

Projects proposed for FY18 - Budget & resources pending

The recommendations and status of each RFP will inform the priority for upcoming stages of the funding and implementation process.

- NOMAD - detector and detector control
- BNAP - new neutron beam - **initiated/Executing**
- ES-SANS - new detector coverage
- TEEMU - detector control
- CD-3 Bio-SANS - new detector coverage
- HEI - polarization upgrade
- CD-3 Bio-SANS - new collimator
- DuPont at FRIB - dynamic nuclear polarization installation

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- FRiD - detector suite-out
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New Instruments at
SNS and HFIR

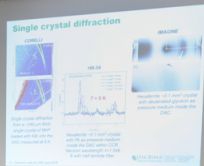


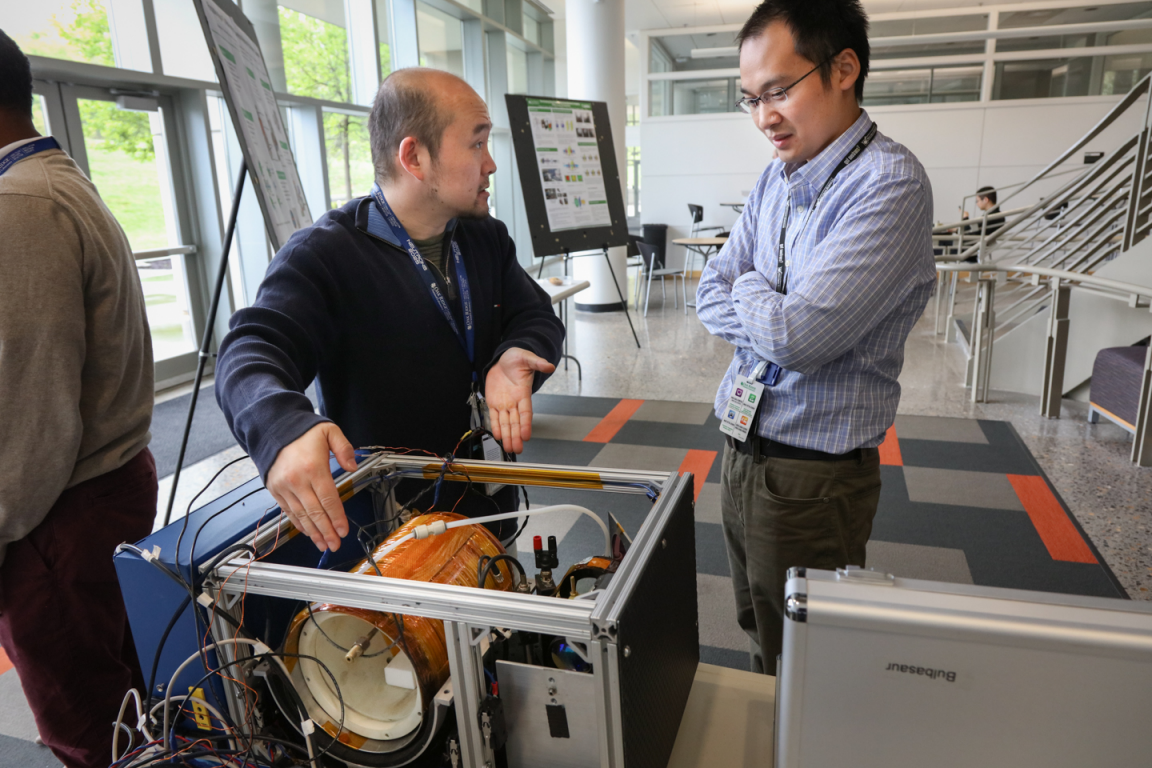
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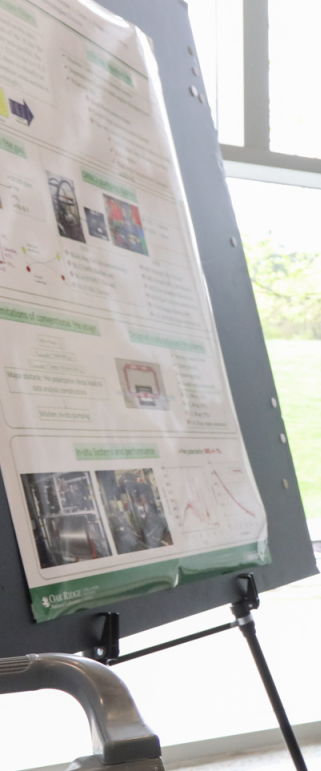


