Committee Minutes

Committee on Research
Duck Pond Room
The Inn at Virginia Tech and Skelton Conference Center
4:15-5:30 p.m.

November 6, 2016

Committee Members Present:

Mr. Mehmood Kazmi
Mr. Stephen Sturgis
Mr. Jeff Veatch
Mr. Horacio Valerias

Guests:

Dr. Timothy Sands, Dr. Thanassis Rikakis, Mr. Dwight Shelton Jr., Mr. James L. Chapman, Ms. Greta J. Harrris, Mr. Charles T. Hill, Ms. Deborah Petrine, Mr. Michael J. Quillen, Rev. Wayne H. Robinson, Dr. J. Thomas Ryan, Mr. Mehul Sanghani, Mr. Dennis H. Treacy, Dr. Monty Abbas, Dr. Daniel Crawford, Mr. Martin Daniel, Dr. Karen DePauw, Mr. Gannon Davis, Mr. Viet Bien Doung, Dr. Srinath Ekkad, Dr. Lance Franklin, Dr. Michael Friedlander, Ms. Kay Heidbreder, Dr. Michael Hochella, Mr. Tim Hodge, Ms. Elizabeth Hooper, Dr. Ed Jones, Dr. Mike Lambur, Dr. Steven McKnight, Dr. Scott Midkiff, Ms. Kim O'Rourke, Mr. Mark Owczarski, Dr. Patty Perrillo, Mr. Charles Phlegar, Dr. Ellen Plummer, Mr. J. Scot Ransbottom, Ms. Tracy Vosburgh, Dr. Sherwood Wilson and Ms. Beth Tranter.

1. **Opening Remarks and Approval of August 28, 2016 Minutes.** Mr. Kazmi called the meeting to order and welcomed those in attendance. The minutes were unanimously approved.

2. **Remarks from the President.** Dr. Sands welcomed those in attendance, noting that the discussion on research expenditures will include a more detailed presentation of research scorecard metrics than was included in the information session. He also noted that future meetings will expand on these metrics to include a focus on scholarship and technology transfer outcomes.

3. **Resolution for Exclusion of Certain Officers/Directors**: Mr. Kazmi provided an overview of the Resolution for Exclusion of Certain/Officers/Directors. The resolution was unanimously approved by the committee.

4. **Report on Research and Innovation Metrics:** Dr. Mayer presented an overview of Virginia Tech's National Science Foundation-reported research expenditures, a

bellwether measure of the research productivity of universities. Dr. Mayer also highlighted areas of increased future federal investment, including applied energy, transportation, agriculture, defense and health, all areas in which Virginia Tech has particular strengths. Dr. Mayer identified upward potential for research productivity in Department of Defense and applied energy research, as well as increasing competitiveness in biomedical and life sciences. While research expenditures have increased slightly since 2010, extramural research funding has remained somewhat flat. With proper strategic investments in faculty resources and proposal development infrastructure, the university will be able to capitalize on these opportunities, enabling continued growth in research in the future. The Office of the Vice President for Research and Innovation will also enhance infrastructure for strategic research program support, industry partnerships, and licensing and ventures to foster research growth. Finally, Dr. Mayer presented plans for the development of a business engagement strategy, a joint initiative between the Office of Research and the Office of Advancement, designed to develop deep relationships with selected corporate partners.

5. **Overview of NSF-Funded National Nanotechnology Coordinated Infrastructure Network Site – NanoEarth**: Dr. Michael Hochella delivered a presentation on NanoEarth, a National Center for Earth and Environmental Nanotechnology Infrastructure. This network includes sixteen national sites representing an $81 million investment. Facilities include the Virginia Tech Center for Sustainable Nanotechnology and the Nanoscale Characterization and Fabrication Laboratory. To date, the Center is a resource for more than 20 institutions, domestic and international, including community colleges and four-year liberal arts institutions.

6. **Overview of NSF-Funded Molecular Software Sciences Institute** Dr. Daniel Crawford, professor in the College of Science's Department of Chemistry, heads the Molecular Sciences Software Institute, an initiative being funded by the National Science Foundation and in part inspired by the White House's year-old National Strategic Computing Initiative. The institute, housed at Virginia Tech's Corporate Research Center, is a $19.4 million initiative to build a national team of software scientists to design and build new, powerful software tools that can help researchers across a diverse array of disciplines to tackle wide-ranging, complex, data-heavy issues, such as cancer, diabetes, and Alzheimer's disease, as well as create new energy storage systems that can help stem climate change.

Adjournment.

There being no further business, the meeting adjourned at 5:41 p.m.

