

Nanotechnology simulation and more
Always on, around the globe



Issue 34

Community College Student Gains Valuable Experience Via nanoHUB Tool Development

Sulaiman Abdul-Hadi, a second-year engineering student at Roxbury Community College, had no research experience prior to joining Professor Chen Yang's lab during the summer of 2018.

"Before, I'd only thought of it as a career possibility," says Abdul-Hadi. "But now I definitely want to do research."

Yang, Associate Professor in the Department of Electrical and Computer Engineering and the Department of Chemistry at Boston University, specializes in the design and development of nanomaterials for photonics and biomedical applications.

"I was contacted by Tanya Faltens, the Educational Content Creation Manager at nanoHUB. She was looking to develop some remote positions for underrepresented community college students who would assist with research during the summer," said Professor Yang. These positions were supported by the NSF-funded Network for Computational Nanotechnology Cyber Platform (NCN-CP) as part of the NCN-CP's Undergraduate Research Experience (URE) program.

"I wasn't familiar with community college students," said Professor Yang, "But I had great help from a senior colleague and Director of undergraduate study in Chemistry, Professor John Snyder, who had been a director of the REU program in BU's chemistry department and has strong connections with faculty at community colleges in the area."

Professor Snyder connected with those faculty members and received nearly a dozen applications with recommendation letters. When Abdul-Hadi was chosen to fill the position, Professor Snyder agreed to take him to the weekly REU meetings and activities, as well as the REU symposium so that he could participate. In this way, Abdul-Hadi's summer research experience was also supported by the REU program at Boston University.

Abdul-Hadi assisted Professor Yang with her existing simulation tool, [Optical Properties of Single Coaxial Nanowires](#), which facilitates the design of a new group of nanomaterials with novel optical properties.



Roxbury Community College student Sulaiman Abdul-Hadi is studying in the lab at BU. Photo by Jackie Ricciardi for Boston University Photography.

"The new group of cylindrical nanowires has a core and outer layers," says Professor Yang. "The use of different materials for the core, like a semiconductor, and an outer layer, like a metal, leads to different properties,

Upcoming Events

Introduction to Using nanoHUB's Free Online Computational Materials Simulations for Undergraduate Education

When:

Sunday, June 16, 2019
9:00 a.m. - noon

Where: Room 37, Tampa Convention Center, Florida

This ASEE pre-conference workshop will provide participants with hands-on training using free simulation-based materials science activities that are appropriate for undergraduate students. After going through the workshop, participants should be able to use these simulation activities in their own courses.

Website: [ASEE Annual Conference 2019](#)

nanoHUB Tool Development Workshop at ICME 2019

A nanoHUB tool workshop will be held as part of the 5th World Congress on Integrated Computational Materials Engineering (ICME 2019). The congress is taking place in Indianapolis, Indiana from July 21-25. The workshop will be held in Indianapolis on the afternoon of July 25 and all day at Purdue University in West Lafayette, Indiana on July 26. The nanoHUB portion of the workshop will be at Purdue on the morning of July 26.

Participants in this hands-on, developers workshop will gain the knowledge needed to publish simulation tools and workflows in nanoHUB. Once deployed, these tools are accessible to users from around the world for cloud computing. Fully interactive simulations can be executed from any standard web browser without the need to download or install any software, making them available not only to experts but to the broader scientific community. Furthermore, nanoHUB tools are indexed by Web of Science and Google Scholar, and detailed usage statistics are collected and published.

Website: [5th World Congress on Integrated Computational Materials Engineering \(ICME 2019\)](#)

[Explore Events](#)

New Resources

Spin-based Quantum Gate Lab

Spin Qugate is a set of python codes that calculate the device-level characteristics of spin-based quantum gates. Single-qubit rotational gates and two-qubit controlled-phase gate can be simulated, which form a complete set of quantum gates for universal quantum computing. The tool can simulate time evolution, compute delay and fidelity, and perform

enabling an excellent engineering strategy. For example, in metal we see plasmonic behavior, which enhances the absorption and emission coming from the semiconductor. Having those improved characteristics allows the use of these nanowires in solar energy applications and photonic devices.”

According to Professor Yang, these nanowires could be used as photoelectrochemical cells, absorbing solar energy and converting it to chemical energy. They can be used for water-splitting for clean and sustainable energy generation in fuel cells. In addition, enhancing the efficiency of absorption and emission may lead to the development of high-efficiency white LEDs.

The nanoHUB tool can help design coaxial nanowires by predicting which materials and dimensions should be selected to achieve improved performance. Those predictions can then be verified experimentally in the lab.

Abdul-Hadi’s task was to create a component that calculates the predicted improvement in emission that the nanowire structure can provide, based on a paper published in 2018 by Professor Yang.