ORNL
Oak Ridge

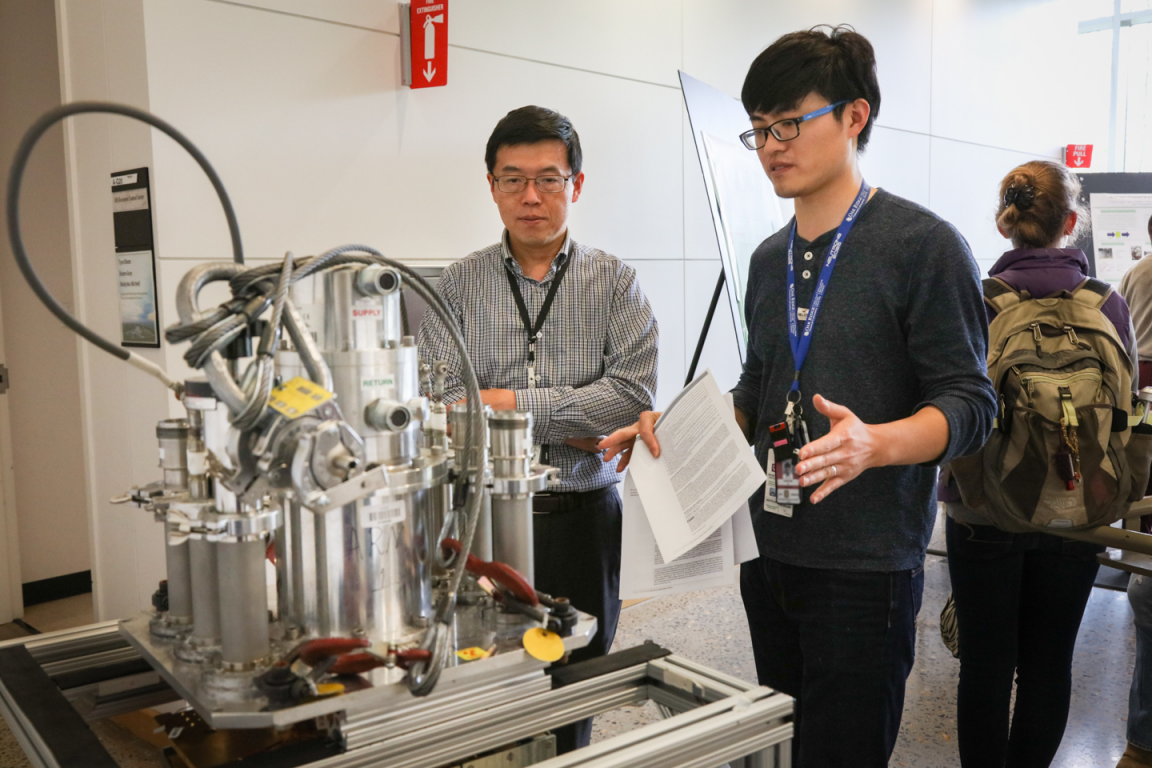


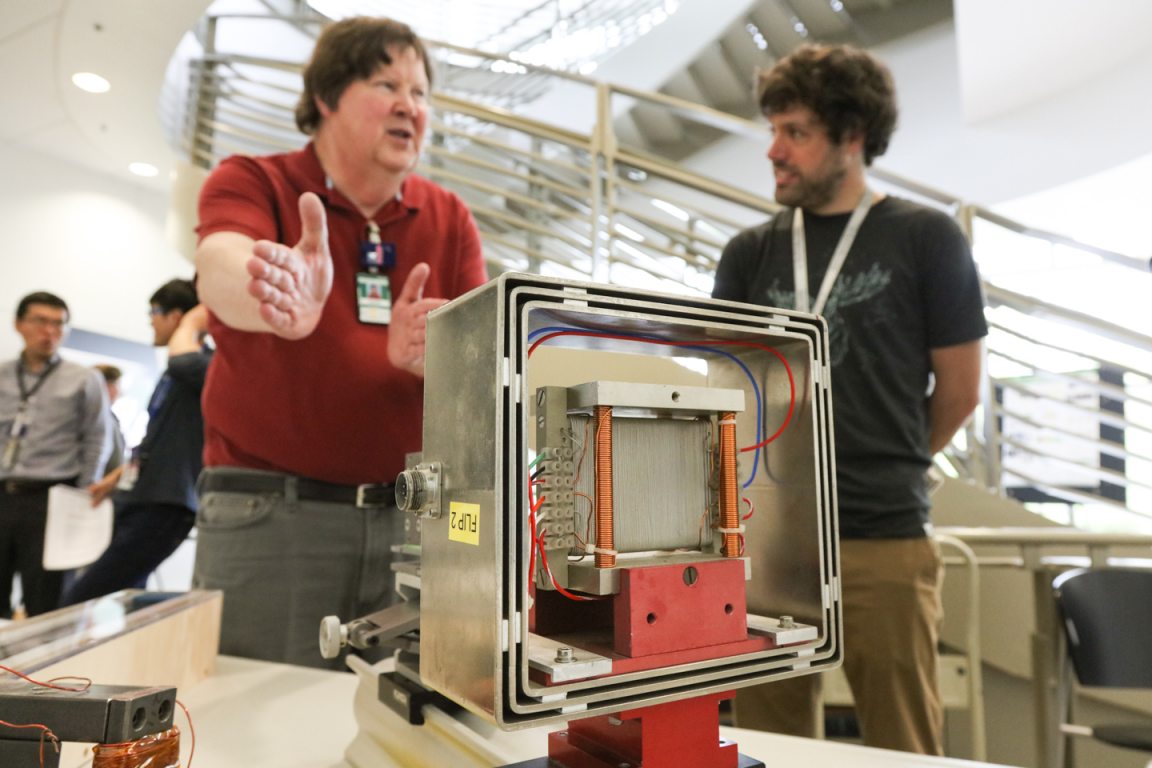




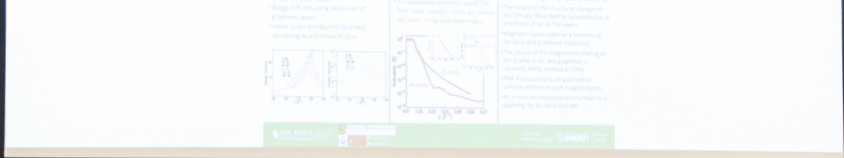


EXIT









OAK RIDGE
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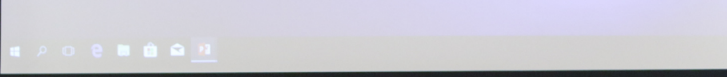


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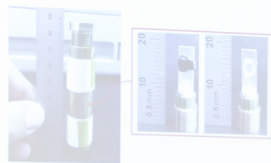




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➤ DLCB

- (i) Determine the critical pressure P_c where the long-range magnetic ordering disappears.
- (ii) Study effect of hydrostatic pressure on spin dynamics with inelastic neutron scattering.



