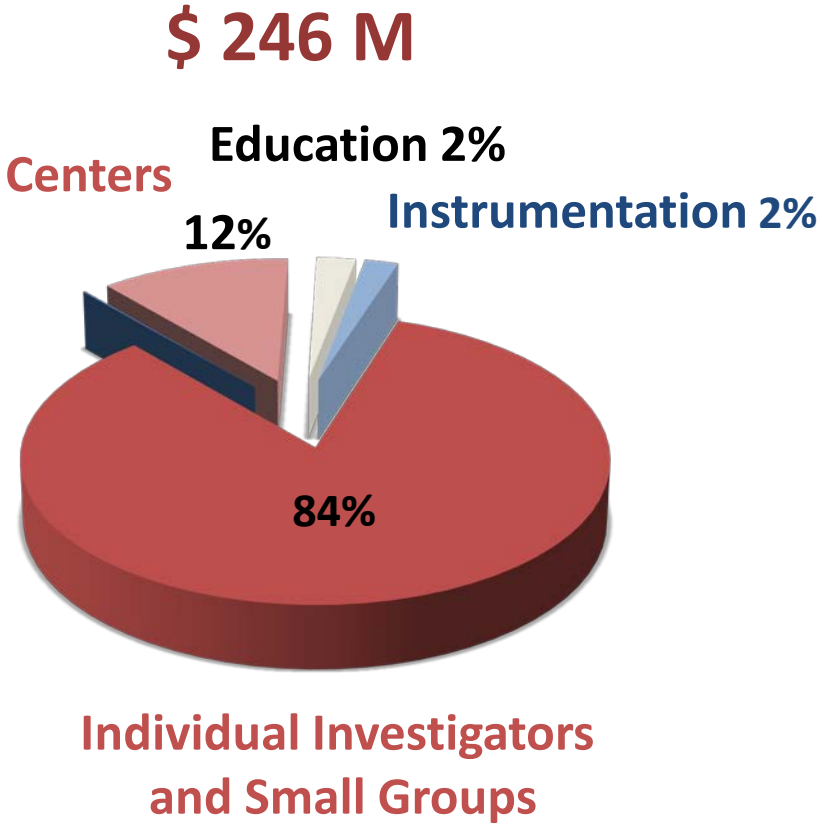
National Science Foundation
Division of Chemistry

Angela K. Wilson
Division Director
Division of Chemistry

MPS AC Meeting
Thursday, November 16, 2017

Overview of the Division of Chemistry (CHE)



The CHE individual investigator program is critical to the field as well as to the economy of our country.

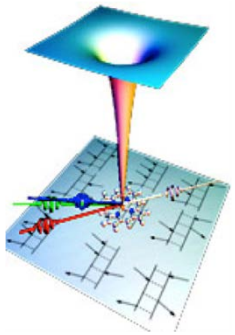
The primary programs include:

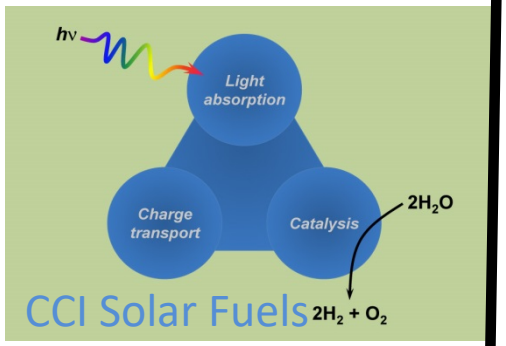
- Chemical Catalysis
- Chemical Measurement and Imaging
- Chemical Structure, Dynamics, and Mechanisms (two programs)
- Chemical Synthesis
- Chemical Theory, Models and Computational Methods
- Chemistry of Life Processes
- Environmental Chemical Sciences
- Macromolecular, Supramolecular and Nanochemistry

Centers for Chemical Innovation (CCI)

Phase II Centers:
Up to $40M investments over 10 years

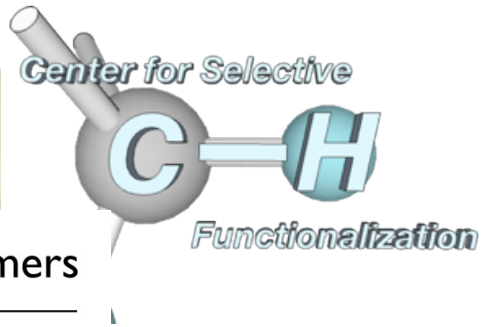
Center for Chemistry at the Space-Time Limit





CCI Solar Fuels

CENTER FOR CHEMICAL EVOLUTION



Center for Sustainable Polymers

The Center for Sustainable Nanotechnology

CAICE
CENTER FOR AEROSOL IMPACTS ON CLIMATE AND THE ENVIRONMENT

Phase I Centers: $1.8M over three years

- Center for First Principles Design of Quantum Processes
- Center for Chemo-mechanical Assembly
- Center for Genomically Encoded Materials
- Center for Autonomous Chemistry
- Synthetic Organic Electrosynthesis Center

First CCI to sunset:

Have begun assessment of CCI program.

Center for ENABLING NEW TECHNOLOGIES CENTC THROUGH CATALYSIS

Harnessing Data for 21st Century Science

NSF Ideas for the Future - "Big Ideas"

Pursuit of **fundamental research in data science and engineering**, the development of a **research data infrastructure**, and the development of a 21st-century **data-capable workforce**.

- What **new information can be obtained** from better utilization of data (including data from multiple laboratories, techniques, and/or chemical systems)?
- How can this lead to **new research directions**?

