NSF Division of Chemistry

Division Director David Berkowitz; Deputy Director Lin He

External Office Hour, January 26, 2024

Chemical Theory, Models, and Computational Methods Program

3-4 PM

Schedule

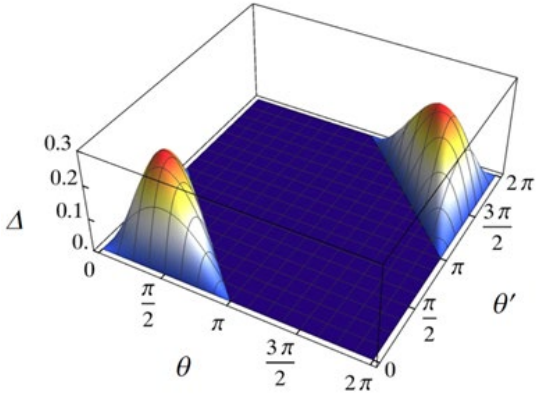
3:00-3:05 Opening Remarks

3:05-3:20 CTMC Program Presentation

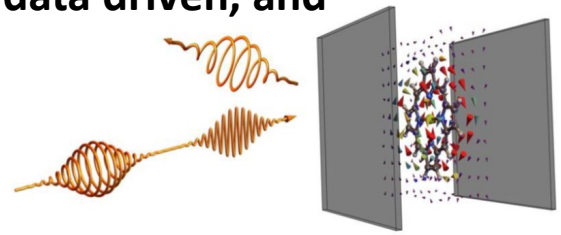
3:20-4:00 Community Q&A

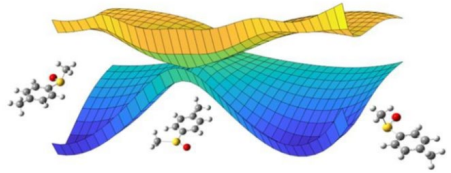
Chemical Theory, Models, and Computational Methods Program

The Chemical Theory, Models, and Computational Methods (CTMC) Program supports the discovery and **development of theoretical and computational methods or models** to address a range of chemical challenges, with emphasis on emerging areas of chemical research. Areas of interest include, but are not limited to, **electronic structure, quantum dynamics and spectroscopy, statistical mechanics, molecular dynamics and simulation, machine learning and data driven, and biosimulation.** The complete current program description is available on the program webpage. https://new.nsf.gov/funding/opportunities/chemical-theory-models-computational-methods-ctmc



Regions where Bell's inequalities are violated in spin-projection measurements in entangled qubits.



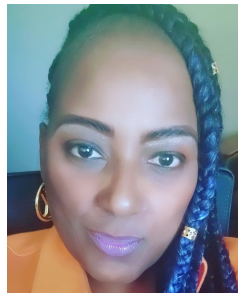


Chiral cavity modes induce selective enantiomer interconversion

Richard Dawes

Michel Dupuis

Ryan Jorn



Monique Moore

Chemical Theory, Models, and Computational Methods (CTMC)

Program description under revision: taxonomies encompass evolving priorities, but the description will be updated

The Chemical Theory, Models, and Computational Methods (CTMC) Program supports the discovery and **development of theoretical and computational methods or models** to address a range of chemical challenges, with emphasis on emerging areas of chemical research. Proposals that focus on established theoretical or computational approaches should involve innovations that substantially broaden their applicability. Areas of interest include, but are not limited to, **electronic structure, quantum reaction dynamics, theoretical/computational spectroscopy, statistical mechanics, molecular dynamics and simulation**, and modeling techniques for isolated molecular systems and systems in complex environments. Areas of application span the full range of chemical systems from single molecules to mesoscopic aggregates. Proposals that develop approaches to bridge multiple spatial or temporal scales are welcome. Despite the diverse application areas, the goal of the program is to support the **development of new theoretical and computational methodologies** that are broadly applicable to a range of challenging chemical problems. The CTMC Program is interested in fundamental areas of chemical research that are difficult or impossible to address using current synthetic, experimental, and/or computational methodologies.