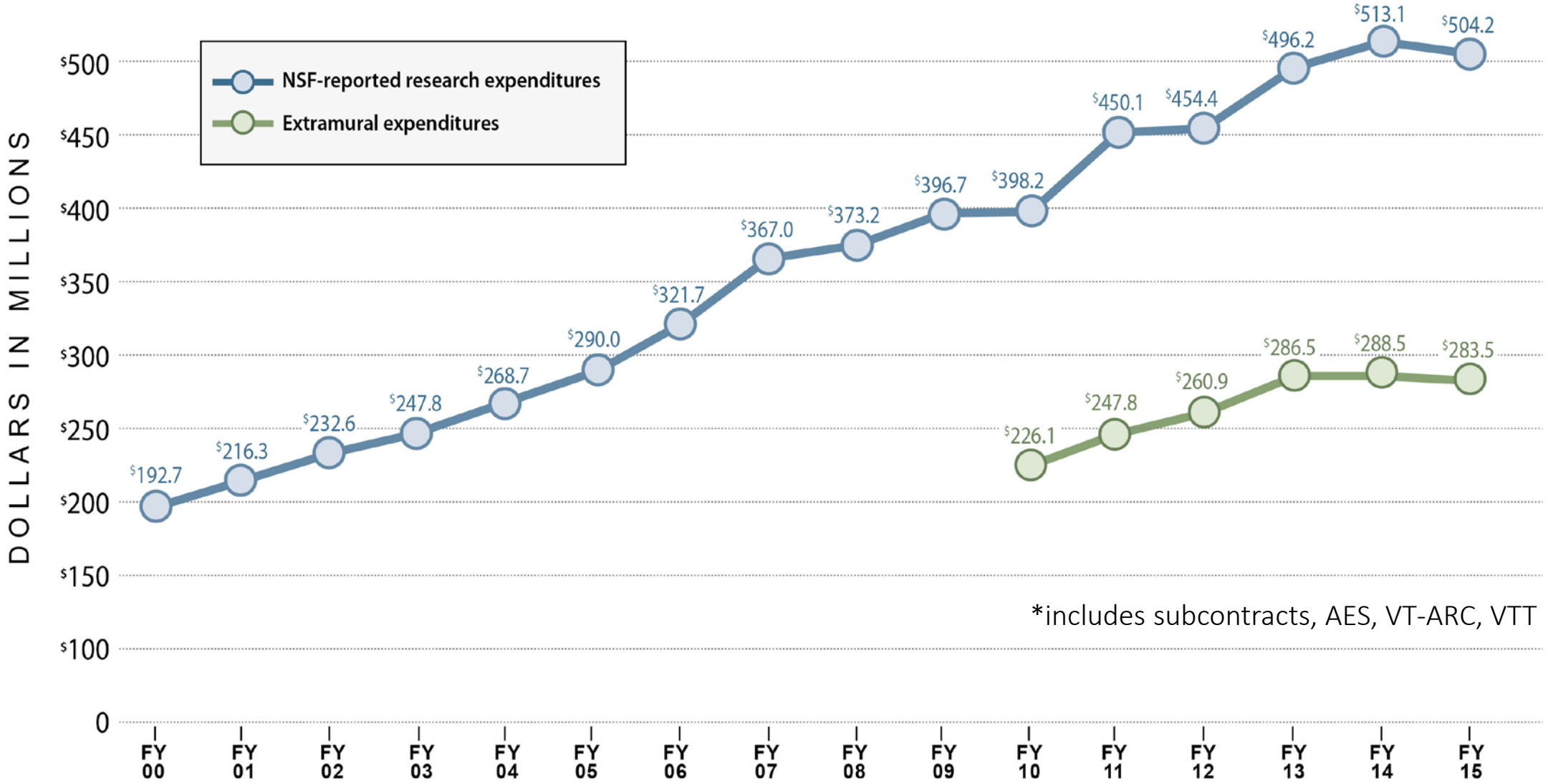
BOV Research Committee Report

November 6, 2016

Priorities for Research & Innovation

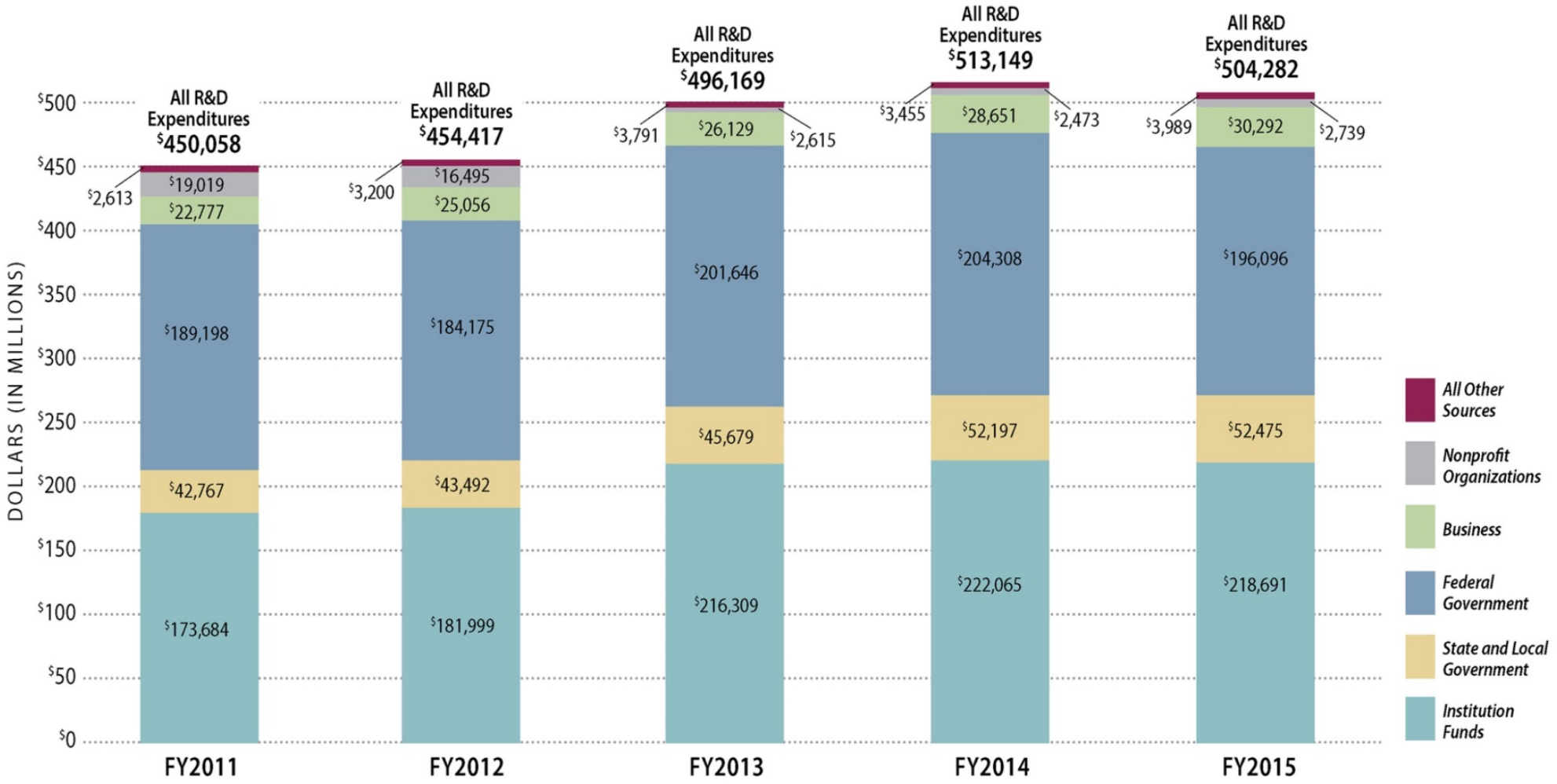
- Reverse recent trend of flat extramural research support and resume growth commensurate with targets
- Enhance the impact of research and innovation through scholarly works, communications, and marketing
- Increase the strategic cross-sector partnerships and entrepreneurial ventures

Research Expenditure History



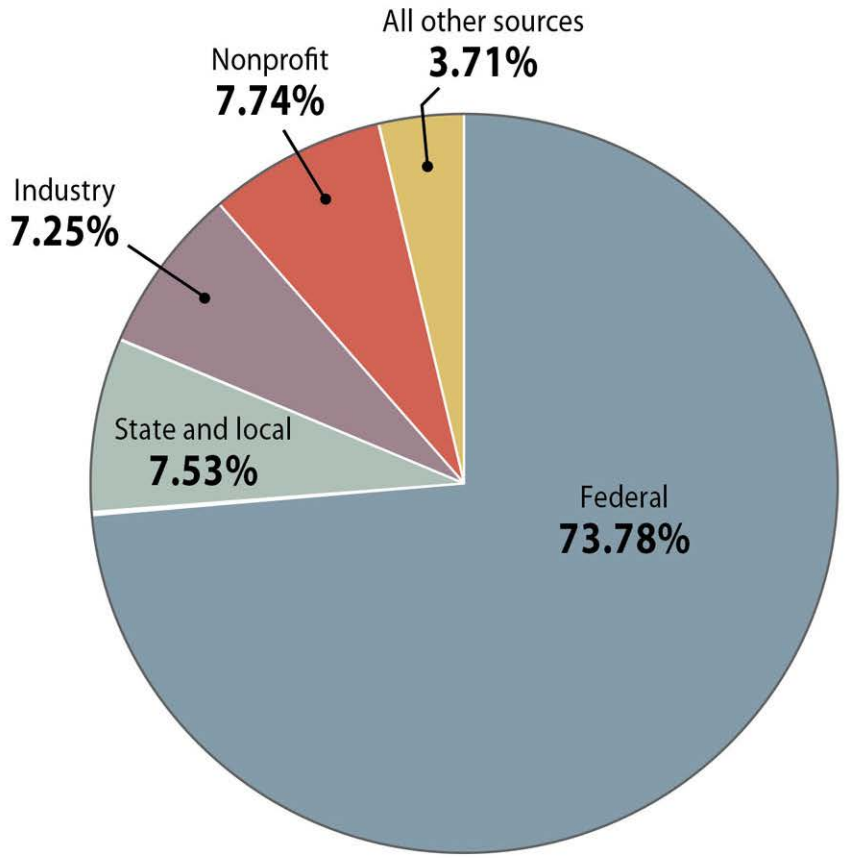
*includes subcontracts, AES, VT-ARC, VTT

Resources to Support Research Enterprise

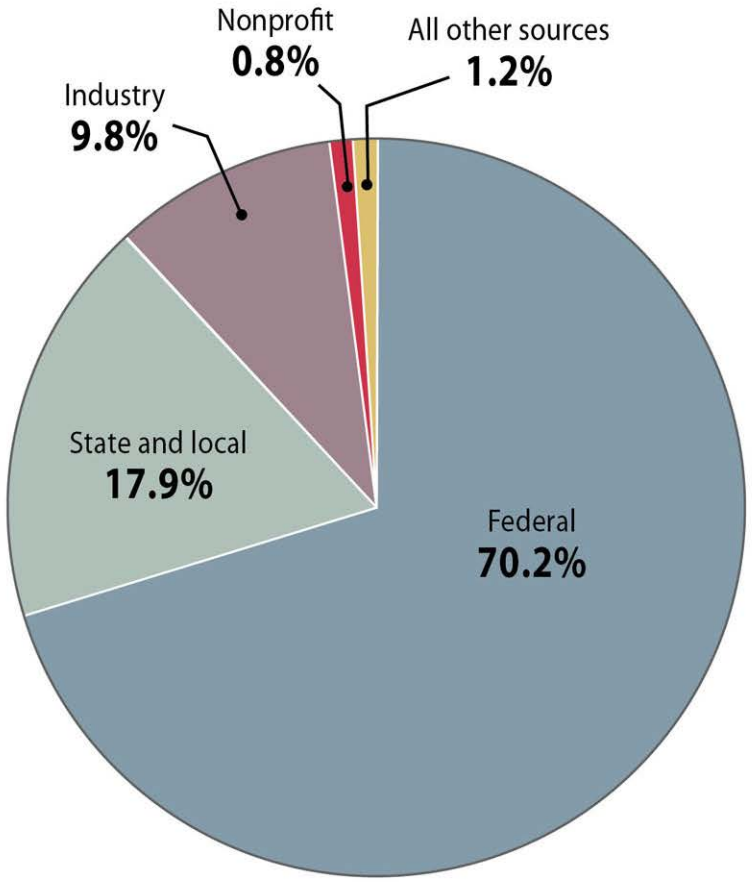


External Sponsors of Research

ALL UNIVERSITIES



VA TECH*



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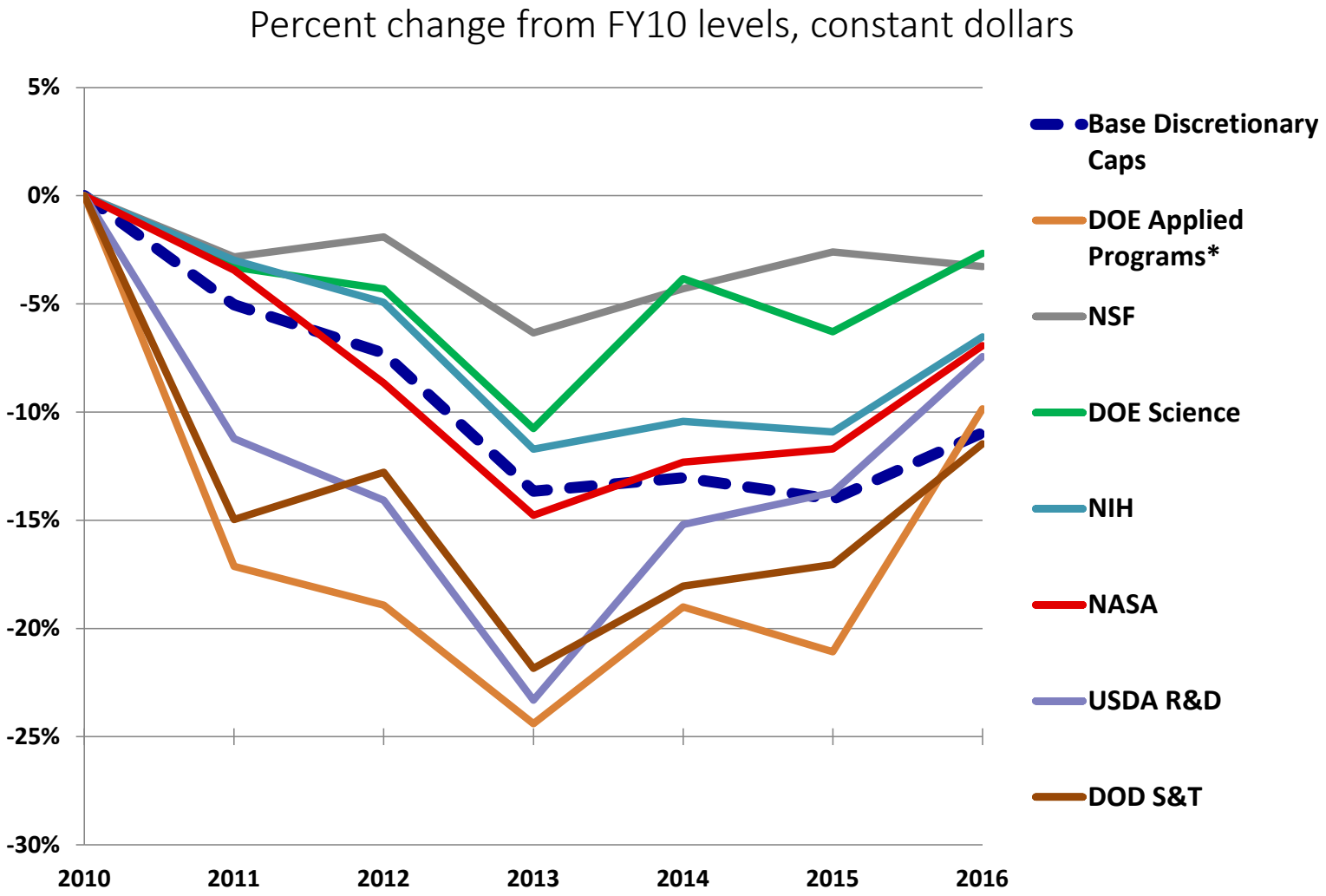
Federal Spending Since FY2010

