

# BLUE WATERS

## Blue Waters Education Allocations Final Report



UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

As a component of your application for a Blue Waters education allocation, you agreed to provide a report at the end of your project. Now that your project is complete, we would appreciate your submission of the following information within two weeks. Please send this report, and any supporting documents, to Scott Lathrop, [lathrop@illinois.edu](mailto:lathrop@illinois.edu).

This information will be shared with the Blue Waters team and the National Science Foundation. Portions of the report (we will omit names of participants) will be posted on the Blue Waters portal for public access.

### Project Information

Project Name	Surface-deposited molecules and clusters: structure, surface-patterning, and bonding analysis
Names of project staff (instructors, TAs, etc) and their department and institutions	Instructor: Prof. Anastassia Alexandrova
URL for the project	n/a
Provide links to or attach materials made available to participants (e.g. slides, articles, exercises, etc.) that may be made publicly available	see attached bundle of pdf files. Also see: <a href="http://cms.mpi.univie.ac.at/vasp/vasp.pdf">http://cms.mpi.univie.ac.at/vasp/vasp.pdf</a> <a href="http://www.gaussian.com/g_ur/g03mantop.html">http://www.gaussian.com/g_ur/g03mantop.html</a> (manuals)
Provide links to or attach any photos (with captions to describe activities)	n/a
Start date	May 21, 2015
Completion date	June 1, 2016

### Information about the Participants

# Participants	# Faculty or staff	# students	# other (e.g. industry)	# under-represented (e.g. women, minorities)	# institutions represented by participants
2	1	1		1	UCLA

Please describe the scope and purpose of this project. Also, please indicate if there were any changes implemented from the original proposed plan, and briefly describe why they were made.

Dr. Anastassia Alexandrova lab was hosting one student for the XSEDE Scholars program, Olivia Irving, with a focus on studying small clusters/molecules on surfaces. Specifically we focused on carboranedithiols adsorbed on Au(111), which have been shown to assemble and form two-dimensional monolayers. Olivia was trained to perform highly parallel simulations of extended surfaces, adsorptions, surface-patterning, and STM image simulations. We ended up dropping the development of Wannier functions that was originally proposed, as it appeared too challenging for now. The extensive need for scripting within the supercomputer environment was instead a valuable coding training component for Olivia.

Please describe the learning outcomes of the participants. How did this project enhance the learning of the participants? What did the participants learn as a result of the use of Blue Waters system that they could not have learned using other systems?

Olivia mastered all the mentioned computational techniques proposed for this allocation. Moreover, she then went on to meaningfully contribute to the research project done in collaboration with Prof. Weiss in UCLA (experimental STM imaging). I consider Olivia well-trained now to perform surface and STM simulations in supercomputing environment, which will be the focus of her research in graduate school.

Please describe lessons learned from the project. What would you do differently next time?

My choice for the project would be better measured for the abilities of the students that I plan to supervise. Part of this project appeared to be too challenging. However, overall we have a very good experience with Blue Waters. The application part of the proposal is completely fulfilled and the outcome even surpassed all our expectations.

What would you recommend that the Blue Waters team do to enhance the success of education projects in the future?

n/a

Please provide a summary of any surveys or evaluations you conducted of the participants. Feel free to attach any related documents.

Weekly (or sometimes even daily) meetings with the student were part of our routine. During those, continuous feedback was given, and directions for improvement have been provided, but without written records. Perhaps what speaks the most about Olivia's success and growth is that she got admitted to UCLA graduate school, after completing her training with the support of Blue Waters.

Please provide any anecdotal stories we may share with NSF and the public.

Oh no

How would you rank the overall experience?

	<b>Excellent</b>	<b>Very Good</b>	<b>Good</b>	<b>Fair</b>	<b>Poor</b>	<b>N/A</b>
<b>Education allocations process</b>	x					
<b>Blue Waters support</b>	x					
<b>Blue Waters computing system</b>	x					
<b>Blue Waters documentation</b>	x					
<b>Blue Waters training</b>	x					

Do you plan to request an education allocation for other future events that will use BW?

Please describe the plans for future events, including the frequency (each semester, yearly, etc.).

I would like to, but at the moment do not have specific plans

Please provide any other comments or suggestions.

n/a