Chemical Theory, Models, and Computational Methods (CTMC)

We also encourage proposals that **develop innovative computational and theoretical approaches** to exploring the chemical basis of life; proposals that involve **novel approaches based on machine learning or other data-enabled methods** with broad applicability to significant chemical problems; proposals focused on theory and approaches to advancing molecular science where novel quantum mechanical effects play an important role; proposals on **quantum information science (QIS)** that either focus on **applying QIS concepts** to theoretical and computational chemistry or on **developing quantum algorithms** for chemical systems.

The CTMC Program encourages the integration of innovative software development with methodological and algorithmic development, especially computational approaches that allow efficient utilization of emerging computer architectures. Such proposals may be submitted to the CTMC Program either directly or through the **Computational and Data Science and Engineering** (CDS&E) **funding opportunity**.

Note: Relevant proposals should have a title starting with "CDS&E:" to be distinguished from other CTMC proposals.

Proposals that utilize established theoretical and modeling approaches to solve problems in chemistry without significant theoretical or methodological development, or that focus on the development of biology or materials design, may be more appropriate for other programs in either the Chemistry Division or in other NSF Divisions or Directorates.

Chemical Theory, Models, and Computational Methods Program Research Portfolio Topic Areas (fine-grained)

a. Quantum Chemistry/Electronic Structure (methods and applications)
b. Electron Dynamics
c. Quantum Dynamics
d. Spectroscopy
e. Photochemistry
f. Molecular Simulation Methods
g. Biomolecular Theory and Simulation
h. Statistical Mechanics (Particularly nonequilibrium)
i. Simulation and Theory at the Nanoscale.
j. Model (Force Field) Development
k. Model (Multi-Scale) Development
l. Charge Transfer, Excitonics, Polaritonics, Spintronics, etc.
m. Optics and Photonics
n. Data-Driven Chemistry including Machine Learning
o. Quantum Information Science, Quantum Algorithms for Quantum Chemistry

Chemical Theory, Models, and Computational Methods Program Research Portfolio Taxonomies

Quantum Chemistry

Wavefunction theory for ground and excited states; Monte Carlo methods, Green's function, other. Density Functional Theory (DFT); semi-empirical models; Machine Learning to augment all of the above.

Quantum Dynamics & Spectroscopy

Wide range of approaches to treat nuclear quantum effects on different scales. Some electron dynamics (also in QC). Calculations of rovibrational states, simulation of spectroscopies…multi-D. Polaritons, strong coupling, manipulation of quantum effects…QIS.

Molecular Simulation & Statistical Mechanics

Methods for molecular dynamics simulation, including acceleration and advanced sampling.

Biomolecular Simulation

Bio-inspired methods and models to treat extended length and time scales including coarse-graining, non-equilibrium stats mech, cell level processes.