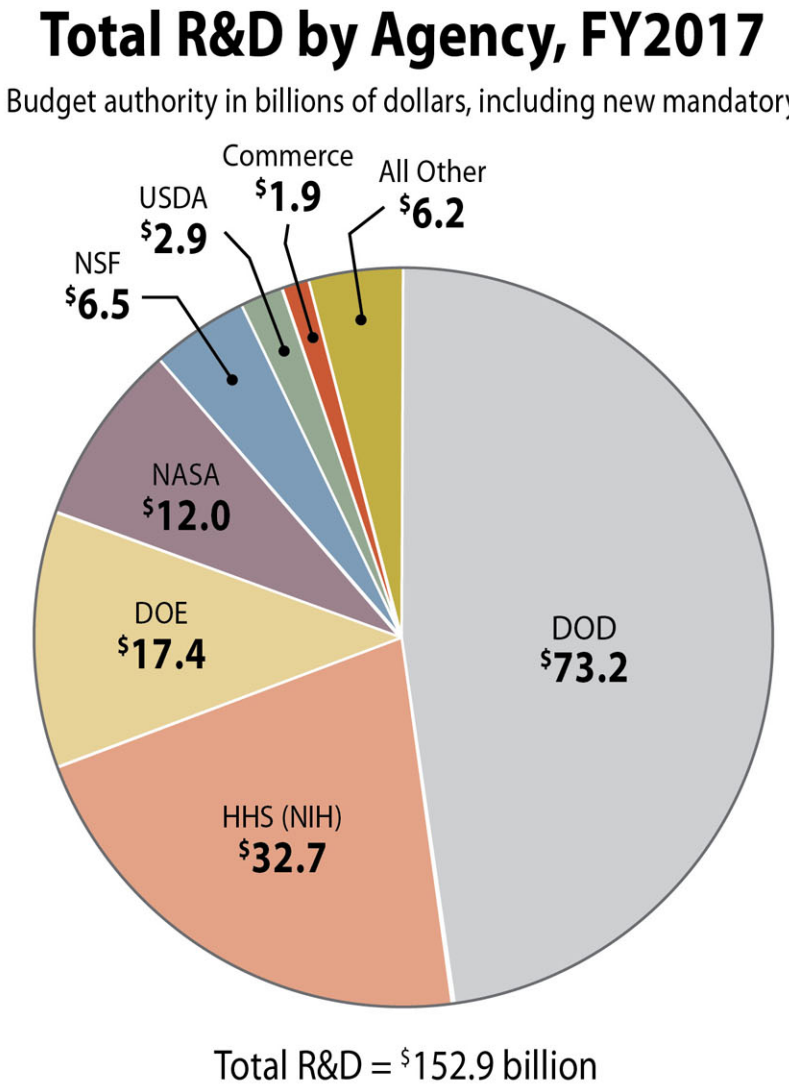


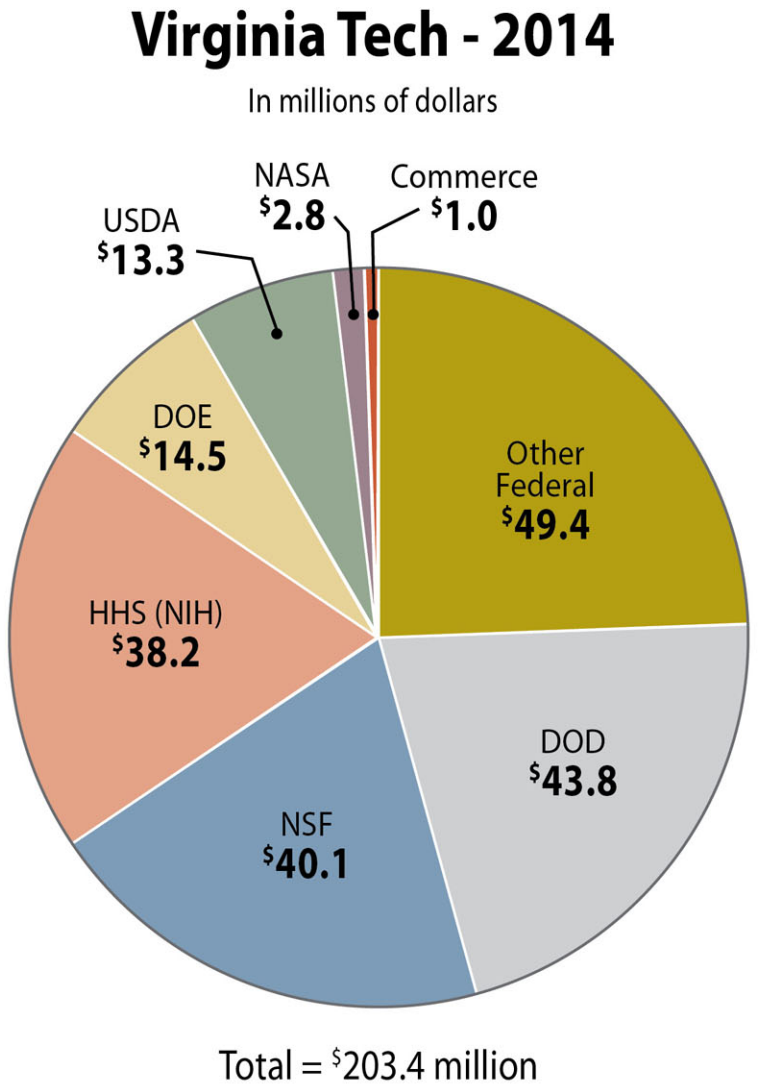
Percent change from FY16

Applied energy:	38.6%
Transportation:	22.8%
Agriculture:	11.5%
General Science:	6.4%
Defense:	4.0%
Health:	2.6%

*Includes EERE, OE, Fossil, Nuclear; excludes ARPA-E (regular appropriations began in FY 2011).