Abundant New Energy Sources

Recent studies with materials under high pressure, as well as other volume measurements, are leading to discovery of potential new energy sources. Such studies have revealed the never-before-seen feature of gap hybridization that produces energy, as well as a superlattice structure.

Cures for Disease

Investigation of Ions and Induced Magnetism in Epitaxial Multi-layer Graphene

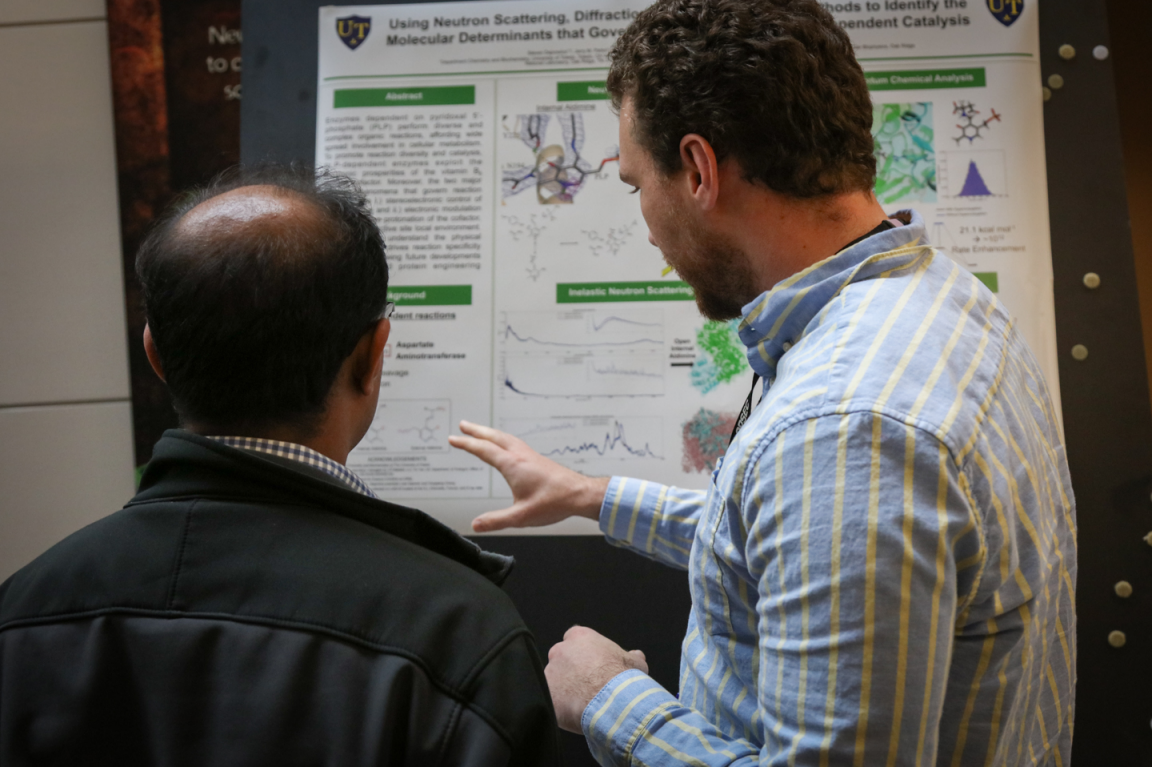
Importance of Structure in Understanding Altered Drug Effects
 Effects due to hydrogen ions, and other ions, and other molecules, and other molecules.