Data-Driven Research

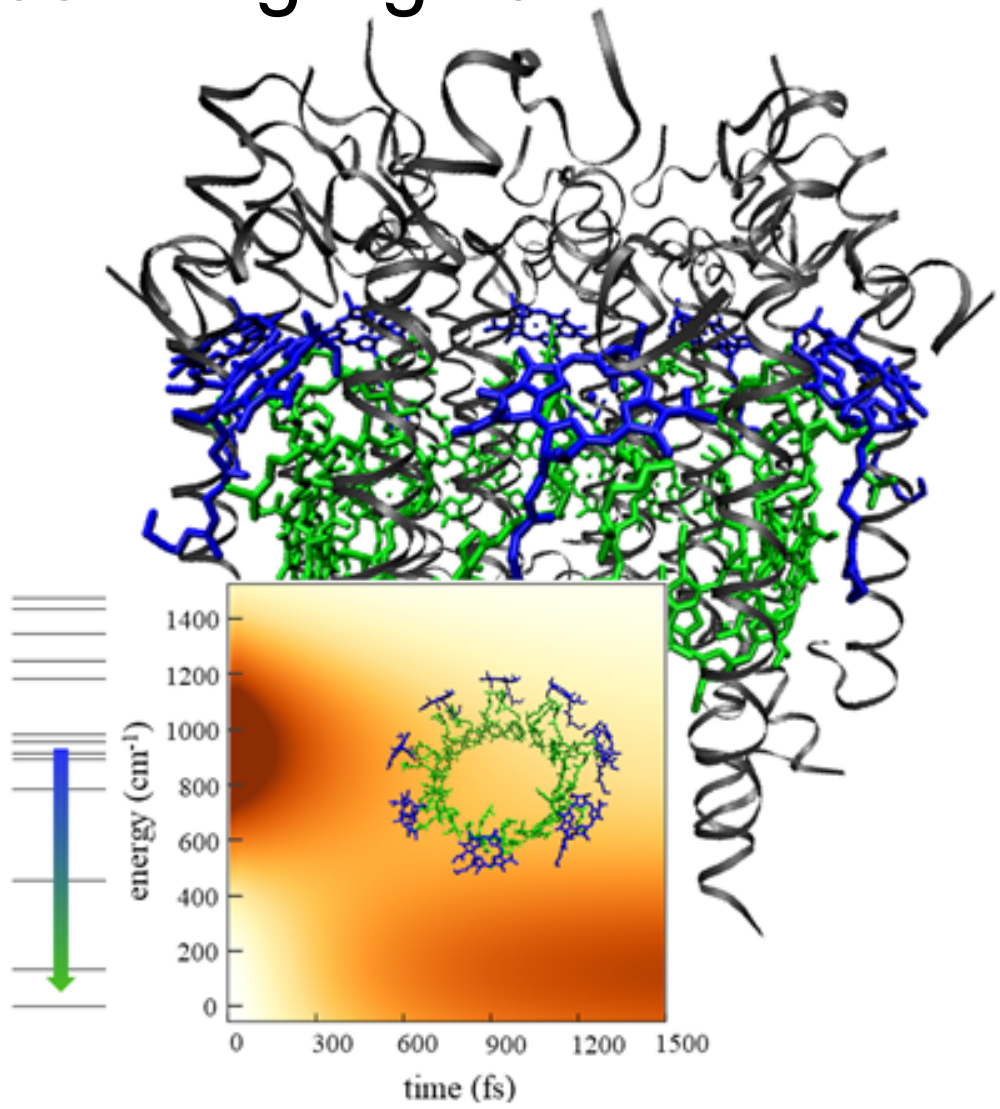
Overlapping all other taxonomies and application areas. AI, Machine Learning, Neural Networks, Automated theorem proving. Used to bolster other methods with low-cost components.

Chemical Theory, Models, and Computational Methods Program: A few recent Highlights

Fully quantum path integral dynamics simulations of energy relaxation in the light harvesting complex 2 (LH2) of purple bacteria. Explicit treatment of many excited states and 50 coupled vibrational modes in each of the 24 bacteriochlorophyll molecules.

Nancy Makri (UIUC)