Dear Colleague Letter: Data-Driven Discovery Science in Chemistry (D3SC)

- Data-driven development of fluorescent sensors for bio-imaging (CHE-1738305)
- Automatic force field parameterization from experimental data (CHE-1738975)
- Using deep learning to optimize chemical reactions (CHE-1734082)
- Modular synthesis of natural products (CHE-1739016)
- Molecular model design to aid chemical data analysis (CHE-1738990)
- Machine-learning approach to explore structure diversity in solid state synthesis (CHE/DMR-1709351)

Recent CHE Workshop Reports

- Framing the Role of Big Data and Modern Data Science in Chemistry
- Measuring the Brain from Synapse to Thought
- Quantum Information and Computation for Chemistry
- Mid-scale Instrumentation (two workshops)

Links are available via the NSF Division of Chemistry website.

NSF Ideas for the Future - "Big Ideas"

Harnessing Data for 21st Century Science and Engineering
Understanding the Rules of Life: Predicting Phenotype
The Quantum Leap: Leading the Next Quantum Revolution
Mid-scale Research Infrastructure

CHE Outreach

- CHE Early Career Workshop
- Conferences – ACS National Meeting, NOBCCHE, specialty meetings
- Visits – Border schools, HBCU's, HSI's

NSF Big Ideas – The Quantum Leap

"**Chemistry is quantum computing's killer app**: Quantum computers could help chemists better understand and develop catalysts, photovoltaics, and more"

- *Chemical & Engineering News*, v. 95(43), 27-31, October 30, 2017

"**Google Debuts Software to Open Up Quantum Computers for Chemists**"

- *Bloomberg*, October 23, 2017

Rules of Life

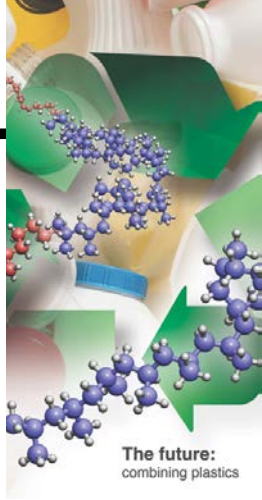
ChemMatCARS

(CHE-1662777)

- Structure-function relationships applied to biological systems.
- Chemistry of Life Processes (CLP) program. (~$25M)
- Understanding the Brain (~$5M)
- **ChemMatCARS** - A beam line at the **Advanced Photon Source** that supports >500 researchers used to look at crystal structures of biologically relevant structures. Examples of projects: identification of mechanisms important for immune regulation, towards therapeutics, and new antibiotics.

Sustainable Chemistry

Sustainable chemistry has led to many partnerships, both internally and externally, and has also led to new start-ups, and significant steps in basic research, that in turn, could impact the economy and the environment.



Extraction of glass-making materials from food waste. **(CHE-1360565)**

Biomass to degradable polymers that can be used as plastics (won the 2015 Presidential Green Chemistry Challenge Award) **(CHE-1300267)**

Lithium ion battery material redesigned to retain function and reduce toxic impacts. **(CHE-1503408)**

Only 2% of the 78 millions tons of plastic used annually for packaging get recycled and reused. This results in a $80-120B annual materials value loss. New catalysts and additives to make plastics recycling effective and economical have been designed. **(CHE-1413862)**

Over 2% of the global energy consumption goes towards the production of fertilizers. A sustainable route for the production of ammonia has been identified, using electrochemistry. This may be more affordable than the current unsustainable process. **(CHE-1205189)**

Detergents found in household cleaning to remediating oil spills are acutely toxic and persist in water supplies and the soil long after they are used. New biodegradable detergents from renewable sources of sugars and natural products have been developed. **(CHE-1339597)**

GLYCOSURF Stonybrook PURIFICATION inpria™ EASTMAN

CHE Budget Decisions

FY18 Presidential Budget Requests

Amount: -$25.47M (-10.3%)

NSF CAREER - Decrease by $2.7M (10.0%)
REU – Decrease by $2.4M
Research resources (CHE supplements to MRI program) – Decrease by $2.4M
CCI – Decrease by $6.5M (centers are sunsetting)
Individual Investigator program (including CCI support) – Decrease by $18.5M (8.0%)

LINKS

Links to Recent Workshop Reports

- **Mid-scale Instrumentation**

http://nsfmidscale.chem.wisc.edu/sites/nsfmidscale.chem.wisc.edu/files/report/MSIregionalcenters_ FINALworkshopreport_5_1_17.pdf
https://advanceddiagnostics.nd.edu/opportunities/nsf-workshop/

- **Quantum Information and Computation for Chemistry**

https://arxiv.org/pdf/1706.05413.pdf

- **Measuring the Brain from Synapse to Thought**

https://beckman.illinois.edu/Content/uploads/files/groups/neurotech-memory-cognition/measuring-the-brain-from- synapse-to-thought-nsf-10-2016.pdf

- **Framing the Role of Big Data and Modern Data Science in Chemistry**

Report is coming soon.

For the links: Also available via the NSF Division of Chemistry website.
https://www.nsf.gov/mps/che/c_newsletters_and_workshops.jsp

Other Links

"**Chemistry is quantum computing's killer app,** *Chemical & Engineering News*, v. 95(43), 27-31, October 30, 2017

https://cen.acs.org/articles/95/i43/Chemistry-quantum-computings-killer-app.html

"**Google Debuts Software to Open Up Quantum Computers for Chemists**"
- *Bloomberg*, October 23, 2017

https://www.bloomberg.com/news/articles/2017-10-23/google-debuts-software-to-open-up-quantum-computers-for-chemists

NSF Centers for Chemical Innovation – Phase II Centers

http://www.nsf-cci.com/