Structural Relationships to Magnetism and Ion Dose
 The Bragg from XRD depends on the structure depth. The center of the ion dose for various with the graphene the shift in the treatment process.

What we did:
 Investigated the relationship between the total dose (in graphene and SiC) scales with magnetism. It has been shown to become magnetic with dose in SiC, suggesting possible changes in the expansion of the ion dose in SiC. The Bragg peak shifts in SiC, and the expansion of the ion dose in graphene.

Concluded Range & ray Effectivity
 Various studies were treated with ion doses 100 and 1000 to vary the ion dose range. The shift indicating expansion of graphene layers. The ion dose distribution obtained increasing as a function of dose.

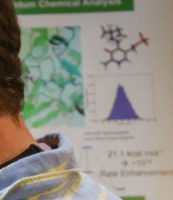
Graphs:
 - A graph showing Bragg peak shift vs. ion dose.
 - A graph showing magnetism vs. ion dose.
 - A graph showing expansion vs. ion dose.



Using Neutron Scattering, Diffraction, and X-ray Crystallography to Identify the Molecular Determinants that Govern Independent Catalysis

Abstract

Enzymes dependent on pyridoxal 5'-phosphate (PLP) perform diverse and complex organic reactions, affording wide spatial involvement in cellular metabolism. To provide reaction diversity and control, P-dependent enzymes exploit the unique properties of the vitamin B₆ cofactor. Moreover, the two major determinants that govern reaction specificity are (1) stereoelectronic control of the cofactor and (2) electronic modulation of the cofactor. We have identified the physical basis for reaction specificity by using future developments in protein engineering.



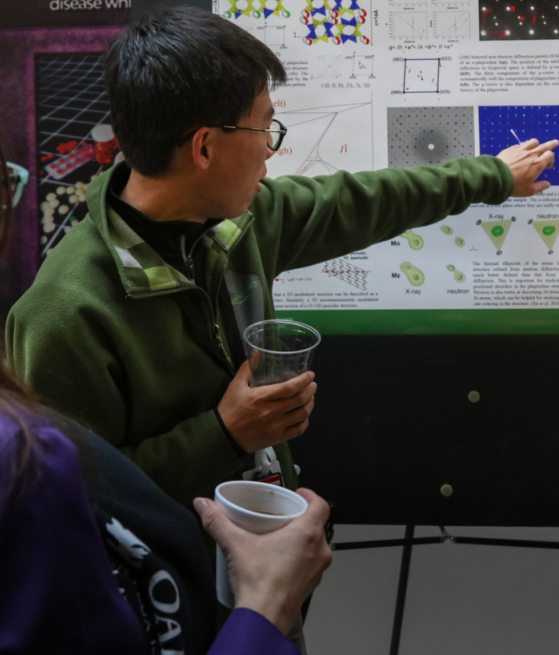
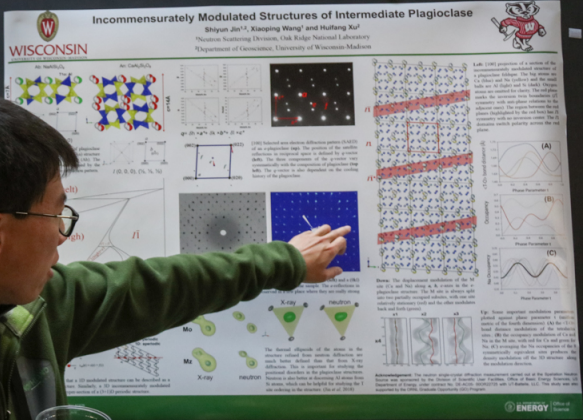
Background