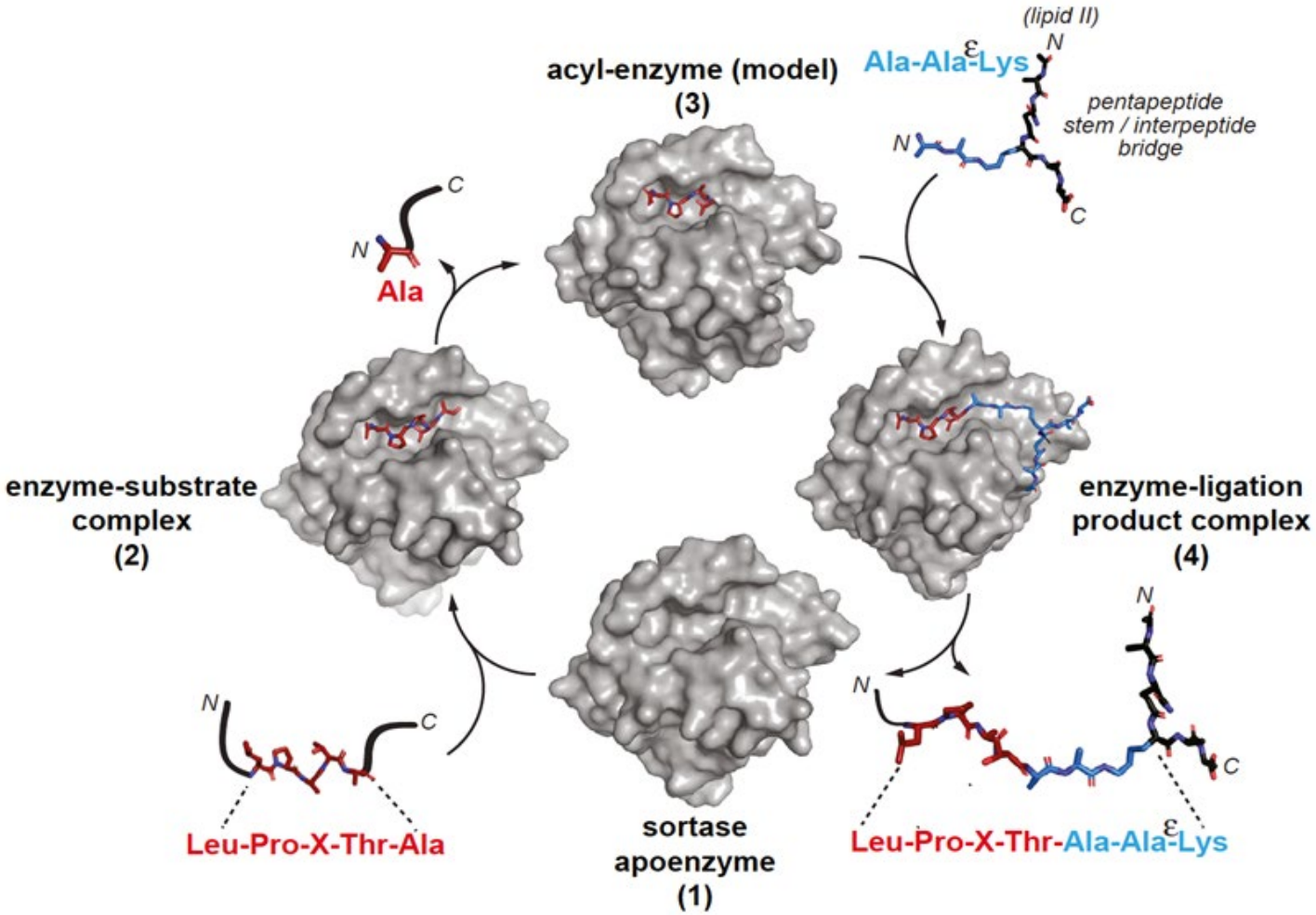
CHE-1955302



Chemical Theory, Models, and Computational Methods Program: A few recent Highlights

A comprehensive structural view of the *Streptococcus pyogenes* Class A sortase catalytic mechanism

