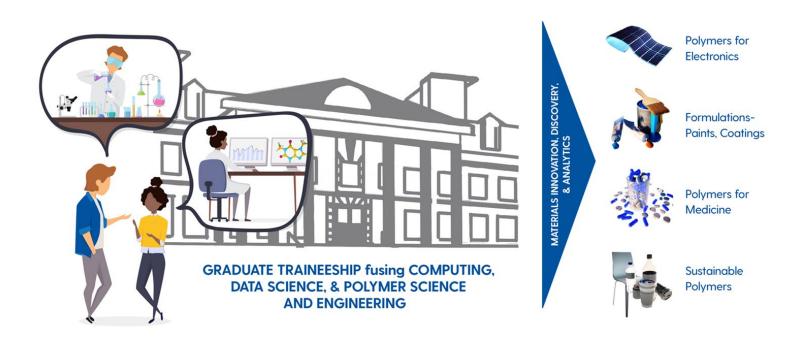
# NSF-funded NRT: Computing and Data Science Training for Materials Innovation, Discovery, & Analytics (MIDAS) program

by

NRT Director: Prof. Arthi Jayaraman & NRT Program Coordinator: Ms. Jennifer Johnston





# NRT Director & NRT Program Coordinator

NRT Director
Prof. Arthi Jayaraman
PI, NSF-NRT grant

NRT Program Coordinator Jennifer Johnston





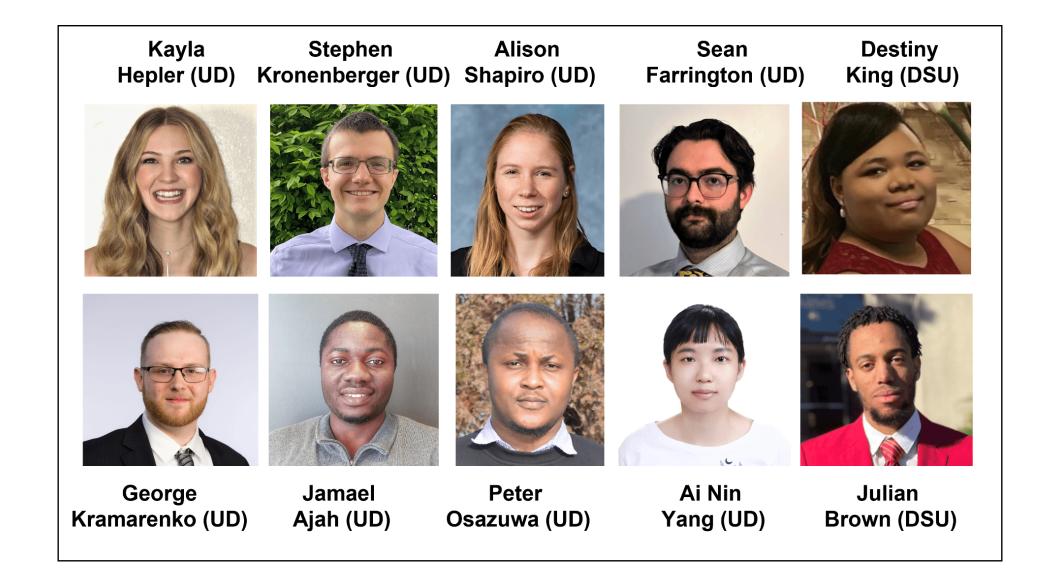
# https://sites.udel.edu/midas-nrt



# Interdisciplinary traineeship for doctoral students

- For admitted 1<sup>st</sup> year doctoral students in UD Chemical Engineering (CBE), UD
   Materials Science & Engineering (MSEG), UD Computer Information Sciences (CIS),
   UD Electrical & Computing Engineering (ECE) and DSU Chemistry (CHEM)
- Research themes combine to different extents high-performance computing (HPC),
   data science (DS), and soft materials (mostly polymers)
- NRT traineeship fits in the timeline of the individual UD graduate programs

## NRT Trainees – 1<sup>st</sup> cohort



# NRT Trainees - 2<sup>nd</sup> cohort

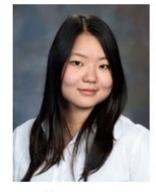
Erik Anderson (Chemical & Biomolecular Engineering UD)



Sonia Li (Chemical & Biomolecular Engineering UD)

Shweta Burgula (Chemical & Biomolecular Engineering UD)





Juliana Nam (Chemical & Biomolecular Engineering UD)

Jamie Holmes (Chemistry DSU)





Mosquera Rodriquez
(Materials Science &
Engineering UD)

Kelsey Koutsoukos (Materials Science &





Jay Shah (Chemical & Biomolecular Engineering UD)

