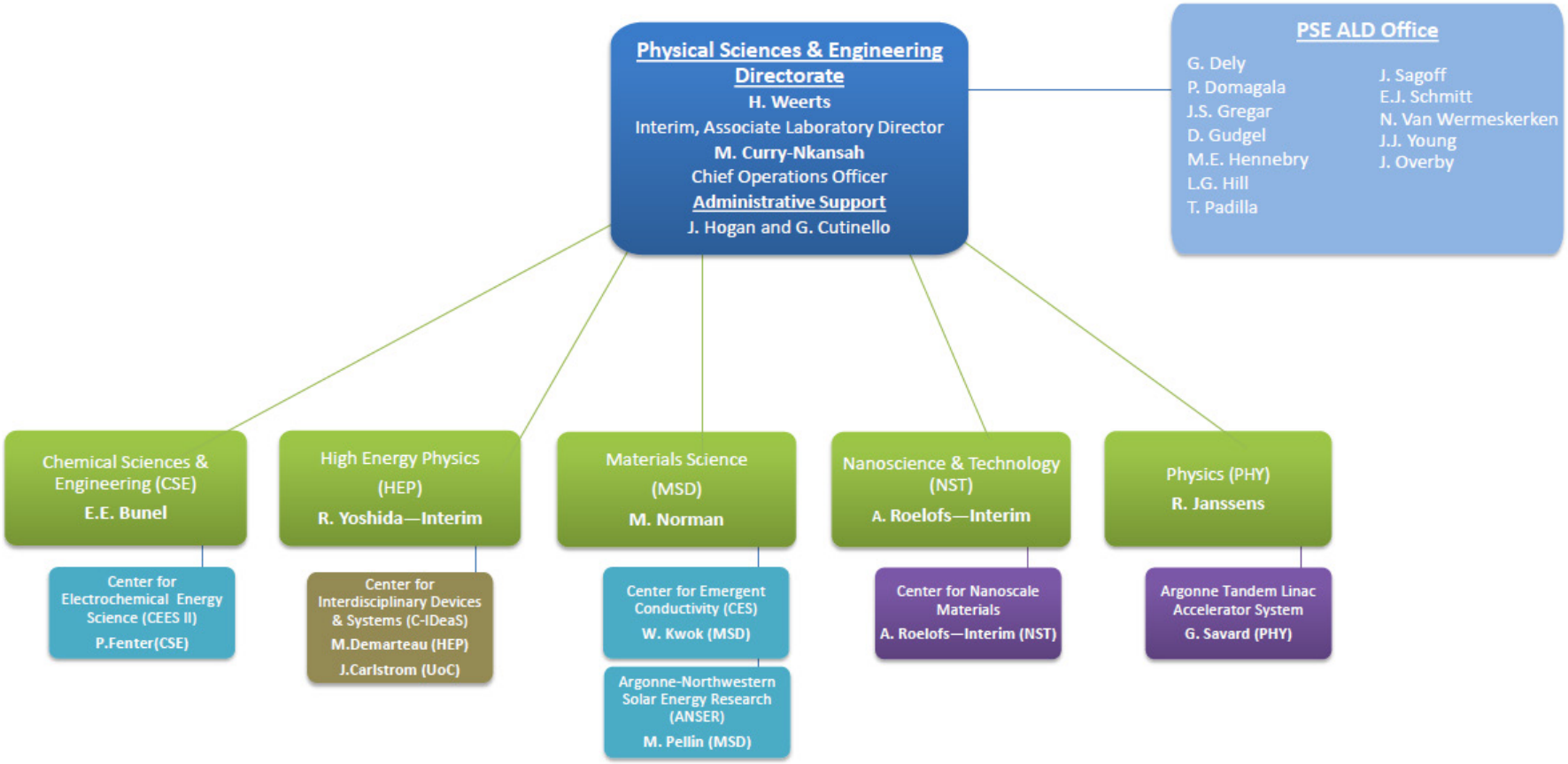
~ $255M

~ PSE

Mission execution

investments in people, infrastructure, and research **~ $160M**

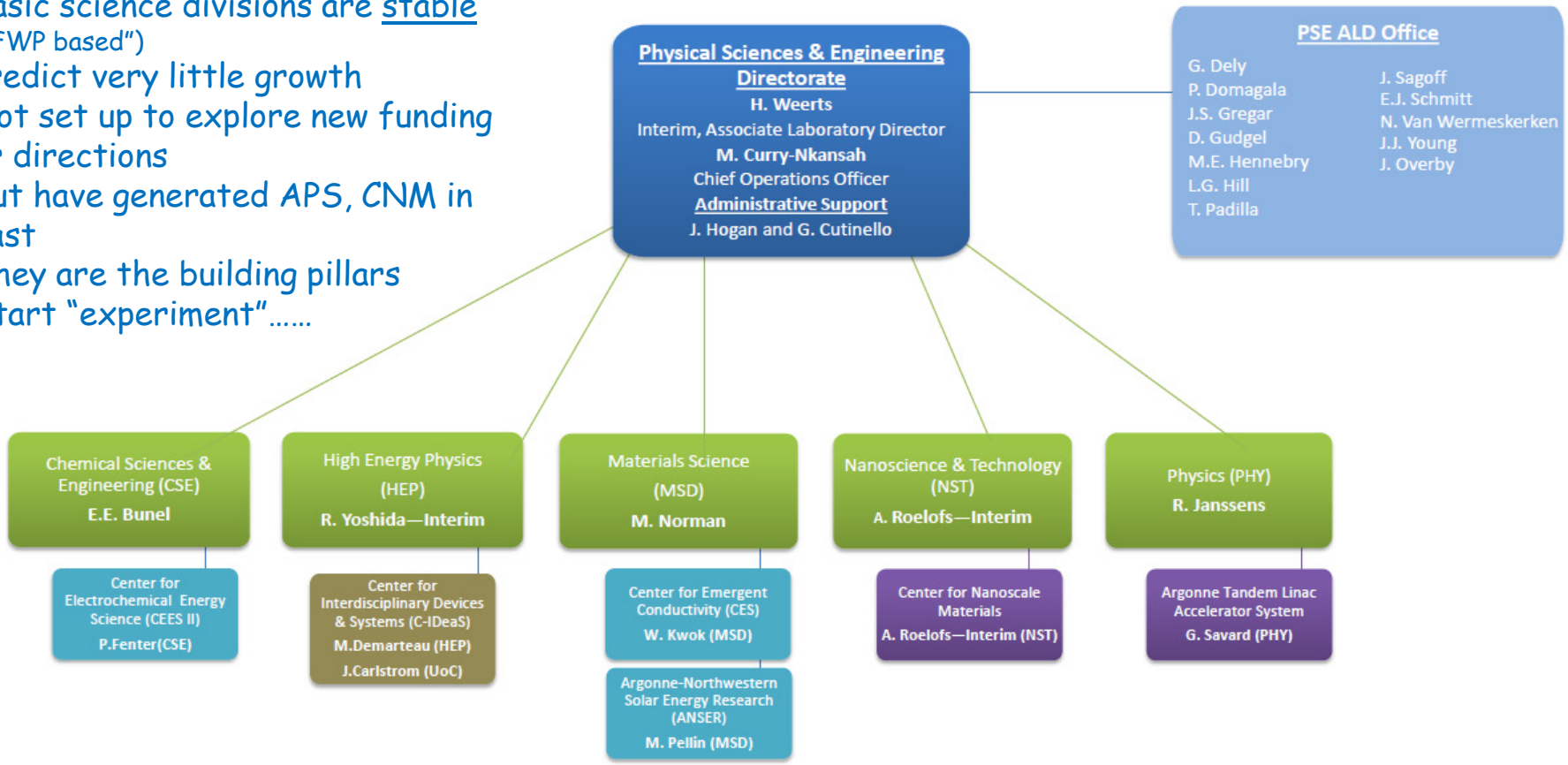
PSE – in FY15


Physical Sciences & Engineering Directorate
H. Weerts
Interim, Associate Laboratory Director
M. Curry-Nkansah
Chief Operations Officer
Administrative Support
J. Hogan and G. Cutinello
PSE ALD Office
G. Dely
P. Domagala
J.S. Gregar
D. Gudgel
M.E. Hennebry
L.G. Hill
T. Padilla
J. Sagoff
E.J. Schmitt
N. Van Wermeskerken
J.J. Young
J. Overby
Chemical Sciences & Engineering (CSE)
E.E. Bunel
High Energy Physics (HEP)
R. Yoshida—Interim
Materials Science (MSD)
M. Norman
Nanoscience & Technology (NST)
A. Roelofs—Interim
Physics (PHY)
R. Janssens
Center for Electrochemical Energy Science (CEES II)
P.Fenter(CSE)
Center for Interdisciplinary Devices & Systems (C-IDeaS)
M.Demarteau (HEP)
J.Carlstrom (UoC)
Center for Emergent Conductivity (CES)
W. Kwok (MSD)
Argonne-Northwestern Solar Energy Research (ANSER)
M. Pellin (MSD)
Center for Nanoscale Materials
A. Roelofs—Interim (NST)
Argonne Tandem Linac Accelerator System
G. Savard (PHY)