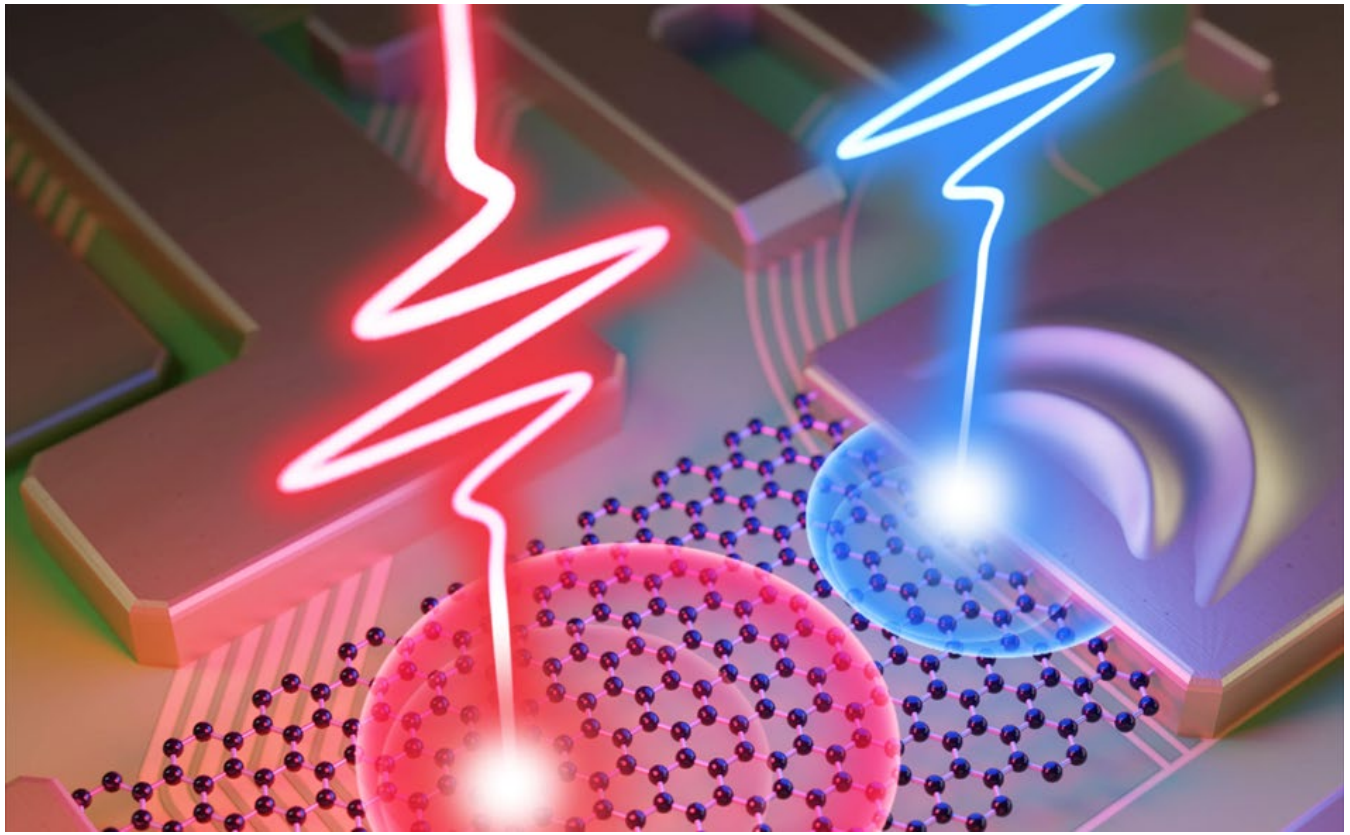
Jeanine Amacher, CHE-2044958 (CLP) and Jay McCarty, CHE-2102189 (CTMC) both from Western Washington University



Chemical Theory, Models, and Computational Methods Program: A few recent Highlights

Laser pulses generate charge carriers in graphene that are absorbed by gold metal to create a current. Theory and simulation helps pave the way to ultrafast logic gates.

Ignacio Franco, University of Rochester
CHE-2102386



Petahertz Logic gates

Chemical Theory, Models, and Computational Methods Program: A few recent Highlights

The relationship between quantum chemistry calculations on conventional and quantum computers was solved using identities from quantum optics. The 'exponential disentangling identity' was used to determine the correspondence between a coupled cluster algorithm on the two different computing architectures.

James Freericks, Georgetown University and Dominika Zgid, University of Michigan, CHE-1836497

Image of the Summit computer, which is one of the world's most powerful conventional computers, and is housed at the Oak Ridge National Laboratory.

The image credit is to Oak Ridge National Laboratory and is approved for all non-proprietary uses.