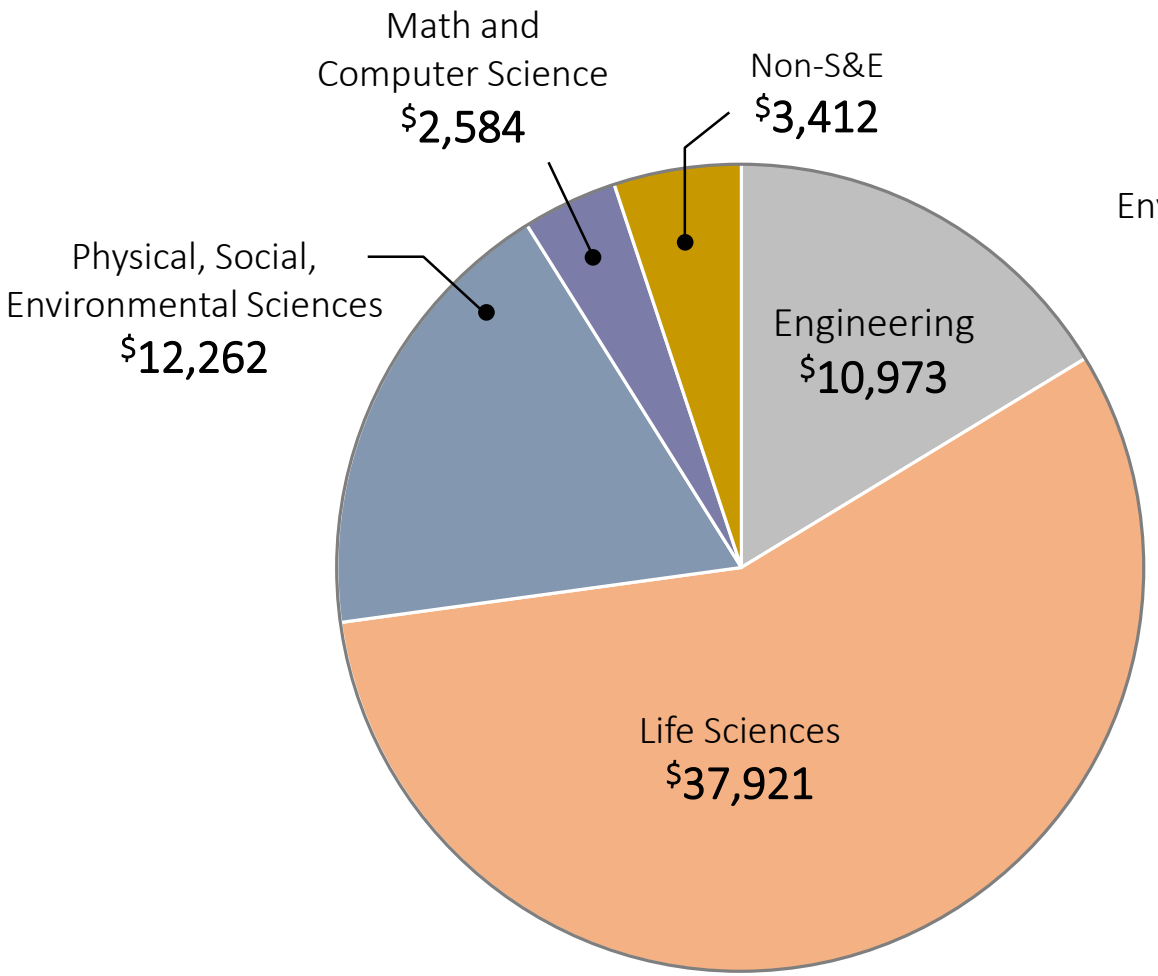
Federal Sponsors of Research





External Sponsors by R&D Field

ALL UNIVERSITIES



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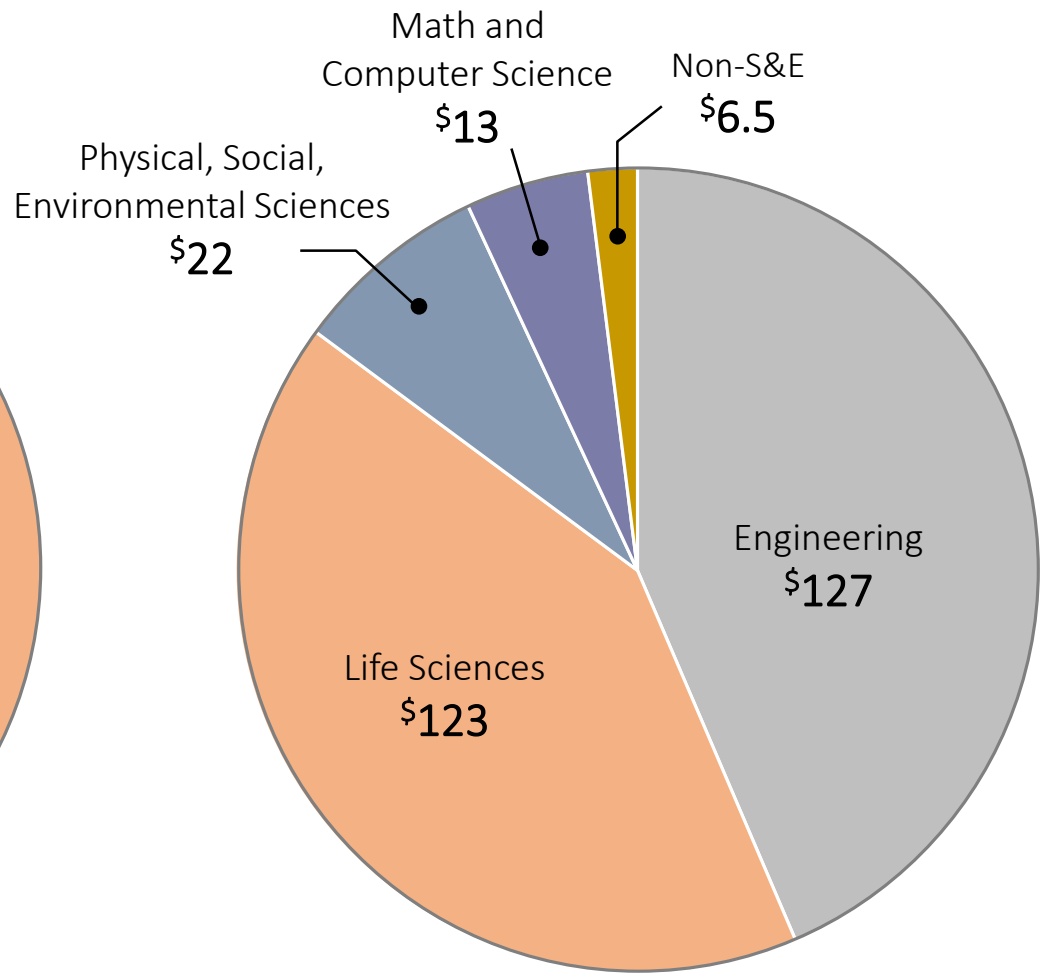

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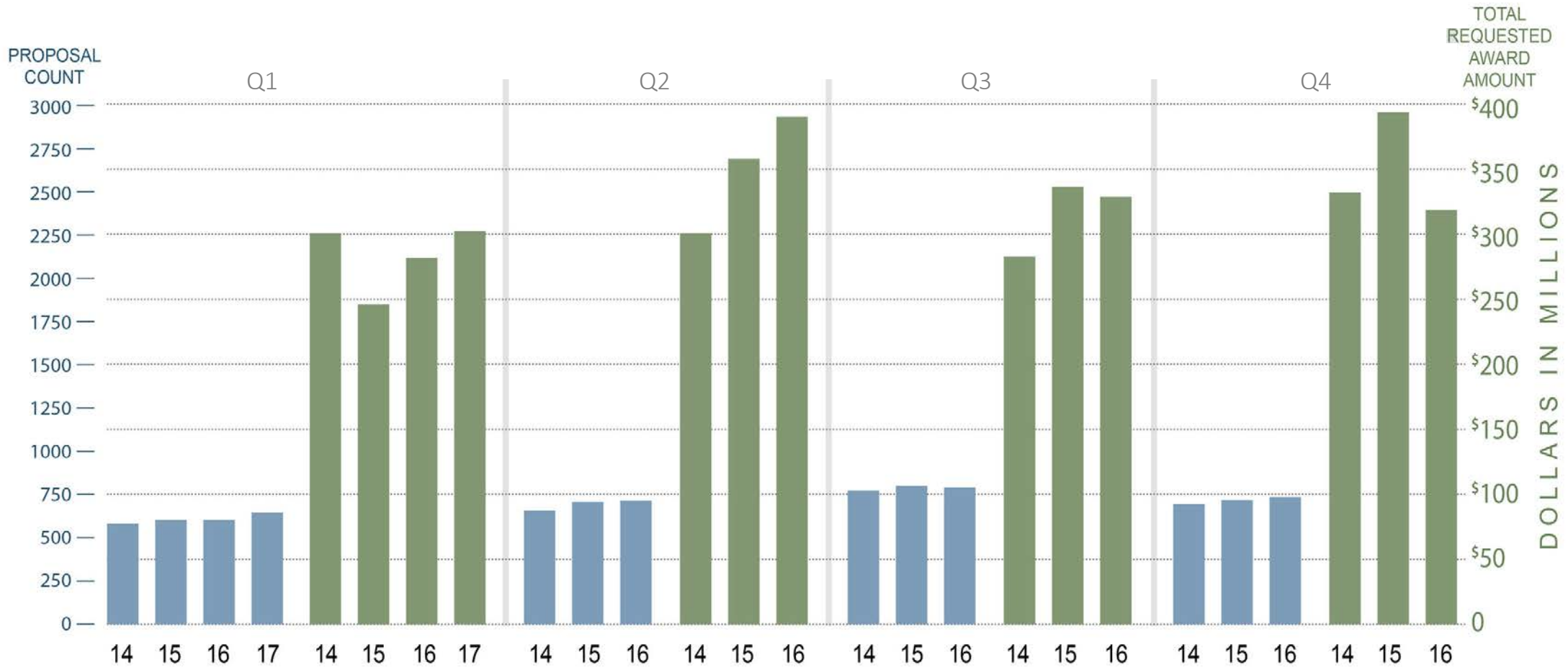
Proposals Submitted and Requested Amount

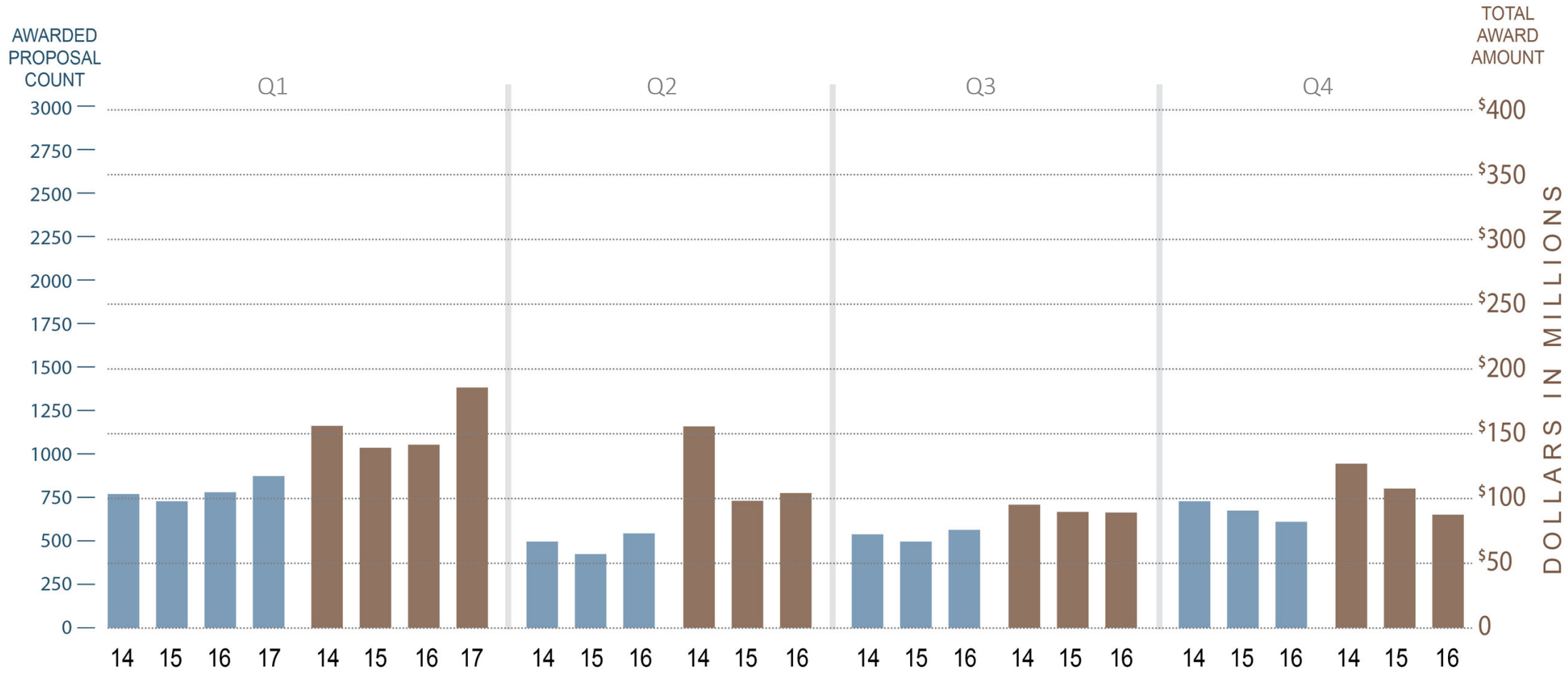
	Number Submitted	Total Requested Award Amount
FY14	2691	$1,218 M
FY15	2815	$1,339 M
FY16	2867	$1,323 M