Justin Labombard (Electrical & Computer Engineering UD)





Tasia Walker (Chemistry DSU)

# Interdisciplinary traineeship for doctoral students

- NRT traineeship augments the experiences that PhD students have beyond what they experience in their own graduate programs.
  - Funded NRT trainees get faculty co-advisors (assigned by the NRT) with expertise complementary to the expertise of their primary faculty advisor
  - NRT trainees participate in NRT industry internship or teaching certificate program (mandatory for funded trainees)
  - All NRT trainees participate in regular community hours that include networking events, technical talks by experts, & professional skills workshops
  - All NRT trainees plan & execute community/public outreach activities

# NRT MIDAS traineeship timeline (Year 1)

## Fall Before Year 1 in NRT program

NRT trainees selected in mid-December

#### Year 1 of NRT program - Winter & Spring

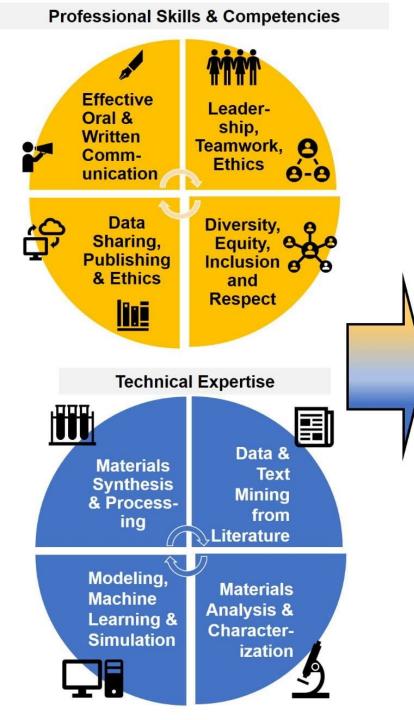
- NRT trainees continue to take their PhD core & elective courses in their respective departments
- NRT trainees start their research (same timeline as other non-NRT students in your departments)
- NRT trainees attend NRT community hours (workshops, talks, RCR training)

#### Year 1 of NRT program- Summer

• Community outreach: All NRT trainees pair up to plan and create activities for outreach to the public/local community – learn to effectively communicate their research work with public and non-scientist audience

## Year 1 of NRT program - Fall

- Present a poster on their ongoing thesis work in one community hour.
- By the end of Year 1 Fall, the NRT trainees should have completed at least **one technical elective in the primary discipline** and **one technical elective in secondary discipline**.





Core discipline courses and interdisciplinary (HPC, DS & MAT) electives





Career counseling with experts from academia, national lab, industry, patent law, science policy, etc.

#### **Professional Skills & Competencies**





Leadership, Teamwork, **Ethics** 



Data Sharing, & Ethics



**Publishing** 

#### **Technical Expertise**



**Materials Synthesis** & Processing

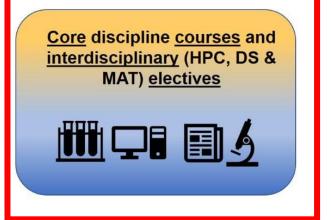


Modeling, Machine Learning & **Simulation** 



**Materials Analysis &** Characterization







Career counseling with experts from academia, national lab, industry, patent law, science policy, etc.

#### **Professional Skills & Competencies**



#### **Technical Expertise**



& Ethics

Data & Text Mining from Literature and Respect

Modeling, Machine Learning & Simulation

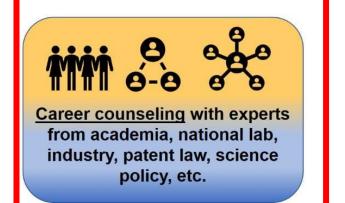
ing

Materials Analysis & Characterization



Core discipline courses and interdisciplinary (HPC, DS & MAT) electives





# NRT community activities – throughout the traineeship

# Fall & Spring NRT Community Hours

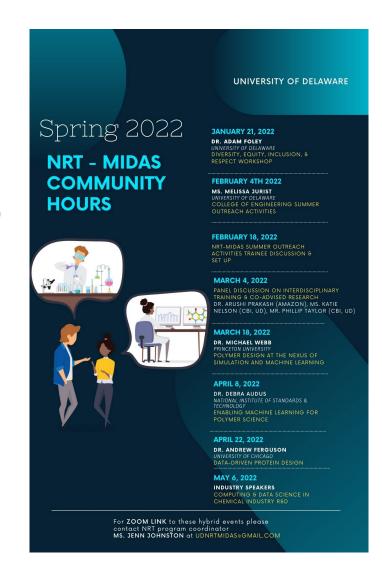
#### **Professional workshops**

- RCR (Responsible Conduct in Research)
- Diversity, Equity, Inclusion
- & Respect (DEIR)
- Ethics in Data Science
- Effective Communications