Enzymatic reactions

Aspartate Aminotransferase



Neutron studies
interact with their
tailor medicine
body. The ability
delivered allow
disease whi



Capturing Hyper-Rotated Solution Structure of the E. coli Ribosome

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¹Department of Microbiology, University of Colorado Boulder, Colorado, USA; ²Center for Molecular Systematics, University of Colorado Boulder, Colorado, USA; ³Center for Environmental and Estuarine Science, University of Colorado Boulder, Colorado, USA; ⁴Center for Environmental and Estuarine Science, University of Colorado Boulder, Colorado, USA



Abstract

The structure of a biological cell, and its organelles, tissues, and membranes, are the result of the self-assembly of the cell. The assembly of the cell is a complex process that involves the self-assembly of the cell's components. In this study, we have used cryo-EM to capture the hyper-rotated solution structure of the E. coli ribosome. This structure is essential for understanding the function of the ribosome and its role in protein synthesis.

Introduction

Structure 1: 50S subunit (PDB: 1J7J)
Structure 2: 30S subunit (PDB: 1J7K)
Structure 3: 70S ribosome (PDB: 1J7L)

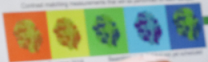


Methods

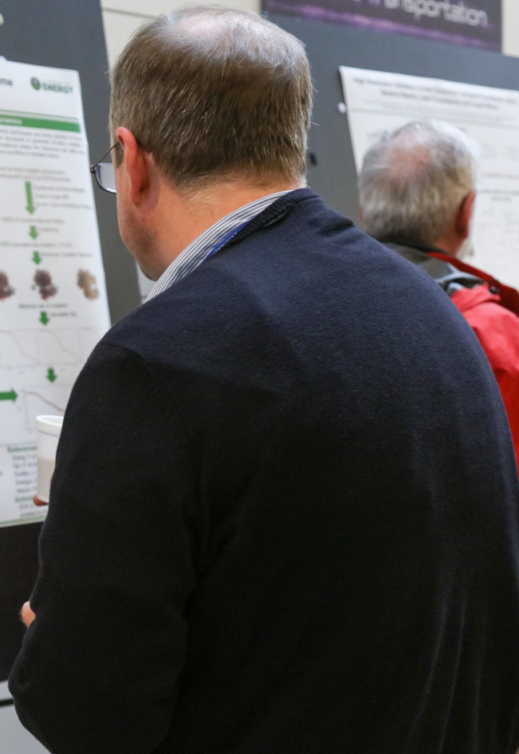
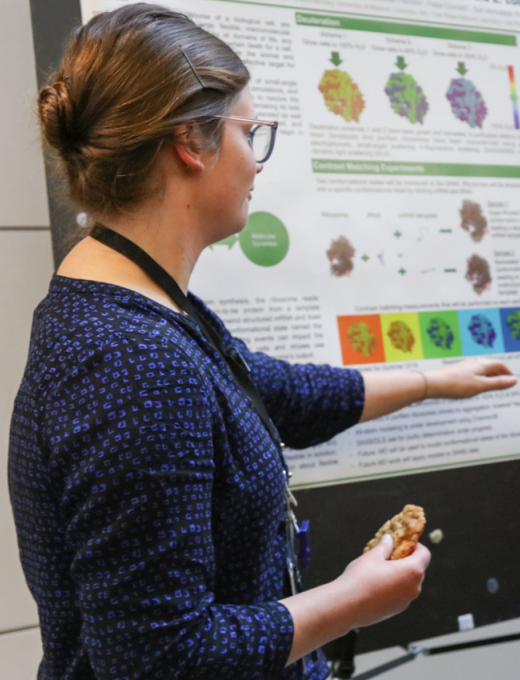
Sample preparation: Ribosomes were purified from E. coli cells and flash-frozen in liquid nitrogen. Cryo-EM data was collected using a Titan Krios microscope at 300 kV. Data was processed using cryoSPARC and 3D reconstruction was performed using cryoSPARC and RELION.