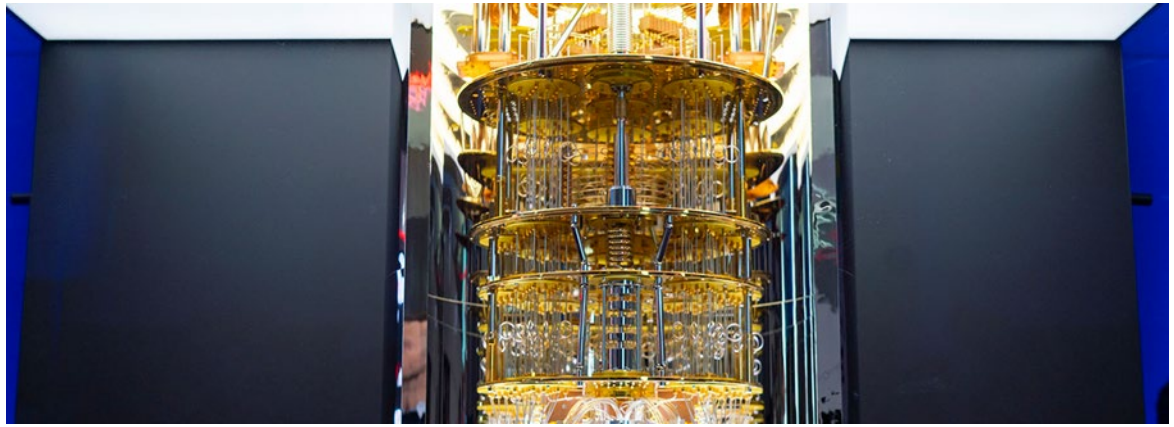


Image of an IBM quantum computer, which is one of the world's most powerful quantum computers.

The image credit is to IBM media center and is approved for broadcast, print, and online use.

How to Engage with CTMC

- A new PI? (new to NSF or new to sponsored research)
- or New to CTMC?
  - Please email the program. (Richard Dawes, rdawes@nsf.gov; Michel Dupuis, mdupuis@nsf.gov; Ryan Jorn, rjorn@nsf.gov) Copy all three of us. Briefly explain who you are and your affiliation. You may attach a CV. You may also attach a 1-2 page description of your interests and plans.
  - Please volunteer to join our reviewer community. Serving on panels is a great way to serve the community while gaining valuable insight into the proposal review process.
- CTMC PI with new research avenue in mind?
  - Please touch base with the program and tell us about your plans. We can help advise with respect to program fit, and also let you know about other opportunities at NSF.

Opportunities at NSF for CTMC PIs within the program

- **NSF 22-586 - Faculty Early Career Development Program.**
- In recent years, CTMC has made 6-8 Career awards per year (details of recent awards can be found on the program webpage).
  - **Upcoming Deadline, July 24, 2024**
  - PIs are encouraged to consider participating in our CHE division Early Career Workshop (usually held in May)
- **NSF 22-606 - Division of Chemistry: Disciplinary Research Programs: No Deadline Pilot (CHE-DRP:NDP)**
  - Yes, CTMC is currently part of a no deadline pilot. That means that you may submit your proposal at any time. There is no preferred time to submit, but keep in mind typical processing time is roughly 6 months. Some limitations apply to the number of proposals allowed in a 12-month period, and how soon you can resubmit a revised proposal (please check the solicitation). There is a 4-month 'cooling off' period after serving on a panel, so please let us know about your intention to submit a proposal.
  - We welcome collaborative proposals with multiple funded PIs either within CTMC, or across another CHE program (*e.g.*, a joint CTMC/CSDM-A award could fund a theory/experiment project).

Other Opportunities for CTMC PIs across NSF

- **Computational and Data-Enabled Science and Engineering (CDS&E)**
  - This opportunity can be confusing. There is a program website, and a solicitation number, PD 23-8084. However, this is what we call a 'meta' program and you still submit your proposal to one of our programs, but flag it as CDS&E. e.g., Simply make the title of your CTMC proposal "CDS&E: My great plan …".
- **Cyberinfrastructure for Sustained Scientific Innovation (CSSI) 22-632**
  - Supports CI development, e.g., an open source package to share your methods.
  - Please contact us as CSSI program goals and review process are quite different from CTMC
- **Pathways to Enable Open-Source Ecosystems (POSE) 23-556**
  - Supports open source communities (ecosystems). Please contact us for guidance.
- **Expanding Capacity in Quantum Information Science and Engineering (ExpandQISE) 24-523**
  - Connects a PI from a non-R1 institution who is new to QIS with a PI from an R1 who is active in QIS research, to form new collaborations. Please contact us.
- **National Artificial Intelligence Research Resource (NAIRR) Pilot;** https://new.nsf.gov/focus-areas/artificial-intelligence/nairr/ ; allocations of HPC resources available…