*includes subcontracts

Awarded Programs and Anticipated Amount

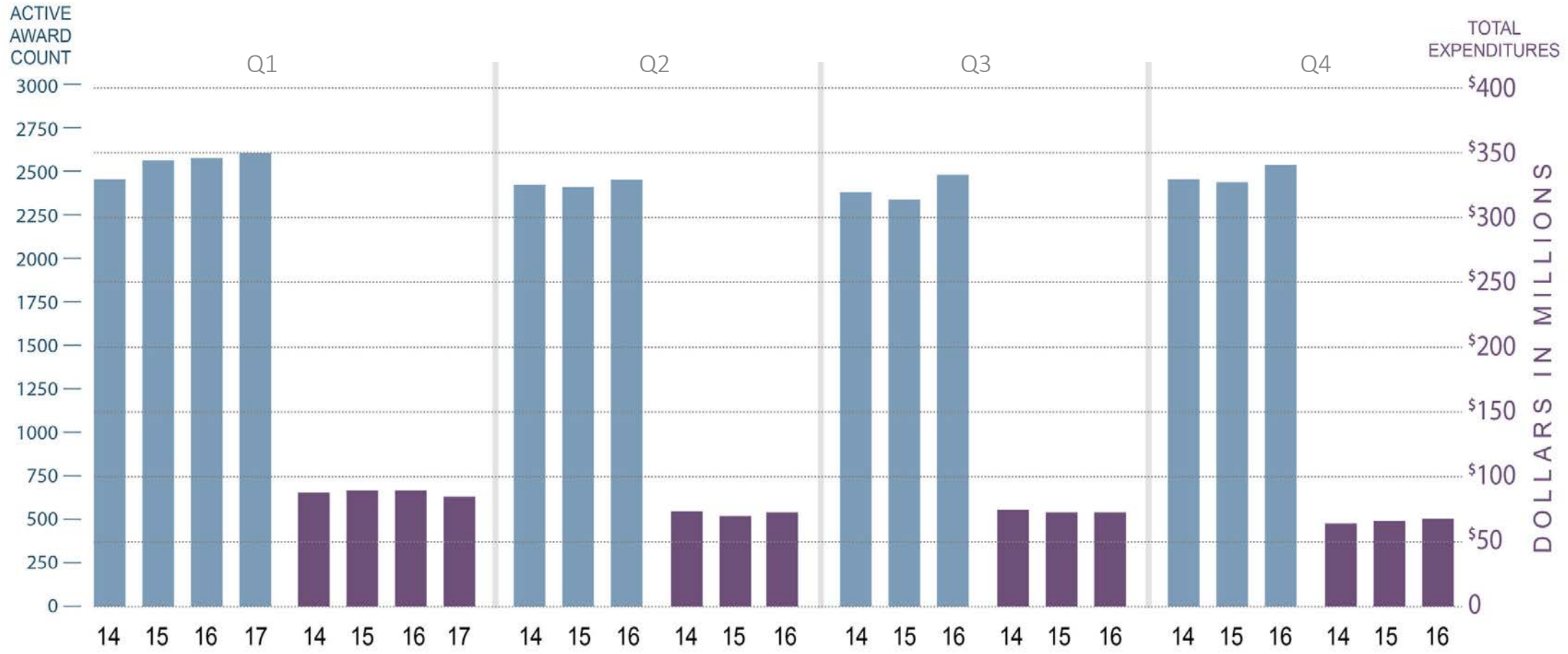
	Number Awarded	Total Anticipated Award Amount
FY14	1935	$531 M
FY15	1839	$432 M
FY16	1966	$385 M



*includes subcontracts

Active Awards and Expenditures

	Number Active	Research Expenditures
FY14	3420	$250 M
FY15	3483	$248 M
FY16	3651	$249 M



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Office of Research and Innovation

- Research Administration
- Research Compliance and Ethics
- Communications and Marketing
- Research Institutes and Affiliated Corporations
- Strategic Research Program Support
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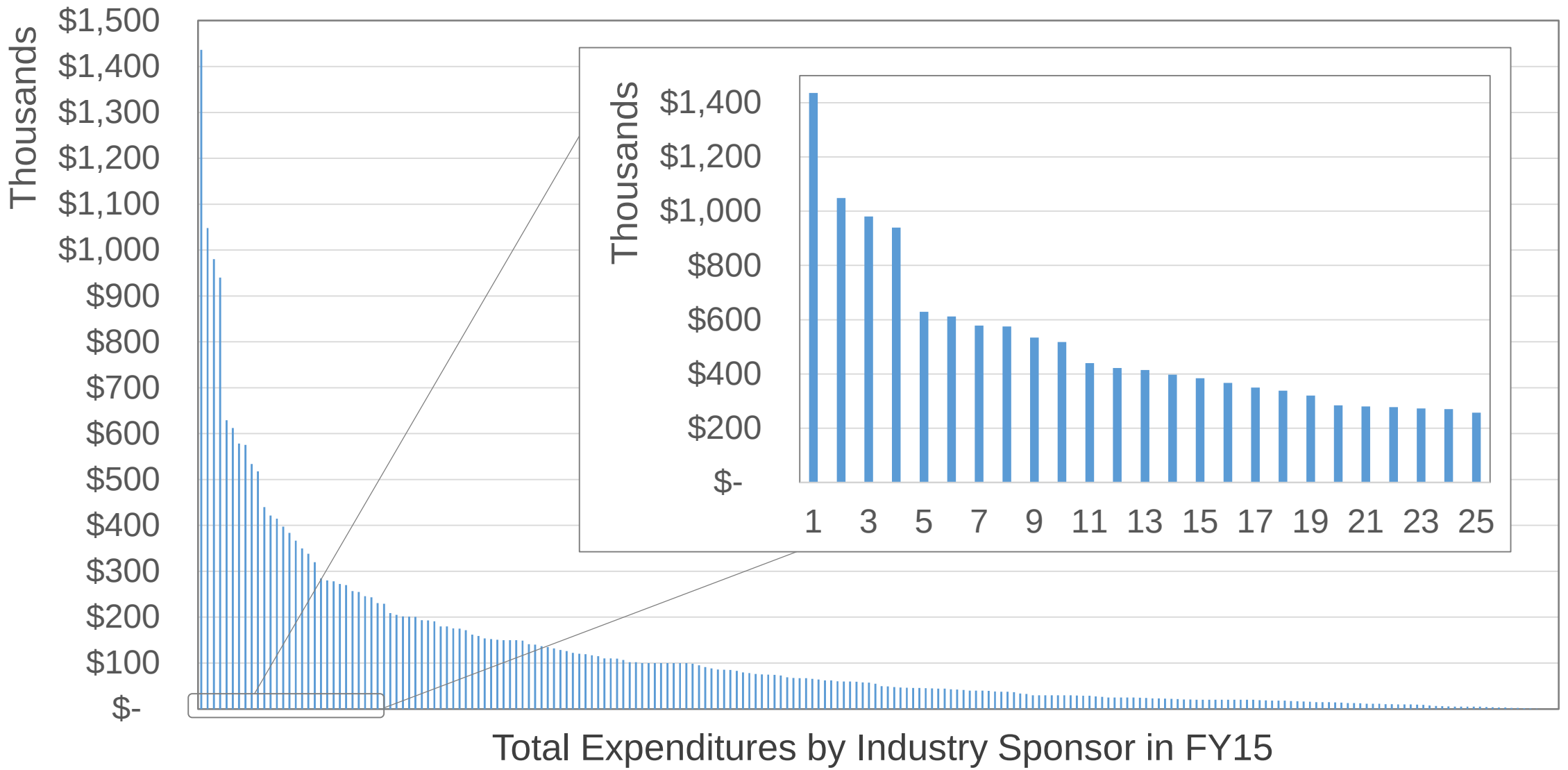
Current Research Portfolio with Industry



Business Engagement Center

- Identifying alignment between needs and expertise
- Connecting talent across both organizations
- Catalyzing innovation through collaboration

Business Engagement Center

- Renew traditional Corporate and Foundation Relations (CFR) approach to industry relations
- Collaboration between Advancement & Research Offices
- Central BEC team members will support strategic cross-university relationships, data curation and analysis
- College-level BEC team members will support focused relationships in the units

Research & Outreach Highlights

Press Release 15-112

$81 million to support new National Nanotechnology Coordinated Infrastructure

16 sites to give academic, small business and industry researchers access to nanotechnology research

National Center for Earth and Environmental Nanotechnology Infrastructure

Michael Hochella

Press Release 16-088

NSF commits $35 million to improve scientific software

Awards will support long-term hubs dedicated to strengthening scientific software ecosystem

Molecular Sciences Software Institute

Daniel Crawford

The Molecular Sciences Software Institute

Prof. T. Daniel Crawford
Department of Chemistry, Virginia Tech, Blacksburg, Virginia

Virginia Tech Board of Visitors

6 November 2016

The Molecular Sciences Software Institute (MolSSI)

- New project (as of August 1st, 2016) funded by the National Science Foundation (NSF).
- Part of the NSF's commitment to the White House's National Strategic Computing Initiative (NSCI).
- Virginia Tech is the lead with collaborators at Rice U., Stony Brook U., U.C. Berkeley, Stanford U., Rutgers U., U. Southern California, and Iowa State U.
- Total budget of $19.42M for five years, potentially renewable to ten years. The vast majority of these resources remain at VT.
- Designed to serve and enhance the software development efforts of the broad field of computational molecular science.
- We began project concept and development in 2010.

CMS Codes Are Developed and Used Globally

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Gaussian

LAMMPS

NAMD

GAMESS

Dalton

These codes represent **decades** of development by thousands of programmers, and are used by **tens of thousands** of scientists worldwide.

QUANTUM ESPRESSO

CHEM

ORCA

GROMACS

Groningen Machine for Chemical Simulations

TURBOMOLE

MOLPRO

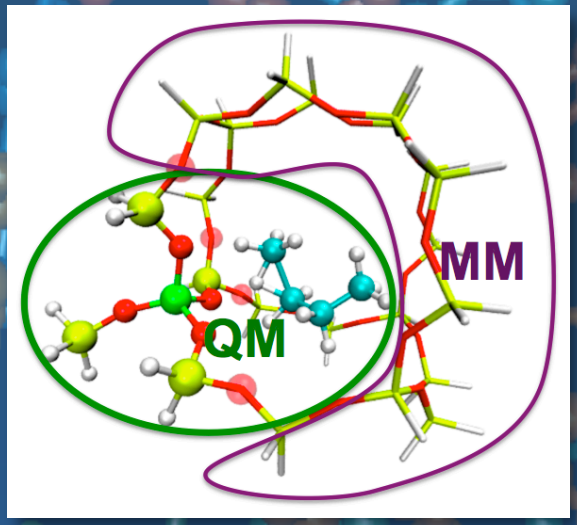
What New Science *Could* We Enable?

- **Intrinsically Disordered Proteins:** Required to understand biochemical function and disease: cellular regulation and signaling; associated with cancer, diabetes, and Alzheimers.

The IDP TAZ1-domain–CITED2 complex (PDB: 1R8U)

What New Science *Could* We Enable?