Results

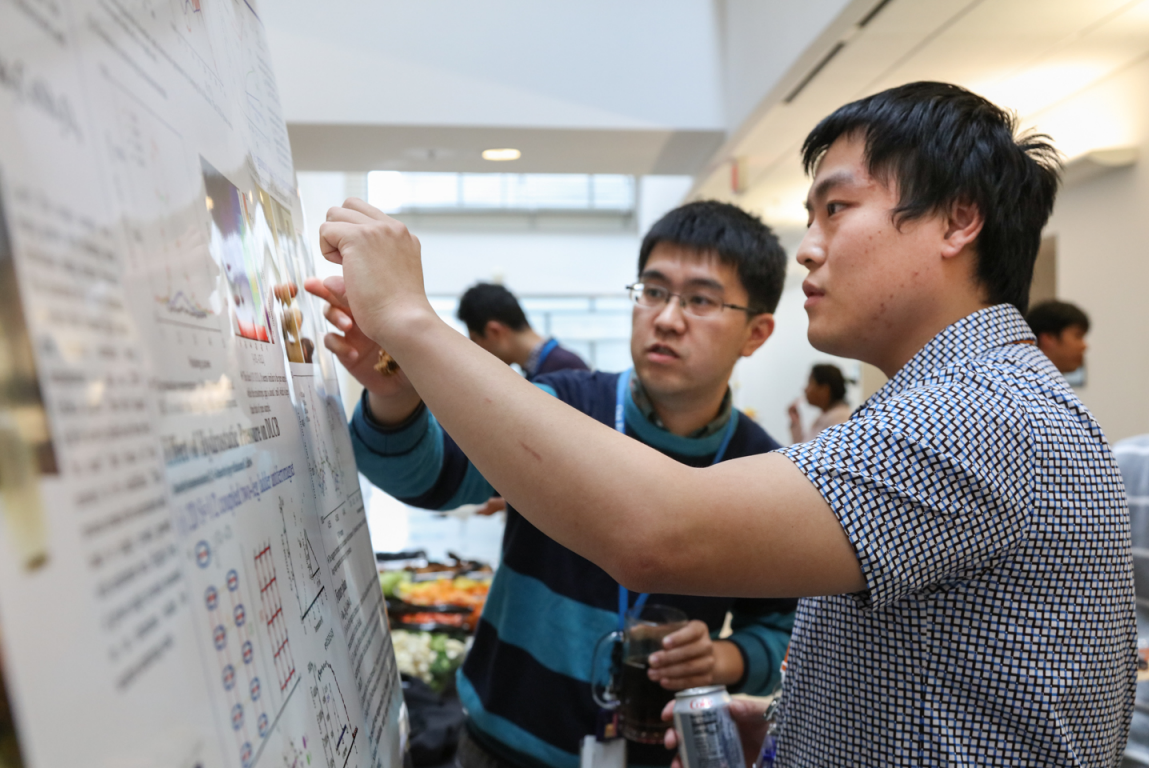
The cryo-EM structure of the hyper-rotated E. coli ribosome shows a significant conformational change compared to the native structure. This change is associated with the binding of the 30S subunit to the 50S subunit, resulting in a more compact and stable structure. The hyper-rotated structure is essential for understanding the function of the ribosome and its role in protein synthesis.