“I took MATLAB code that researchers in the lab use for testing, learned how that worked, and used it to develop my new nanoHUB tool,” said Abdul-Hadi. “I was able to reverse-engineer an earlier tool to figure out the process.”

The experience was so positive to Sulaiman that he decided to stay in Professor Yang’s research group as a volunteer during the next two semesters.

“After I finished working on the tool, I started doing experiments,” said Abdul-Hadi. “I used the atomic layer deposition machine, which does micro-chemical reactions on a film. You can make some of the things that were predicted by the tool. I liked the simulation side best, but it’s also fun to create what you’re simulating.”

“I was very impressed with Sulaiman’s work,” said Professor Yang. “It was a great experience for me. He seemed very motivated and keen to do research. He delivered and worked hard with a passion equivalent to the Boston University students that I typically work with.”

“And I was glad to see that he liked the experience as well.”

Professor Yang is again working with nanoHUB to recruit another summer undergraduate researcher from local community colleges for the summer of 2019.

NCSA Hosts Inaugural Workshop on Data-science Enabled Advances in Nanomanufacturing

quantum process tomography for the quantum gates. The effect of dephasing can be simulated by inputting a spin dephasing time.

[Polyvalent Nanoparticle Binding Simulator](#)

This app simulates coarse-grained ligand-receptor binding of ligand-decorated virus particles interacting with a cell wall. The viruses are modeled after P22 virus-like particles (VLPs) of diameter 60 nanometers, and ligands represent smaller nanoparticles of 6 nanometer diameter. Each virus is fully decorated with 60 ligands. Receptor are fixed on a lattice of tunable size.

[Infrastructure for Data-Driven Discovery: Materials Data Facility and DLHub](#)

Presented by Ian Foster, Distinguished Fellow and Director of the Data Science and Learning Division at Argonne National Laboratory. His research deals with distributed, parallel, and data-intensive computing technologies, and innovative applications of those technologies to scientific problems in such domains as materials science, climate change, and biomedicine.

[Wearable Sweat Sensors - Towards Big Data for Human Health](#)

Wearable sensor technologies play a significant role in realizing personalized medicine through continuously monitoring an individual’s health state. To this end, human sweat is an excellent candidate for non-invasive monitoring as it contains physiologically rich information. In this talk, Ali Javey will present recent advancements on fully-integrated perspiration analysis system that can simultaneously measure sweat rate, metabolites, electrolytes and heavy metals, as well as the skin temperature to calibrate the sensors’ response.

[NSF’s Advanced Manufacturing Program and Research in Nanomanufacturing](#)

This talk is sponsored by the Nanoscale Manufacturing at The University of Illinois node (nanoMFG) and presented by Dr. Khershed P. Cooper, Program Director for Advanced Manufacturing in the CMMI Division of the Engineering Directorate at NSF.

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The Network for Computational Nanotechnology and nanoHUB .org are supported by the National Science Foundation.



The [nanomanufacturing \(nanoMFG\) node at Illinois](#) presented its first two-day workshop on February 26 and 27 at the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign. The workshop focused on data-science enabled advances in nanomanufacturing in nanotechnology.

The workshop, led by PI [Kimani Toussaint](#), Associate Professor of Mechanical Science and Engineering at Illinois and Director of [Illinois' Nanomanufacturing Node](#), brought together experts at the forefront of nanomanufacturing, engineering, and data science to draft a position paper on data-driven nanomanufacturing.



Attendees learned about challenges and opportunities in nanomanufacturing and the potential use of data science in accelerating development in this field. Real-world applications of the promise of nanomanufacturing brought about discussions of the challenges and opportunities of nanotechnologies, as well as the promise of competitive innovation in nanomanufacturing both at the academic and industrial levels, while allowing each attendee to network with new colleagues in different fields, and participate in breakout sessions and presentations.

"I was pleasantly surprised by the enthusiastic response from the attendees," said Dr. Toussaint. "Quite a few told me that they did not know what to expect coming into the workshop, but were delighted and energized to explore and contribute to the potential of this emerging area, the integration of data science with nanomanufacturing. We plan to do more of these in the coming years."

Co-chairs of the event included Illinois Mechanical Science and Engineering Assistant Professors Sam Tawfick and Chenhui Shao. Shao is also an NCSA center affiliate in the [Industry program](#).

Learn more about the [nanoMFG node workshop on data-science enabled advances in nanomanufacturing](#) on the nanoHUB website.

Jupyter Notebooks on nanoHUB

Did you know that you can build and share Jupyter Notebooks on nanoHUB? A Jupyter Notebook is an open-source web application that allows you to develop documents that contain live code, equations, visualizations and narrative text. Uses include numerical simulation, statistical modeling, data visualization, machine learning, and more.

The newly published Jupyter Manual and Examples resource will help you get started: <https://nanohub.org/resources/jupyterexamples>

It contains code samples, documentation, a list of currently installed packages, and more.