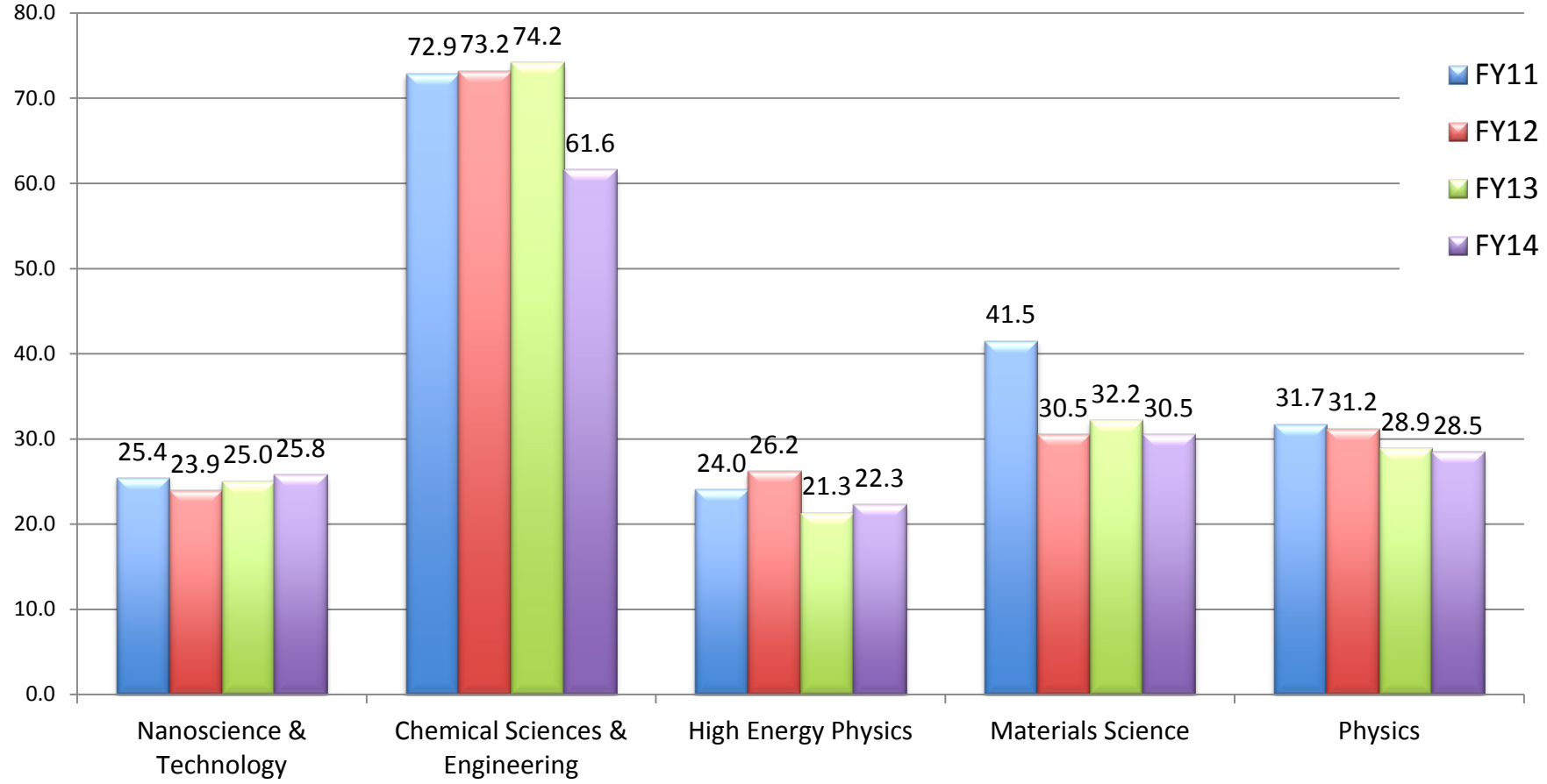
PSE – in FY15 - evolving

Assumptions:

- Basic science divisions are stable ("FWP based")
- Predict very little growth
- Not set up to explore new funding or directions
- But have generated APS, CNM in past
- They are the building pillars
- Start "experiment"……



FY2014 PSE New Budget Authority (estimated, $M)



FY2014 Budget (est.)
PSE = $169M
Argonne = $703M

PSE – in FY15 - evolving

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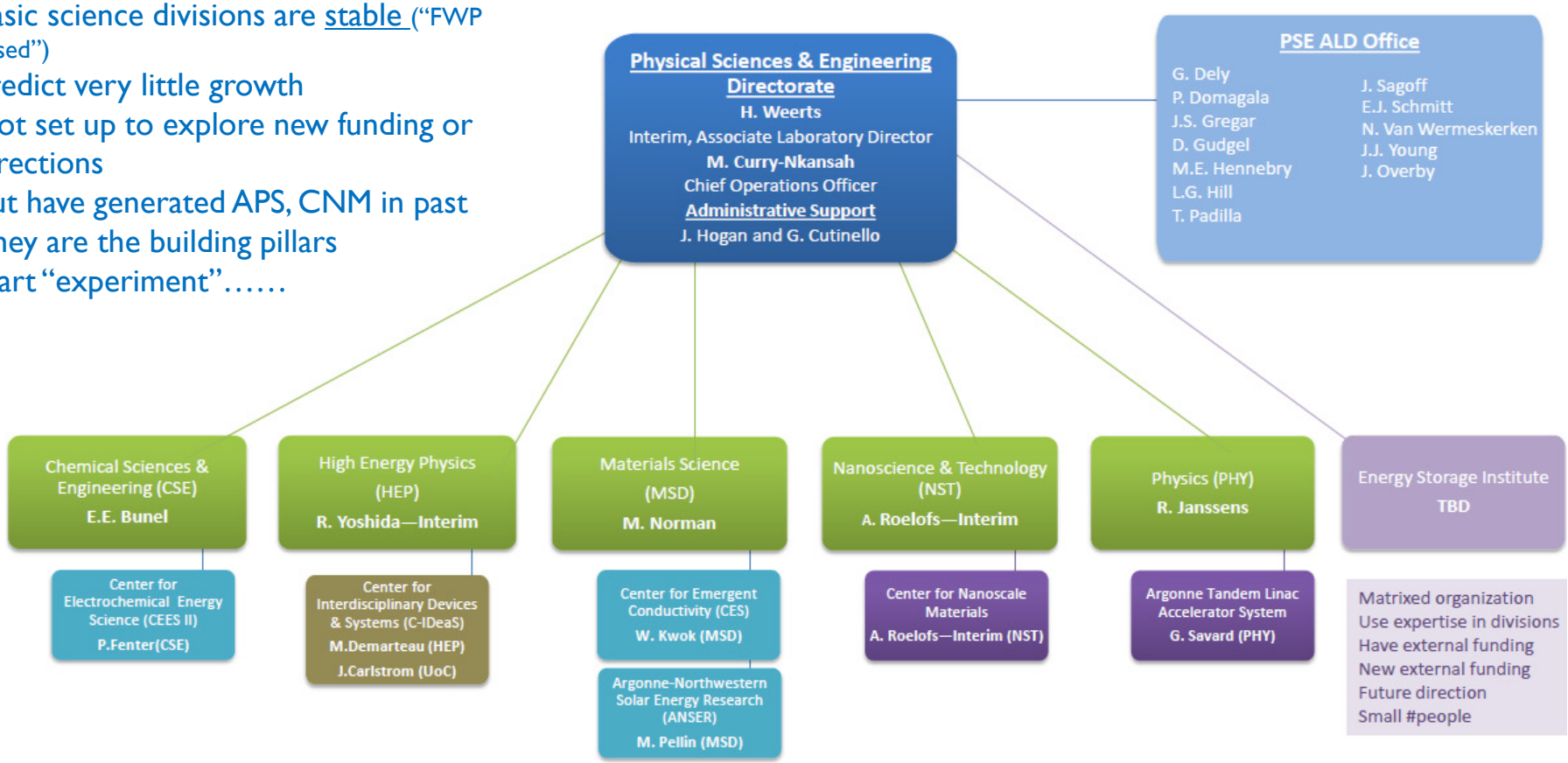
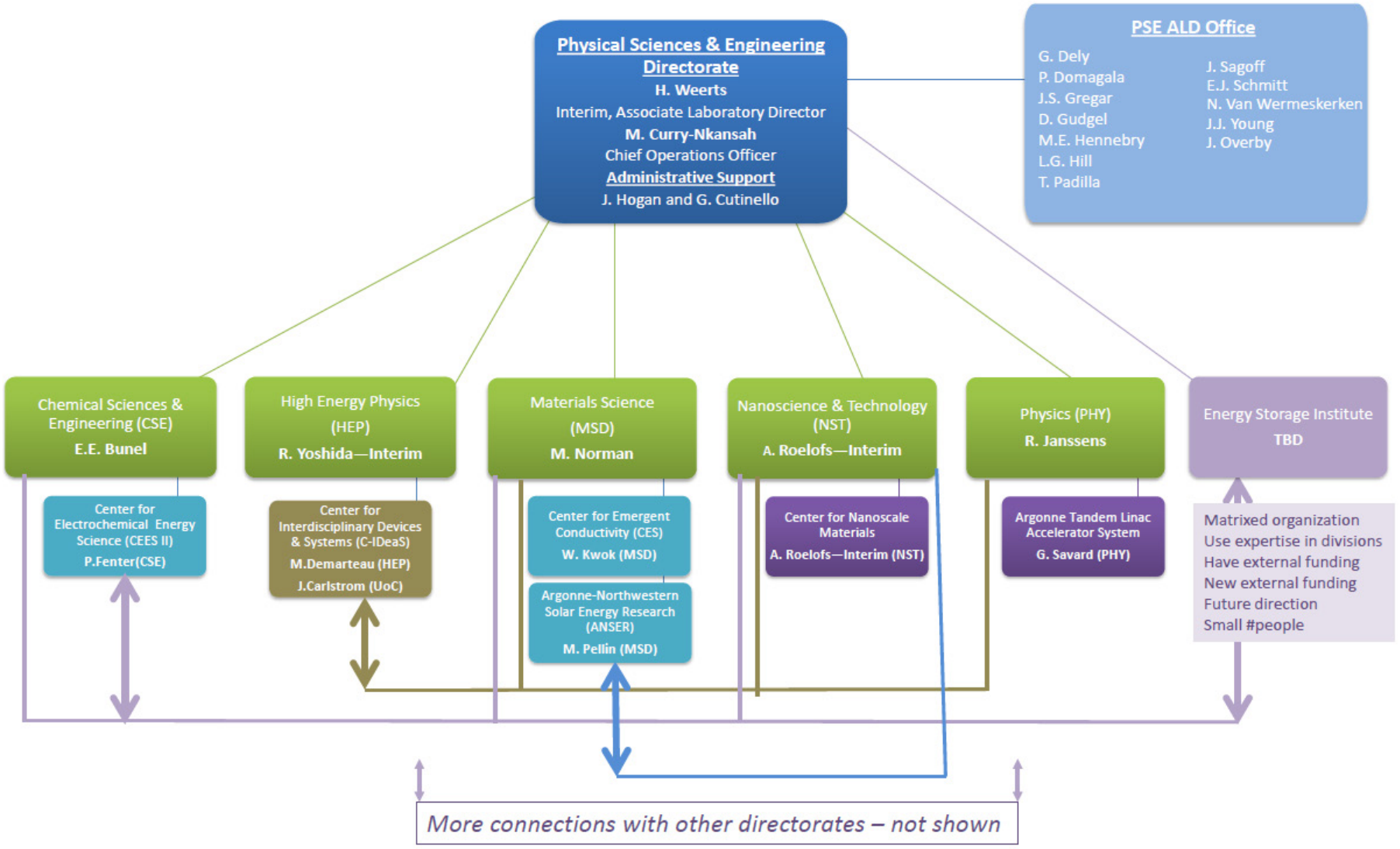