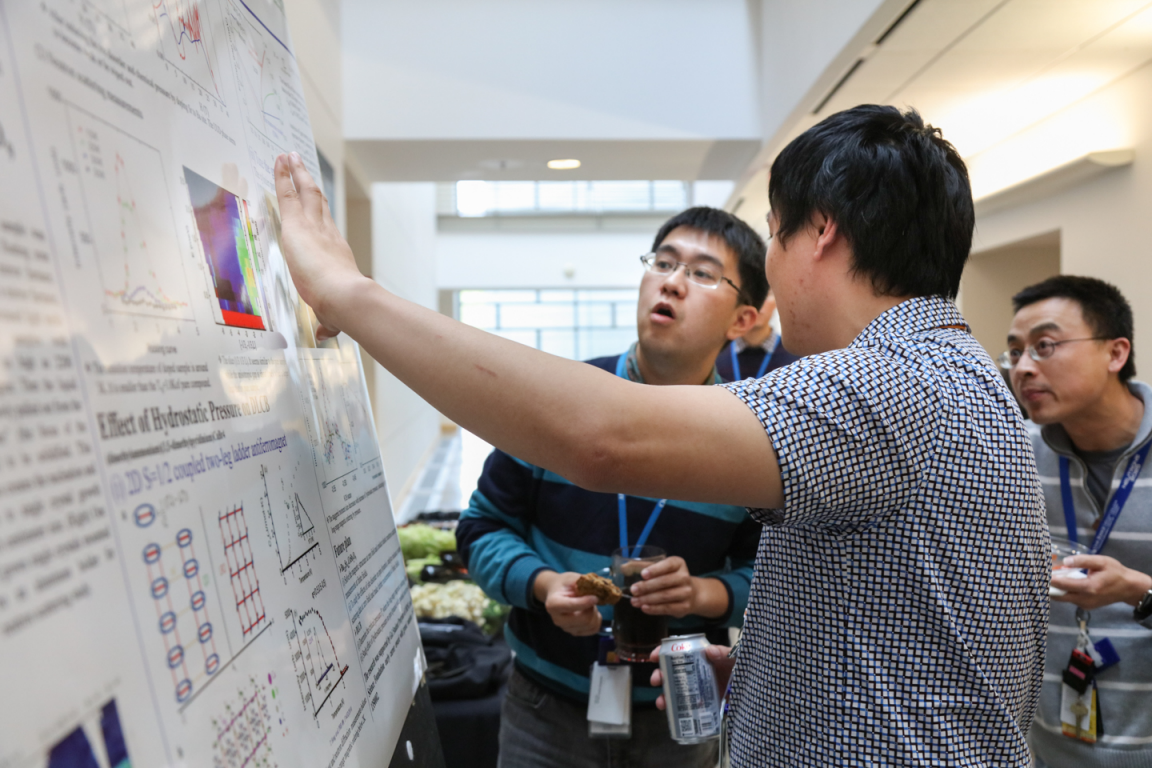


Supporting Information: Additional data and figures are available in the Supporting Information. This information is available for free at <https://doi.org/10.1101/2023.01.10.524567>.



Efficient Transportation





Capturing Hyper-Rotated Solution Structure of the *E. coli* Ribosome

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Abstract
 Problem: The structure of a biological cell in solution and subjected to a large, time-varying mechanical force is unknown. Goal: To determine the structure of the ribosome in a solution state that is hyper-rotated. Approach: We use cryo-EM to capture images of the ribosome in a solution state that is hyper-rotated. We use a high-throughput approach to generate a large number of images of the ribosome in a solution state that is hyper-rotated. We use a high-throughput approach to generate a large number of images of the ribosome in a solution state that is hyper-rotated.



Dehydration

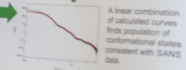
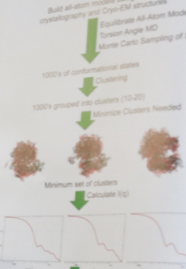


Conformal Matching Experiments



Molecular Dynamics

Molecular Dynamics techniques are being applied to *E. coli* ribosome structures to generate all-atom models of possible conformational states the ribosome can take in solution. Future workflow is detailed below.