- **Intrinsically Disordered Proteins:** Required to understand biochemical function and disease: cellular regulation and signaling; associated with cancer, diabetes, and Alzheimers.
- **Molecular-Level Catalyst Design:** Optimizing catalyst performance is vital to the multi-billion dollar global chemical, biochemical, petrochemical, and pharmaceutical industries.



Present-day hybrid QM/MM model of a zeolite catalyst framework. [Adapted from: P.M. Zimmerman *et al.*, *J. Chem. Theory. Comp.* **7**, 1695 (2011).]

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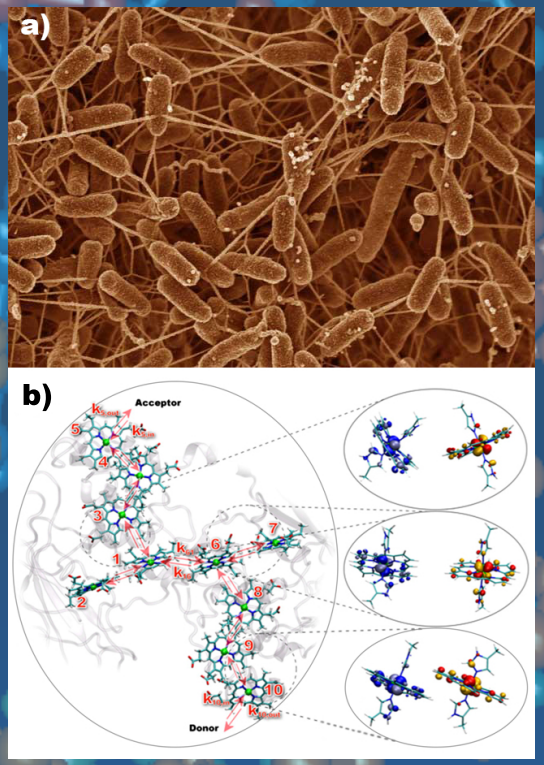
- **Molecular-Level Catalyst Design:** Optimizing catalyst performance is vital to the multi-billion dollar global chemical, biochemical, petrochemical, and pharmaceutical industries.
- **Complex Materials Chemistry:** Critical for mechanistic insight into fuel-cell membranes, light-harvesting plants, data-storage devices, etc.



(a) A bacterium exhibiting 8-10 nm nanowires; (b) Heme cofactors in a protein responsible for electron transport. [Adapted from: M. Breuer *et al.*, *Proc. Nat. Acad. Sci.*, **111**, 611-616 (2014)]

The Molecular Sciences Software Institute (MolSSI)

Expertise

- MolSSI will work with CMS research groups nationwide and internationally to design, develop, test, deploy, and maintain key code infrastructure and frameworks for the entire community.
- MolSSI will interact with partners in industry, NSF supercomputing centers, national laboratories, and international facilities to identify and act on emerging hardware trends, access leading-edge computing architectures, further educational goals, set software priorities, and identify future workforce career paths.

The Molecular Sciences Software Institute (MolSSI)

Education, Outreach, and Training

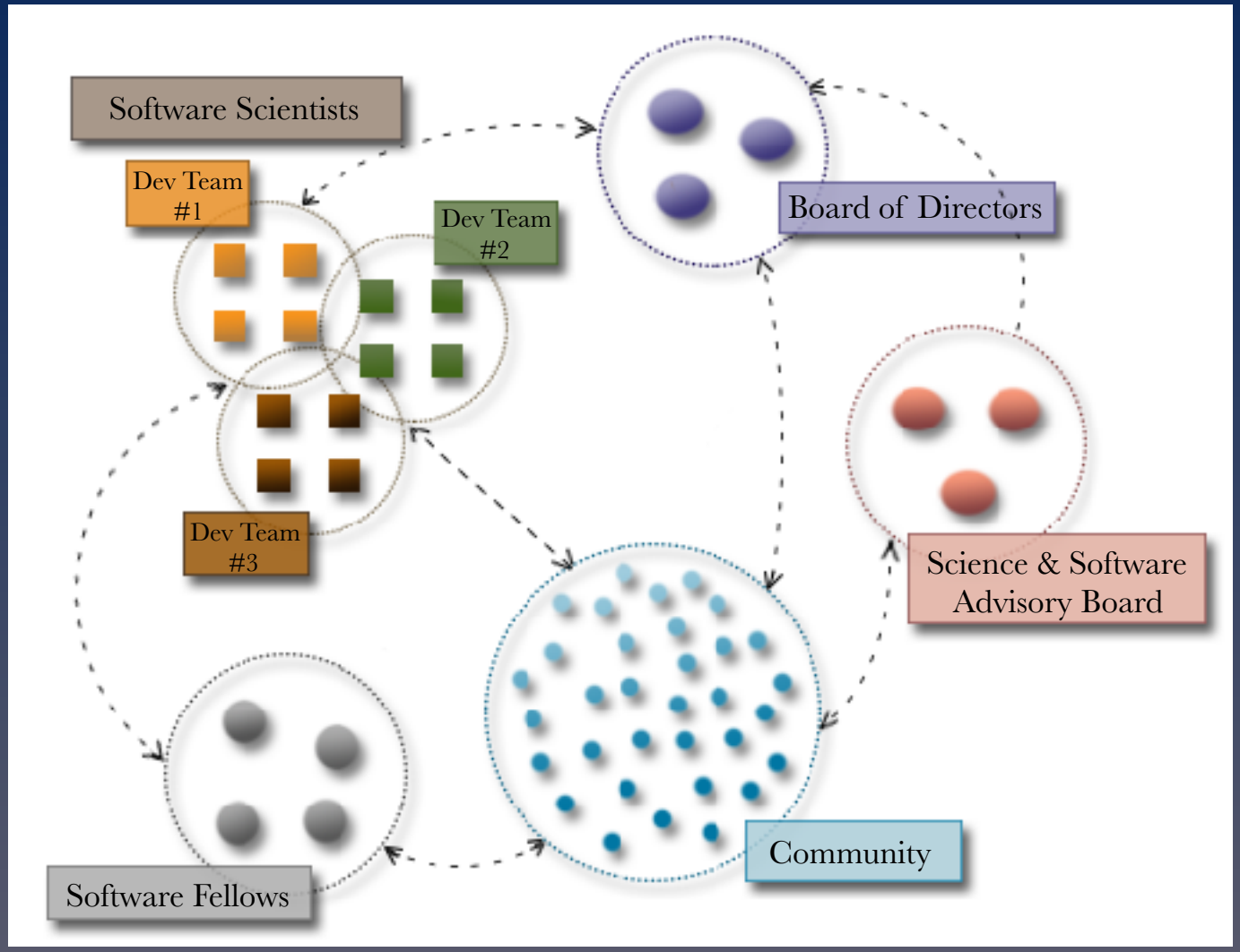
- MolSSI will serve as an education and outreach nexus for the worldwide CMS community.
- MolSSI will organize summer schools, targeted workshops, high-school and undergraduate training programs, and on-line resources and classes to provide current and future CMS students with a modern and complete set of programming skills.
- MolSSI will reach beyond the traditional student cohort to computer scientists and mathematicians seeking interdisciplinary applications.
- MolSSI will deploy a Professional Master's program in Molecular Simulation and Software Engineering.

The Molecular Sciences Software Institute (MolSSI)

Community Engagement and Leadership

- MolSSI will enable the CMS community to establish its own standards for interoperability, best practices, and curation tools.
- Through a "**grass roots**" approach, MolSSI will engage the community broadly using interoperability workshops and focus groups – and ultimately the formation of a Molecular Sciences Consortium – to catalyze the consensus needed for standardization of data structures, APIs, and frameworks for the entire CMS software ecosystem.

The Molecular Sciences Software Institute (MolSSI)



The MolSSI Software Scientists (MSSs)

- A team of ~12 software engineering experts, drawn both from newly minted Ph.D.s and established researchers in molecular sciences, computer science, and applied mathematics.
- Dedicated to multiple responsibilities:
  - Developing software infrastructure and frameworks;
  - Interacting with CMS research groups and community code developers;
  - Providing forums for standards development and resource curation;
  - Serving as mentors to MolSSI Software Fellows;
  - Working with industrial, national laboratory, and international partners;

Approximately 50% of the Institute's budget will directly support the MolSSI Software Scientists.

The MolSSI Software Fellows (MSFs)

- A cohort of ~16 Fellows supported simultaneously – graduate students and postdocs selected by the Science and Software Advisory Board from research groups across the U.S.
- Fellows will work directly with both the Software Scientists and the MolSSI Directors, thus providing a conduit between the Institute and the CMS community itself.
- Fellows will work on their own projects, as well as contribute to the MolSSI development efforts, and they will engage in outreach and education activities under the Institute guidance.
- Funding for MolSSI Software Fellows will follow a flexible, two-phase structure, providing up to two years of support.

Approximately 25% of the Institute's budget will directly support the MolSSI Software Fellows.


Education and Training

Summer Schools and Hack-a-Thons

- Expand and broaden the summer schools we organized over three years of S2I2 conceptualization activities.

- Up to three schools per year will be held at sites across the country in order to provide access to as much of the community as possible.

- High-school hack-a-thons in the model of the SBU IACS will extend MolSSI's educational outreach.
- Emphasize participation by members of underrepresented groups and underwrite costs for students with special financial needs.

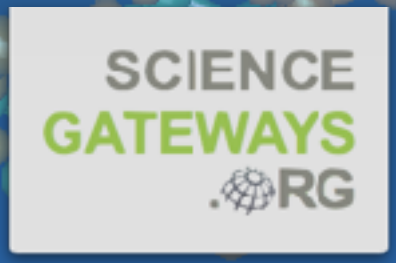
Professional Master's in Molecular Simulation and Software Engineering (MSSE)

- A two-year, self-supporting, part-time Master's program comprised of 26 units including:
  - Computational chemistry
  - Materials science
  - CS294: Software Engineering for Scientific Computing (P. Colella)
  - CS267: Applications of Parallel Computers (J. Demmel)
  - Leadership, management, and communication (Fung Institute):
    - E271/272: Engineering Leadership I & II
    - E273: Ethics and Capstone Project
- MolSSI will engage with industry and government labs for capstone projects, help with outreach for admissions, and provide a career fair at the Virginia Tech Arlington Center that will include remote access.