#### **Technical talks**

- Speakers from Industry, Academia & National Lab
- NRT Trainees' poster presentations

#### **NRT Community Gathering**





# NRT MIDAS traineeship timeline (Year 2)

## **Year 2 of NRT program - Winter**

NRT trainees continue to do their research and attend one NRT community event

#### **Year 2 of NRT program - Spring**

All NRT trainees enroll in a mandatory NRT course CHEG/MSEG/CISC/ECEG
 Computing and Data Science for Soft Materials Innovation

# Year 2 Spring - Interdisciplinary NRT course

NRT MIDAS trainees take CHEG/MSEG/CISC/ECEG Computing and Data Science for Soft Materials Innovation (after their primary discipline elective and secondary discipline elective)

Interdisciplinary group of graduate students work in teams of 3-4 with each team tackling one project submitted by industry/ national lab using computing tools

- o Instructors teach molecular modeling and simulation, high performance computing, and machine learning with emphasis towards application of these tools to soft materials problems.
- Students apply these computational tools to solve the industry or national lab problem throughout the semester
- Students also learn and practice collaborative teamwork, and oral + written communications training regularly; professional skills in interdisciplinary work environment

# CHEG/CISC Computing and Data Science for Soft Materials Innovation











# In Spring 2022

15 MS & PhD students

7 graduate students with computing background

+

8 graduate students with soft materials background

taught by

Arthi Jayaraman (Chem Eng., Mat Sci & Eng.)
Sunita Chandrasekaran (Comp. Sci)

# Spring 2023

# **Computing and Data Science for Soft Materials Innovation**









## In Spring 2023

MS & PhD students

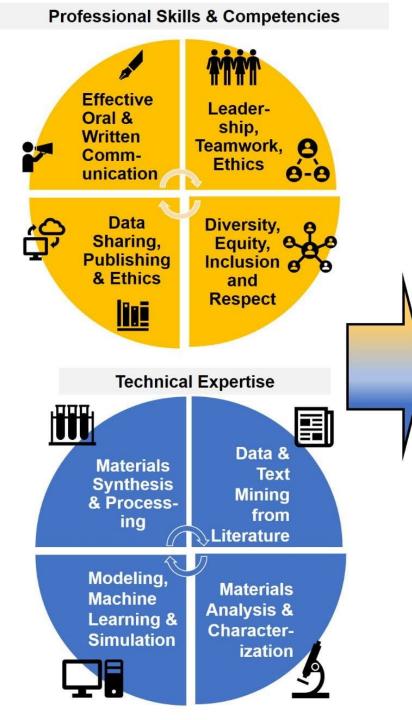
4 graduate students with computing expertise

+

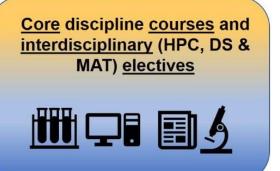
10 graduate students with experimental expertise

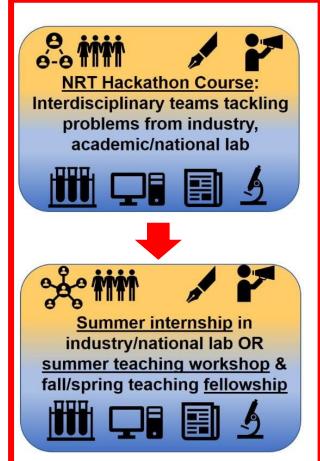
taught by

Arthi Jayaraman (Chem Eng., Mat Sci & Eng.)
Austin Brockmeier (Elec & Comp. Eng. and
Comp. Sci)



Convergent research under two thesis advisors with different research expertise





NRT course in Spring

Internship or Teaching workshop in the summer



# NRT MIDAS traineeship timeline (Year 2 continued)

## **Year 2 of NRT program - Summer**

For those interested in industry or national lab

#### **Industry/National Lab Internship**

For the entire summer, NRT trainees gain on-site experience with one of our partner companies who combine data science and computing for solving materials problems.

Mandatory for NRT-funded UD & DSU trainees interested in industry/national lab career

For those interested in academia

**2-part Teaching Certificate Program** 

Part 1 Effective teaching workshop by NRT core faculty in Y2 summer

Part 2 Teaching fellowship in core/elective/NRT course in Y2 Fall or Y3 Spring semester

Open to all NRT trainees and other students enrolled in UD & DSU

# Year 2 of NRT program - Fall

• **NRT trainees** will present in the NRT community hour what they have learned from Summer internship/teaching certificate (mandatory for funded trainees); we also want to hear how they are combining technical and professional skills they have learned so far in their thesis work.