Experiment:

Start "Energy Storage Institute" as an experiment
Rather small in terms of people; but brings in funding
Relies on and uses expertise in divisions (matrix operation)
Can have a finite lifetime
Have more/other institutes in future (around a direction)

PSE – in FY15 – with connections



Connections, collaboration, multi/interdisciplinary activities = future

Conclusion

PSE growth opportunities are in:

"use inspired" research activities
"applied" research
building core science expertise

Resulting in something that will be manufactured

Batteries are perfect example

Conclusion A

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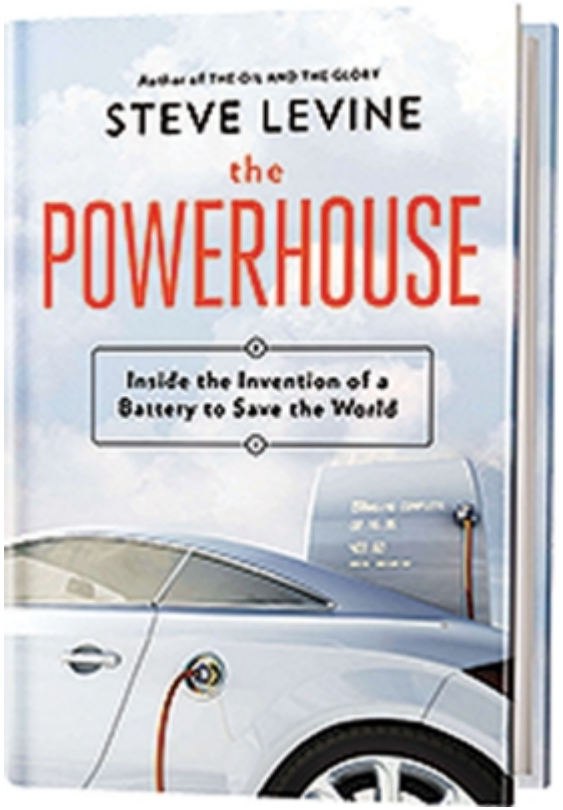

If a book is written about it, it must be a good model

Ingredients of PSE now in FY15 --

PHY | CSE | NST | MSD | HEP

With basically five well run divisions; organization based on these divisions

IME

ATLAS | CNM — User facilities – DOE recognized

CEES | CES | ANSER — EFRC's:

- Center for Electrochemical Energy Science
- Center for Emerging Superconductivity
- Argonne Northwestern Solar Energy Research center

SRF | AWA | ATTA | AAI — Facilities/capabilities

Large, LDRD funded initiative

Materials for Energy

- Materials and Molecular Design & Discovery (M2D2)
- Computational Materials
- Integrated Imaging Initiative

Ingredients of PSE – future vision/directions

PHY CSE NST MSD HEP

IME

With basically five well run divisions; organization based on these divisions

ATLAS CNM User facilities – DOE recognized

CEES CES ANSER EFRC's:

Center for Electrochemical Energy Science
Center for Emerging Superconductivity
Argonne Northwestern Solar Energy Research center

SRF AWA ATTA AAI Facilities/capabilities

AKHAN AKHAN Research Center – diamond – Carbon Research Center (CRC) Being put in place

Future vision/direction:

CMB-S4

BioIm

CoMaCh

BioIm

Combust

ASCES

BRAIN

AM(3D)

M2D2

C-IDeaS

IntIm

?????

Ingredients of PSE – future vision/directions

CMB-S4	Cosmic Microwave Background – Stage 4 – large science project
M2D2	Materials and Molecular Design and Discovery
IntIm	Integrated Imaging Initiative
CoMaCh	Computational Materials & Chemistry
AM(3D)	Additive Manufacturing
BioIm	Bio-inspired Hybrid Materials for Energy

MfE

Centers

ASCES	Argonne Strategic Center for Energy Storage
BRAIN	BRAIN initiative -- National Brain Observatory(NBO)
C-IDeaS	Center for Interdisciplinary Devices & Systems -- new devices & applied materials

Combust	The Ultimate combustion engine with EGS/ES (computational aspect)
?????	Future Accelerator based facilities……

Ingredients of PSE – future vision/directions

CMB-S4 Cosmic Microwave Background – Stage 4 – large science project

M2D2 Materials and Molecular Design and Discovery

IntIm Integrated Imaging Initiative

CoMaCh Computational Materials & Chemistry

AM(3D) Additive Manufacturing

BioIm Bio-inspired Hybrid Materials for Energy

"Molecules to Manufacturing"

Centers

ASCES Argonne Strategic Center for Energy Storage

BRAIN BRAIN initiative -- National Brain Observatory(NBO)

C-IDeaS Center for Interdisciplinary Devices & Systems -- new devices & applied materials

Combust The Ultimate combustion engine with EGS/ES (computational aspect)