Community Engagement and Leadership

Engaging the Cyberinfrastructure Community

- National Center for Supercomputing Applications (Ed Seidel, Director)
- XSEDE (John Towns, Director)
- Texas Advanced Supercomputing Center (Dan Stanzione, Director)
- XSEDE Campus Bridging and Jetstream (Craig Stewart, Director)
- Science Gateways Community Institute (Nancy Wilkins-Diehl, Director)



Engaging National Labs and Industry

- PNNL (Allison Campbell, Associate Lab Director)
- ORNL (Jeff Nichols, Associate Lab Director)
- BNL (Robert Harrison, Center for Computational Science Director)
- LBNL (Kathy Yelick, Associate Laboratory Director for Computing Science)
- NVIDIA (David Leubke, Sr. Director of Research)
- Intel (Timothy Mattson, Principal Engineer, Parallel Computing Lab)
- IBM (Jed Pitera, Principal Research Manager)
- Cray, Inc. (Ryan Olsen, Performance Engineering)

Engaging the International Community

- MolSSI's Board of Directors and SSAB have established numerous community code partners worldwide.
- EPSRC: ARCHER eCSE
- EU Computational Materials Centers
- EU Center of Excellence on Biomolecular Simulation (BioExcel)
- Our S2I2 Conceptualization workshops prompted the UK's EPSRC to report on how the British CMS community could interface to MolSSI.
- The SSAB will maintain an international representative.

NOMAD

NOVEL MATERIALS DISCOVERY

archer

Horizon 2020

MolSSI Management and Oversight

The MolSSI Board of Directors

- T. Daniel Crawford (Virginia Tech, Director)
- Cecilia Clementi (Rice University)
- Robert Harrison (Stony Brook University)
- Teresa Head-Gordon (U. California, Berkeley)
- Shantenu Jha (Rutgers University)
- Anna Krylov (U. Southern California)
- Vijay Pande (Stanford University)
- Theresa Windus (Iowa State University)

The Science and Software Advisory Board (SSAB)

The inaugural SSAB membership:

- Sharon Glotzer (U. Michigan, Chair)
- Kathy Yelick (UC Berkeley and LBNL, Vice-Chair)
- Ian Foster (U. Chicago)
- Emily Carter (Princeton)
- Nathan Baker (PNNL)
- Martha Head (GlaxoSmithKline)
- Angel Rubio (MPI – Hamburg)
- Michael Levitt (Stanford)
- Laxmikant Kale (UIUC)
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***Members of the National Academy of Sciences**

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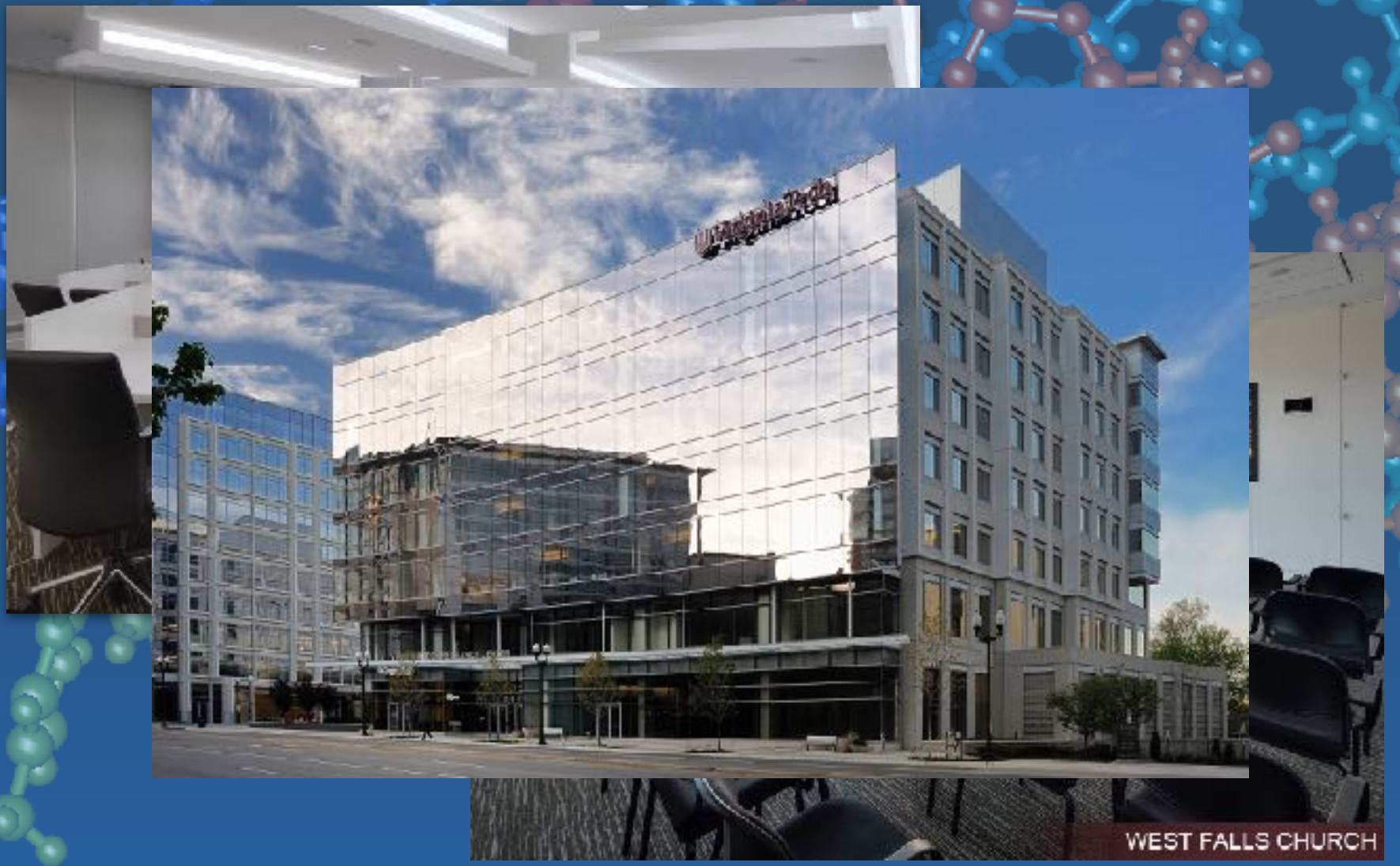
***Winner of the 2013 Nobel Prize in Chemistry**

MolSSI Headquarters

MolSSI will occupy a newly renovated, 6,000 sq. ft. facility adjacent to campus.

Virginia Tech's Arlington Research Center



MolSSI: What's Coming Next?

- Hiring ~12 Software Scientists over the next two years;
- First call for Software Fellowship proposals around the end of 2016;
- Call for proposals work community-driven workshops out now!
- Planning multiple targeted workshops before April 2017:
  - Houston, TX, October 8-10, 2016 (Cyberinfrastructure)
  - Palo Alto, CA, January 2017 (Biomolecular Simulation)
  - Berkeley, CA, February 2017 (Materials Science)
  - Arlington, VA, February 2017 (Interoperability)
  - Laguna Beach, CA, May 2017 (Integral/Tensor Infrastructure);
- A launch event at the April 2017 ACS meeting in San Francisco;
- First MolSSI Software Summer School coming in 2017.

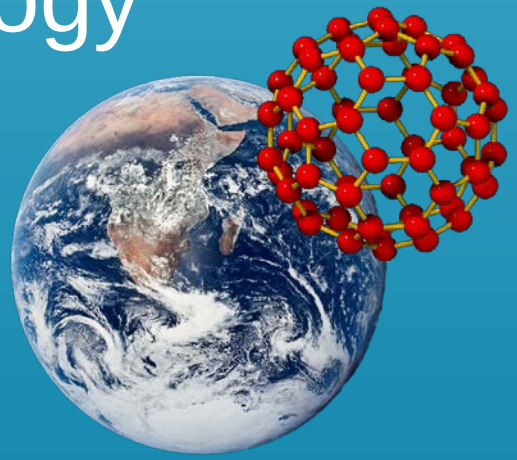
Acknowledgements

- Co-PIs: Cecilia Clementi, Robert Harrison, Teresa Head-Gordon, Shantenu Jha, Anna Krylov, Vijay Pande, Theresa Windus;
- The dozens of members of the CMS community who helped to develop the vision for the Institute over the last five years;
- NSF ACI-1547580;

Watch molssi.org and bit.ly/molssi-g for the latest information!

NanoEarth:

National Center for Earth & Environmental Nanotechnology Infrastructure

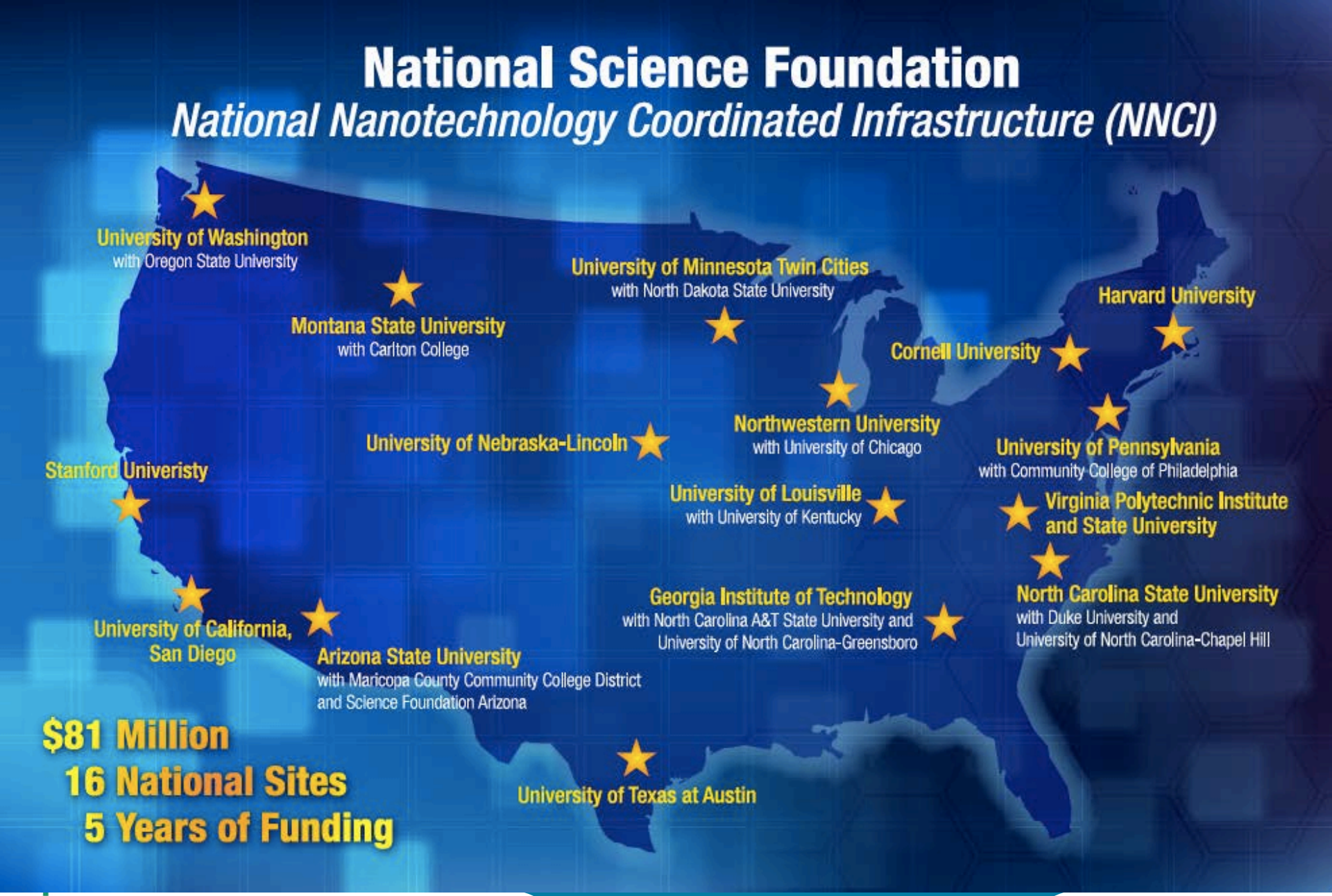


NanoEarth

NanoEarth

National Science Foundation

National Nanotechnology Coordinated Infrastructure (NNCI)



National Nanotechnology Coordinated Infrastructure

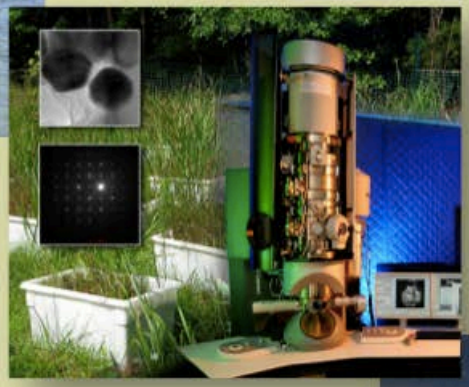
NanoEarth

NSF

CENT
Center for the Environmental Implications of NanoTechnology

ICTAS
INSTITUTE *for* CRITICAL TECHNOLOGY *and* APPLIED SCIENCE *Virginia Tech*

U.S. DEPARTMENT OF ENERGY



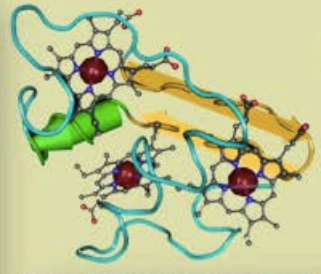
NIH
National Institutes of Health

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY

VTSuN
Virginia Tech Sustainable Nanotechnology

VIRGINIA

Nanoscience and Nanotechnology



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Molecular Biology

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Earth & Environmental Sci.

Scholarship

Core faculty

2 Geosciences, College of Science

3 Civil & Environ Eng, College of Engineering

2 Materials Sci & Eng, College of Engineering

Funding history

$12.5 M in environmental-nano research before 2010

$25.5 M in research awards obtained in 2010 – 2016

$38.0 M total amount raised in this field

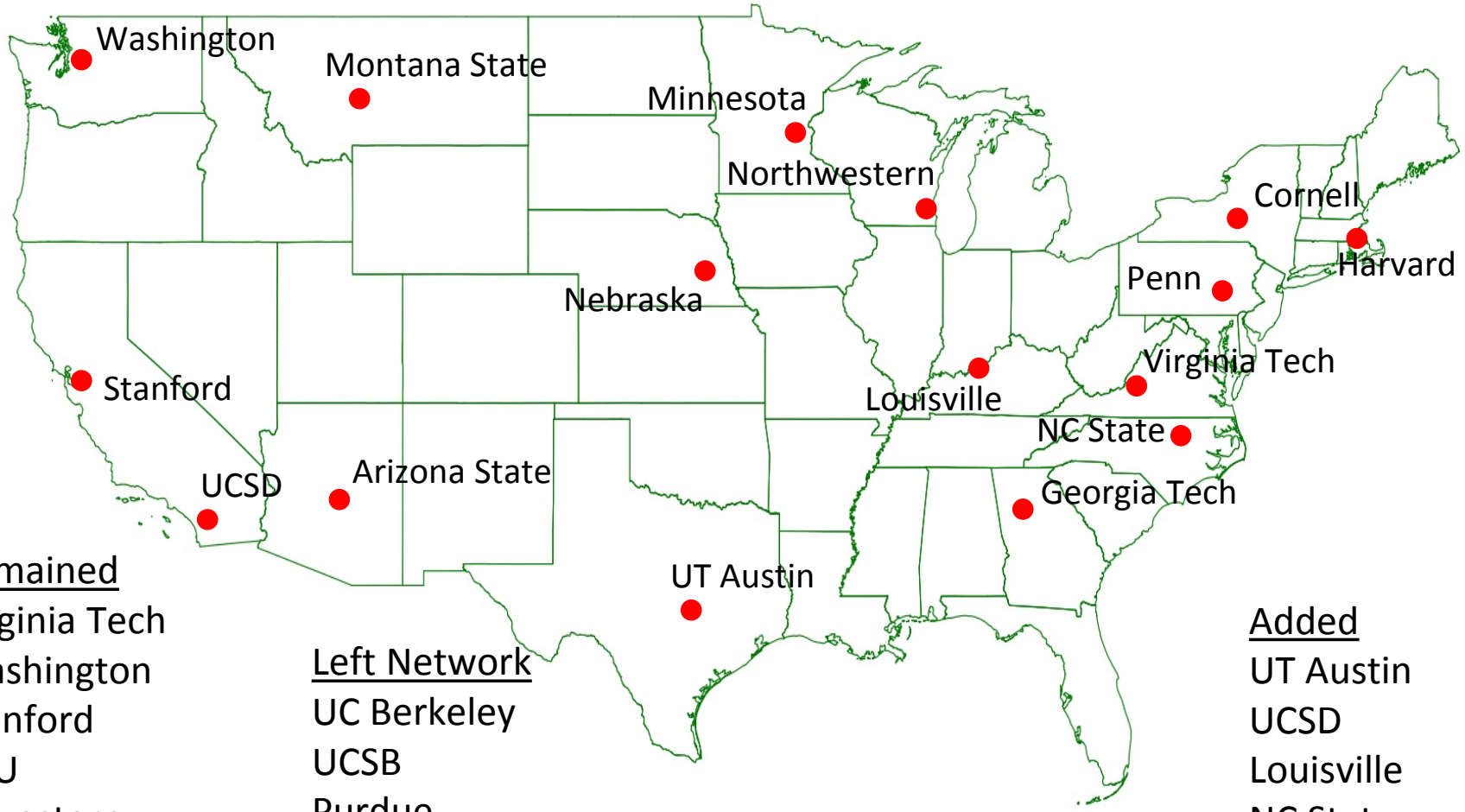
Accomplishments

Combined citations: **>28,000**

One UDP, one PECASE, two CAREER awards

Income: senior faculty/year: **approx. $1M**

A turbulent 2014-15, from NG-NNIN to NNCI



<u>Remained</u>
Virginia Tech
Washington
Stanford
ASU
N'western
Minnesota
Cornell
Harvard
Georgia Tech

<u>Left Network</u>
UC Berkeley
UCSB
Purdue
Michigan
Howard
Rice
Penn State

<u>Added</u>
UT Austin
UCSD
Louisville
NC State
Penn
Montana State
Nebraska

About NanoEarth: Facilities

VTSuN

VT Center for Sustainable Nanotechnology

- 21, 300 sq. ft. (up to 38,000 sq. ft.) of laboratory, instrument, & office space

NCFL

Nanoscale Characterization and Fabrication Laboratory

NanoEarth

About NanoEarth: Facilities – EMSL

- **Environmental Molecular Scientific Laboratory**: A national scientific user facility operated by Battelle for DOE BER.

Statistics: 234,000 square feet, 150+ instruments, roughly 220 staff

Keys:

- Mass spectroscopy
- Microscopy
- Molecular Science Computing
- NMR and EPR
- Spectroscopy & Diffraction
- Subsurface flow & transport
- Cell isolation & systems analysis

NanoEarth Progress to Date: Establishing New Collaborations

Research Universities (21 to date)

- Cambridge University (UK)
- Duke University
- East Tennessee State University
- Florida Institute of Technology
- Georgia State University Geosciences & WIC
- Howard University
- Hampton University
- Kyushu University, Japan, URC and Dept. of Chemistry
- Laurentian University, Canada
- Montana State University
- Rutgers University
- University of Alabama
- University of Copenhagen, Denmark
- University of Delaware
- University of Kentucky
- University of Illinois, Chicago
- University of New Mexico
- University of South Carolina Geosciences & School of Public Health
- University of Texas, El Paso
- United States Geological Survey, Boulder
- Wichita State University

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NanoEarth Progress to Date: Establishing New Collaborations

Community Colleges (2 to date)

- City University of New York, Kingsborough Community College
- Virginia Western Community College

Four-year Liberal Arts Colleges (5 to date)

- Hope College
- Longwood College
- Penn State Erie, The Behrend College
- Roanoke College
- Washington and Lee University

NanoEarth Outreach:
MUNI (Multicultural and Underrepresented Nanoscience Initiative)

Already received many new visitors (undergrad, grad, faculty) from:

- Georgia State University
- Howard University
- Hampton University
- Penn State Erie, The Behrend College
- University of South Carolina
- City University of New York, Kingsborough Community College

- NanoEarth Outreach: Pulse of the Planet

JIM METZNER'S
PULSE OF THE PLANET
The Sound of **Life** on Earth

Heard over 270 radio stations by 1.1M listeners per week, including Armed Forces Radio and the World Radio Network

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