#### Successful completion of all of the above NRT training elements will earn you a

# University of Delaware's **Graduate Certificate** in **Computing and Data Science for Soft Materials**

This certificate program was proposed by Prof. Arthi Jayaraman & Ms. Jennifer Johnston.

It has now been approved (after multiple rounds of reviews and interviews) by University of Delaware to be effective Fall 2023!

# How and when to apply to the NRT?

- Go to <a href="https://sites.udel.edu/midas-nrt">https://sites.udel.edu/midas-nrt</a> and click on "How to apply" in the menu
  - Has all the relevant information who can apply, how to apply, selection process
- A google form + information on what is needed before you fill the google form
  - This year's deadline November 30<sup>th</sup> 2022, 5pm
- Selection process will take place December 1 December 15
  - Alignment in thesis topics with NRT research themes, CV, personal statement
  - Short interview (virtual/in person) of finalists before final list of trainees are selected

# **NRT** decision letters

- Final decision that every applicant will get will inform them if they have been
  - Selected as a "NRT Trainee funded by NRT grant" for 2 years and then by their primary advisor
  - Selected as "NRT Trainee, not funded by NRT grant" (funded by primary advisor through out)
  - Not selected for NRT program

# Trainees funded by NRT

- 2-3 (UD) + 1-2 (DSU) domestic students (US citizen, green card holder)
  - NRT grant provides 2 years of stipend + tuition covered (Jan AY1 through December AY3) travel support (~\$500 per trainee) once;

#### **OR 1-2 International students**

- Will receive 1 semester of tuition + stipend from Univ. funds + travel support (\$500 once)s
- Must have an assigned primary advisor who will support the trainee outside of any NRT/COE funding
- 2-yr funded trainees will have secondary advisor will be assigned by NRT team
  - will bring in complementary expertise to that of primary advisor and work with the trainee and primary advisor in IDTP preparation, mentoring, & research direction
- These trainees are expected to do an internship in industry OR teaching certificate program

# Trainee not funded by NRT grant

- ~4-5 International or domestic students who are interested in participating in this program
  - Trainees should have other sources of funding (e.g., primary advisor's grant supports them or the trainee's department TA-ship, etc.)
  - Trainees' primary advisor or source of funding should approve the trainee's participation in the training elements at time of selection
- Trainee commits to (selected) technical and professional training elements (designed to fit well within graduate program timeline)
- NRT grant/COE funds will provide travel support (\$500 per trainee) once
- Access to all professional workshops (including teaching certificate program), other networking opportunities
- Industry internships will be possible only if positions available

# Frequently asked questions

- I am an MS degree student at UD. Is the NRT program only for students in the PhD program?
  - This NRT program is designed for **funding PhD students in their 1**<sup>st</sup> **year**.
  - MS students can participate in all or any of the NRT elements and apply for the Graduate certificate!
- Will I have to select a secondary advisor before applying?
  - No, those who are funded (for 2 years) by the NRT program will be assigned secondary advisor by the NRT program; goal to assign someone with expertise different but complementary to primary advisor expertise so the trainee receives combined computing/data science & soft materials advising
  - Unfunded NRT trainees will not get an assigned co-advisor.
- Do I have to take more courses than expected from my grad program?
  - You only do as many electives as your grad program expects. All that the NRT program expects you
    to do is select those electives with a purpose to bring interdisciplinarity in your training
    - 1 elective of your choice on computing (e.g., molecular modeling & simulations, Intro or advanced machine learning courses, GPU computing course),
    - 1 elective of your choice on soft materials (e.g., polymers elective for CBE/MSEG students or molecular modeling for soft materials for CS students)
    - Mandatory Spring Y2 NRT 'hackathon-style' course "Computing and data science for soft materials innovation"

# Frequently asked questions

- I am an international student. Am I allowed to participate in this NRT program? Can I apply?
  - Yes, an international student can be part of the NRT program. You cannot receive any financial support from the NSF NRT grant (NSF rules).
  - We have an additional pot of money from college of engineering to support international student NRT trainee travel (for unfunded NRT trainees) or 1 semester of stipend & tuition (for funded NRT trainee who is an international student)
- Will I get a special degree or certificate?
  - Your degree will be the same as what you would get from your UD grad program
  - Upon successful completion of expected NRT training elements, you can also receive a graduate certificate from UD Graduate College!
- Who supports me financially after my NRT funding runs out (a question from NRT funded trainees)?
  - Your primary advisor (research support) or your department (TA support)

#### NRT-MIDAS Graduate Traineeship