CHE Division Announcements

A special CHE virtual office hour is scheduled for **Feb 9, 2024,** 3-4 PM Eastern Time to answer any question you may have about a recently issued **Dear Colleague Letter: Planning Proposals for Centers of Research Excellence in Science and Technology (CREST Centers) in Chemistry Research** (**NSF 24-029**). Through this Dear Colleague Letter (DCL), EDU/EES and MPS/CHE jointly encourage the submission of planning proposals for CREST centers to help mitigate potential barriers to the preparation of future competitive Chemistry CREST proposals for the proposing institutions and PIs.

Register in advance for this meeting:
https://nsf.zoomgov.com/meeting/register/vJItd-uhrTIuGQUQUlucWxWywWFLg8T9MsE.

CHE Division Announcements
Future Office Hours

Program	Host	Date (3-4pm, Eastern Time)	Zoom Registration Link
CTMC	Richard Dawes (rdawes@nsf.gov)	1/26/2024	https://nsf.zoomgov.com/meeting/register/vJIsdO-tqzgjEmPSA3jlj6lnpdXHwK6sGwU
SYN	George Richter-Addo (grichter@nsf.gov)	2/23/2024	https://nsf.zoomgov.com/meeting/register/vJIscOqsqTsoHmn2FkiHTZ8qNv1tPxO0pF4
CSDM-A	John Papanikolas (jpapanik@nsf.gov)	3/29/2024	https://nsf.zoomgov.com/meeting/register/vJIsdO6vqTstEx4WmMHEjvlISsxPtr3J5zE
CAT	Ken Moloy (kmoloy@nsf.gov)	4/19/2024	https://nsf.zoomgov.com/meeting/register/vJIsfuyrpzwqE-zVoqp5zSdiWti0xd7H0rk
CSDM-B	Tingyu Li (tli@nsf.gov)	5/10/2024	https://nsf.zoomgov.com/meeting/register/vJIsdO-rrT4qEhSP0xUwuEC-pSy7Lpv4Nzo
REU	Tomislav Pintauer (tompinta@nsf.gov)	6/7/2024	https://nsf.zoomgov.com/meeting/register/vJIscuivpj0iHiKio_5BXDEfhM-7PJlsybE
CCI	Kathy Covert (kcovert@nsf.gov)	6/28/2024	https://nsf.zoomgov.com/meeting/register/vJIscuyqpjIoE-1hYuxJOy8FEMMdRiwkRwY
CMI	Kelsey Cook (kcook@nsf.gov)	7/19/2024	https://nsf.zoomgov.com/meeting/register/vJIsc-uupjMvE9fdyfPEoPGP8FHV9_X5YBw
MSN	Suk-Wah Tam-Chang (stamchan@nsf.gov)	8/16/2024	https://nsf.zoomgov.com/meeting/register/vJIsfuyvrDMqHVeqFzKCscb8URObFxv3SRc
MRI	Tanya Whitmer (twhitmer@nsf.gov)	9/20/2024	https://nsf.zoomgov.com/meeting/register/vJItduCtqjkoEtScSwjEcX8ZoBn2QNkffkg
CLP	Catalina Achim (cachim@nsf.gov)	10/25/2024	https://nsf.zoomgov.com/meeting/register/vJItdO6rpjksHZazsYt8NscT7P7rtS0HVqc
Broadening Participation	Anne-Marie Schmoltner (aschmolt@nsf.gov)	11/15/2024	https://nsf.zoomgov.com/meeting/register/vJItd-qorzstG4pPOdYcuy_tlLt-H9DV2QY
ECS	Anne-Marie Schmoltner (aschmolt@nsf.gov)	12/6/2024	https://nsf.zoomgov.com/meeting/register/vJItc--rz4oEw0TKxGWv0KXz6zHd3Eso_E

Questions??