????? Future Accelerator based facilities……

List provided by PSE:

revisit

1. Institute for Molecular Engineering (IME) IME
2. National Brain Observatory (NBO) BRAIN
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5. Silicon Tracking for LHC Phase II Upgrade
6. Center for Atom Trap Trace Analysis of Noble Gas Radionuclides
7. Novel devices and Applied Materials C-IDeaS → CMB-S4
8. Computational Chemistry and Materials CoMaCh
9. Integrated Imaging IntIm
10. Materials and Molecular Design and Discovery M2D2
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????? Not on list for now --- future

1. Institute for Molecular Engineering (IME)
2. National Brain Observatory (NBO)
3. Argonne Strategic Center for Energy Storage (ASCES)

Institute for Molecular Engineering (IME) IME

These are basically startup funds for IME activities and all support the research of joint positions with IME. Goal: establish funding streams for IME at Argonne thru BES.

National Brain Observatory (NBO) BRAIN

What and how Argonne can contribute to the NIH and NSF led BRAIN initiative. These funds would support an initial group (one) of neuroscientist establishing a bridge on how to make use of Argonne expertise & facilities to enable BRAIN initiative. Hire in progress.

Argonne Strategic Center for Energy Storage (ASCES) ASCES

Center to enhance the battery program even more, bring in more industry work/connections and bring Argonne's leading role in this to next level. This has been discussed for a while and we simply want to start the "experiment".

4. Development of a Multi-User Upgrade of ATLAS
5. Silicon Tracking for LHC Phase II Upgrade
6. Center for Atom Trap Trace Analysis of Noble Gas Radionuclides

These are initiatives to enable specific programs funded by a particular office in Office of Science. It enables a new capability and possibly future funding.

Development of a Multi-User Upgrade of ATLAS (PHY)
ATLAS is a NP user facility. Only stable beam facility in the US. To do its physics, want to run more than one experiment at the same time. NSAC long range plan is due April 2015. Need to show Argonne interest to get upgrade funding in future.

Silicon Tracking for LHC Phase II Upgrade (HEP)
LHC needs to go to high luminosity around 2022, requiring major detector upgrades. Argonne wants to build part of new silicon tracker and needs infrastructure locally to attract upgrade funding. Use for future silicon detectors for APS??

Center for Atom Trap Trace Analysis of Noble Gas Radionuclides (PHY)
Unique capability to do radio-krypton (^{81}Kr) dating and has shown this world class capability, by dating ground water (<100K years). Should we invest in improving method (smaller samples) ? This is of interest to national security applications.
Can we establish a connection to national security?

7. Novel devices and Applied Materials

C-IDeaS → CMB-S4

Novel devices and Applied Materials

Establish a world-leading center to develop novel devices and detectors cutting across the entire lab and including industry. Bring industry & science problems to lab.

Name (C-IDeaS) will most likely change

Together with University of Chicago (narrower scope there)

Together with additional cleanroom space (planned) important ingredient in realizing CMB-S4 at Argonne- University of Chicago- Fermilab.

Replaces "Materials for Energy"

8. Computational Chemistry and Materials
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"Molecules to Manufacturing"

Long term (simple) vision of where materials and chemistry will be in 10 to 15 years and how it will effect manufacturing. Theory/simulation (exascale) -> quantitative predictions of properties of "new materials".
Need "Computational Material and Chemistry" effort over next decade.
Experimental verification effort: M2D2; Imaging.
Take the step to manufacturing "things" (call them devices) by using additive manufacturing tools ("3D printing"), synthesis, atomic layer deposition, etc. Using our unique capabilities
Can only be done with our expertise and facilities .

At some point also include bio inspired materials as well as "quantum' materials.

May be only implement parts at Argonne initially

Integrated Approach to Develop and Optimize Fuel Chemistry

The development of a unified suite of high performance computer (HPC) codes that can *identify* promising biofuels and fuel additives, *develop* their combustion mechanisms in phases of increasing accuracy and reliability, and *simulate for validation* a supporting array of experimental measurements.

This would be in collaboration with Transportation in Energy Systems division.

Long term goal: *The ultimate combustion engine*

Can we set challenging long term goal ?? Like we did for batteries in JCESR ?

Future

This is snapshot where thinking is now

Process rushed

Strategic plan still be formulated

Without your input this will not work

Next year process repeats

Your input is needed during the whole year

Not just input to strategic lab plan but also to:

Future EFRC submissions/planning
LDRD funding/initiatives
……

Really ongoing process and need your input continuously = our future