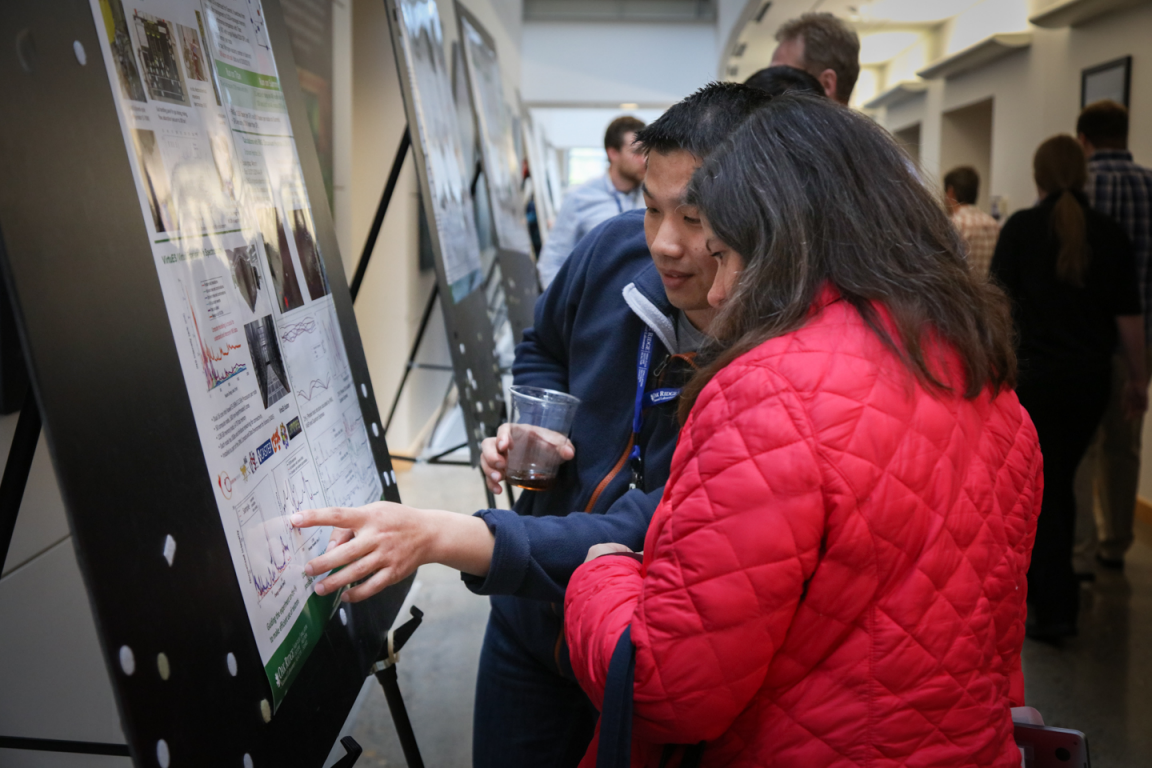
Conclusions & Future Plan

- Successfully expressed ribosomes in cells grown in 100% H₂O & 85% D₂O
- SANS data of purified ribosomes shows no aggregation, however has limited low-Q data.
- Atom modeling is under development using Charmm36.
- SANS/DLS use for purity determination under progress.
- Future MD will be used to model conformational states of the ribosome in solution.
- Future MD work will apply models to SANS data.

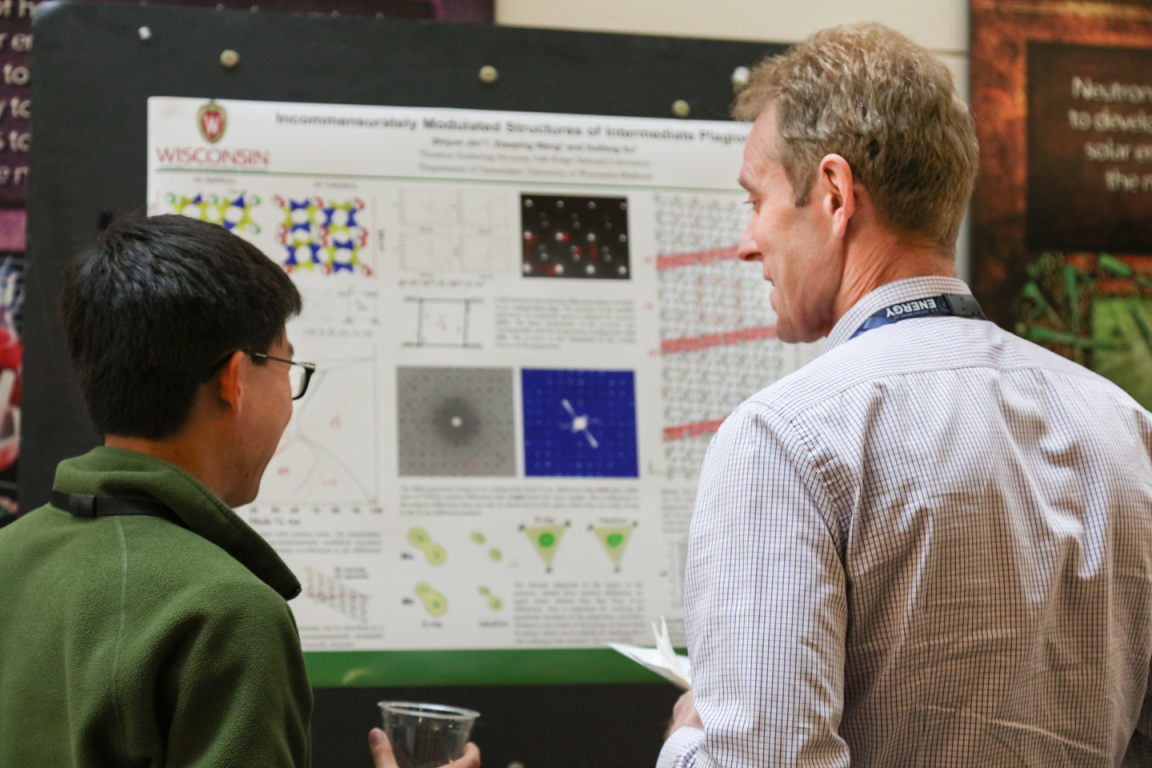
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WISCONSIN
Incommensurately Modulated Structures of Intermediate Phases
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Department of Chemistry, University of Wisconsin-Madison

