

**THE DEPARTMENT OF CHEMISTRY  
PRESENTS**

**A VIRTUAL  
MINI-SYMPOSIUM  
& POSTER  
SESSION**

**SUMMER UNDERGRADUATE  
RESEARCH FELLOWS**

July 31, 2020

## VIRTUAL KEYNOTE PRESENTATION

1:00 PM

**MILLAN WELMAN**

*"Optimizing Effective Potentials with Pure-State Solutions in  
Density-Functional Theory"*

Mentored by Professor Weitao Yang

Zoom Link: [https://duke.zoom.us/j/96933496096?  
pwd=Q1lVdUE4cmF1MVZpOERrSSsxMjZOOT09](https://duke.zoom.us/j/96933496096?pwd=Q1lVdUE4cmF1MVZpOERrSSsxMjZOOT09)

Meeting ID: 969 3349 6096

Password: chemsurf

## VIRTUAL POSTER SESSION: HOW IT WORKS

The virtual poster session is intended to simulate an in-person poster session in which audience members stop by posters, take a look, ask questions, and move on to another poster.

There will be two poster sessions.

Session 1: 1:45-2:30 EDT

Session 2: 2:30-3:15 EDT

Posters are listed below alphabetically by last name (within sessions).

Each student has a listing in the program that includes:

-Title

-Faculty mentor

-Zoom Link, Meeting ID, and Password  
(should be 'chemsurf' for each meeting)

## HOW IT WORKS

Click on the Zoom link provided to join a given student's meeting where she or he will present their poster. If you are prompted to enter a password, please enter 'chemsurf.' Within each session, you may choose which posters you go to and when. Do not worry about joining a meeting that is already in session or ducking out to peruse another poster. Feel free to ask the presenter for a short summary of the poster or for the presenter to zoom in on a specific area of the poster you have more questions about.

An electronic version of each student's poster is also available on the Chemistry Department's website (<https://chem.duke.edu/undergraduate/chemsurf-2020>).

Please click on the link to any poster to view it more easily on your own computer or device (the files are large, so they may take a few minutes to load).

We hope this will make it more convenient for you to review the fellows' work independently of their presentations so you can spend more time talking to them and asking them questions about their work rather than requesting they zoom in on different sections of their posters.

## ACKNOWLEDGEMENTS

The Department of Chemistry would like to thank the faculty and graduate students involved in the research with our participants this summer. In addition, the summer graduate mentor, Brandon Bowser, provided outstanding support to the students in this unprecedented time. Dr. Daniel Fowler excelled in supervising this unique virtual program.

The Department also thanks the Trinity Research Enhancement for support of the Summer Fellowship.

## POSTER SESSION I

1:45 - 2:30 PM

Password: chemsurf

### DANIEL CHEONG

*"Predicting Substrate Specificity for a Fatty-Acyl Adenylate Ligase in Toxoplasma gondii using bioinformatic analysis"*

Mentored by: Professor Emily Derbyshire

Zoom Link: <https://duke.zoom.us/j/96731254053?pwd=aVJjeXY3UFAyb0FIUi9zYmMya2d6Zz09>  
Meeting ID: 967 3125 4053

---

### HALEY HUTCHINSON

*"Identification and Characterization of Novel Cis-Regulatory Elements Controlling PTEN Expression"*

Mentored by: Professor Kris Wood

Zoom Link: <https://duke.zoom.us/j/99565692594?pwd=R3NEeHQwRzN1cWtzL1RaZ00vQXJHZz09>  
Meeting ID: 995 6569 2594

---

### HOLLY KIM

*"Analyzing the Active Sites of SARS-CoV Nonstructural Proteins"*

Mentored by: Professor Lorena Beese

Zoom Link: <https://duke.zoom.us/j/97558582749?pwd=SEhzY1Y4a0FiSnorbktCYzJ6SG5tZz09>  
Meeting ID: 975 5858 2749

**POSTER SESSION I**

**1:45 - 2:30 PM**

**password: chemsurf**

**TOMMY LIN**

*"Virtual Reality Understanding of the Catalytic Mechanisms in SABRE"*  
Mentored by: Professor Volker Blum

Zoom Link: <https://duke.zoom.us/j/96199599732>  
Meeting ID: 961 9959 9732

---

**MICHAEL PUPI**

*"A bioinformatic analysis of PY motif-mediated interactions in  
the Nedd4 family of ubiquitin ligases"*  
Mentored by: Professor Dewey McCafferty

Zoom Link: [https://duke.zoom.us/j/95993404120?  
pwd=NC84aGxwVXh5UXFEOFZqbTB6UUZsUT09](https://duke.zoom.us/j/95993404120?pwd=NC84aGxwVXh5UXFEOFZqbTB6UUZsUT09)  
Meeting ID: 959 9340 4120

**POSTER SESSION II**

**2:30 - 3:15 PM**

**Password: chemsurf**

**OLIVIA LIU**

*"Host-Pathogen Interactions in Toxoplasma gondii Infection"*

Mentored by: Professor Emily Derbyshire

Zoom Link: [https://duke.zoom.us/j/99572740059?  
pwd=Sk93OTJweXlScnZGZXNOTEFrQ1FXZz09](https://duke.zoom.us/j/99572740059?pwd=Sk93OTJweXlScnZGZXNOTEFrQ1FXZz09)

Meeting ID: 995 7274 0059

---

**ANNA SCHWARKOPF**

*"The Role of NADPH Oxidase I in Vascular Disease; a Multi-Omics Approach"*

Mentored by: Professor Francis Miller

Zoom Link: [https://duke.zoom.us/j/91751577672?  
pwd=dU9CVkw5Wkx6NE43VHZwVjg1b2ZYZz09](https://duke.zoom.us/j/91751577672?pwd=dU9CVkw5Wkx6NE43VHZwVjg1b2ZYZz09)

Meeting ID: 917 5157 7672

---

**POSTER SESSION II**

**2:30 - 3:15 PM**

**Password: chemsurf**

**CHARLOTTE THOMAS\***

*"Homology Modeling and Virtual Screening in the C. trachomatis  
Chorismate Biosynthesis Pathway"*

Mentored by: Professor Dewey McCafferty

Zoom Link: <https://duke.zoom.us/j/96254654002>

Meeting ID: 962 5465 4002

\*Selected as 2020's Alvin Crumbliss Summer Fellow

---

**JEFFREY ZHANG**

*"Probing active site specificity of ramoplanin class fatty acyl-AMP ligases"*

Mentored by: Professor Dewey McCafferty

Zoom Link: <https://duke.zoom.us/j/96073603957>

Meeting ID: 960 7360 3957