

Nanotechnology simulation and more
Always on, around the globe



Issue 31

NodeNews – Two Photon Lithography Simulation Tool

The Network for Computational Nanotechnology's partnership with the Nanomanufacturing (nanoMFG) Node continues to be productive with the development and release of a new simulation tool that is available to the entire nanoHUB community.

Published in early July, the [Two Photon Lithography](#) (TPL) tool was developed at the University of Illinois at Urbana-Champaign by Mohammad Kabir, a PhD candidate, Varun Kelkar, a master's student, and Darren Adams, Senior Research Programmer with the National Center for Supercomputing Applications.

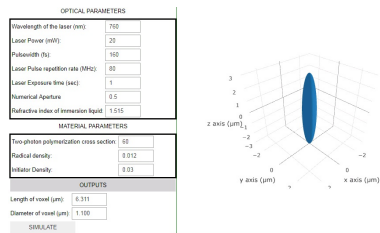
"Two Photon Lithography is a nanoscale manufacturing process that uses a photo-polymer resin and light to create three-dimensional structures," says Kabir. "An important determination for TPL is to discover what would be the smallest structure that can be constructed."

"The user can enter the properties of the light to be used, such as power and wavelength, along with the properties of the polymer material, and that will allow us to calculate the size of the smallest structure that can be expected from the process."

According to Kabir, the TPL process can produce 3D structures faster than standard photo-lithography and can be used to quickly prototype new designs from a CAD file. Combined with the new simulation tool, manufacturers should be able to get a much clearer picture of the nanostructure that will result.

Kabir, Kelkar, and Adams plan to continually refine and update the TPL tool. The first step in that process is to gather feedback from users. "Try out the tool and let us know your thoughts via nanoHUB's feedback system," says Kabir. "The information that we collect from our users will be very important in this development cycle."

Planned future upgrades include the addition of some Uncertainty Quantification based on error, as well as the inclusion of a 3D CAD viewer, allowing users to view the final structure that will be created.



Summer School for Integrated Computational Materials Education

Upcoming Events

[Frontiers In Education \(FIE\) 2018 Conference](#)

When: Oct. 3-6, 2018

Where: San Jose, California

The 48th Annual Frontiers in Education (FIE) Conference is a major international conference focusing on educational innovations and research in engineering and computing education. The theme for 2018 is Fostering Innovation Through Diversity. Thematic tracks include: diversity/equity/inclusion in engineering/computing, encouraging and teaching innovation, innovation in software engineering education, upward mobility, and EPICS/service-learning. FIE 2018 continues a long tradition of disseminating results in engineering and computing education. It is an ideal forum for sharing ideas, learning about developments and interacting with colleagues in these fields.

[Applied Nanotechnology and Nanoscience International Conference \(ANNIC\) 2018](#)

When: Oct. 22-24, 2018

Where: Langenbeck Virchow Haus, Berlin, Germany

The Applied Nanotechnology and Nanoscience International Conference is an annual event. It hosts high-profile plenary speakers, world-class researchers, oral and poster presentations, workshops, sponsor exhibits and afterworks. This event is a great opportunity to share your research findings with a wide audience, promote knowledge exchange, and network. Come to share during this fourth edition.

[Explore Events](#)

New Resources

[Modeling a Deep Reactive Ion Etching \(DRIE\) Process](#)

This Learning Module introduces Deep Reactive Ion Etching (DRIE) used in the fabrication of microsystems, an overview of how DRIE can be computationally modeled, and a brief conclusion of the Design for Nanomanufacturing at UC Berkeley's research on modeling a DRIE process. Activities in this module allow you to demonstrate and apply your understanding of the basic concepts of these processes.

[Two Photon Lithography](#)

Two-photon lithography (TPL) is a nanoscale 3-D fabrication technique. TPL depends upon the two-photon polymerization process, whereby two incident photons of light are absorbed by a precursor material leading to polymerization. The smallest feature size

It is widely recognized that nanoHUB's simulation tools can be used for serious research, but more and more often the tools are finding an important second role as teaching resources.

Since 2011, they have proven their usefulness in the Summer School for Integrated Computational Materials Education (ICMed) at the University of Michigan, during which attendees learn how to use computational simulation in education.

In this, the seventh full year of the program—one year featured a short course rather than the typical two-week session—the ICMed Summer School ran from June 4 – 15 with 20 attendees.

Professor Katsuyo Thornton, the L.H. and F.E. Van Vlack Professor of Materials Science and Engineering at the University of Michigan organizes the conference along with colleagues Mark Asta of UC Berkeley and Raúl Enrique of the University of Michigan. The participants consist of graduate students, postdocs who are interested in becoming faculty, and current faculty who would like to learn more about incorporating many different types of simulation resources into their classrooms.

“nanoHUB has the advantage of not having to install software on computers,” says Thornton. “So it’s one of the easiest ways to implement simulation in the classroom because all you need is a web browser.”

Thornton teaches an array of learning modules, including several using the following nanoHUB simulation tools:

- [DFT Calculations with Quantum ESPRESSO](#)
- [Virtual Kinetics of Materials Laboratory](#)
- [Semiconductor Doping](#)

Throughout the years, Thornton has continued to teach others how to incorporate nanoHUB resources into their classes. “I believe it is important to keep nanoHUB in the school because of its ease of use.”

For more information, see the program's website (<https://icmed.engin.umich.edu>) or contact the organizers at icmed2018@umich.edu.



NCN Undergraduate Research Experience Wrap Up

Congratulations to our NCN URE cohort of 2018! The summer is over but the memories, the friendships, and the research outcomes live on.

Watch the [New Resources](#) page on nanoHUB to see the posters and tools contributed by our URE students to the community.



Tool Statistics and Citations

(voxel) achievable in a IPL process is typically observed in the form of an ellipsoid and depends upon the incident laser beam parameters and the properties of the precursor material. A ultrafast, femtosecond pulsed laser beam is used as the optical source of polymerization.

This tool calculates the expected voxel dimensions - axial length and cross-sectional diameter - under given experimental conditions provided by the user.

[Computational Catalysis with DFT](#)

This tool utilizes the Atomic Simulation Environment (ASE) Python library and Quantum Espresso to calculate properties of interest for catalysis. Outputs include adsorption energy, density of states (DOS), projected density of states (PDOS), s-, p-, and d-band centers, and a visualization of the atomic structure and unit cell using the Visualization Toolkit (VTK). The tool has two modes of operation: Basic and Advanced. Basic Mode has relatively few inputs and is intended for use in educational settings, while Advanced Mode offers more customizability and is intended for use in research.

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



Publishing your simulation tool is an excellent step to disseminating your content to a broader audience. Did you know that you can find detailed usage statistics on your tool's resource page?

These quantitative statistics provided on the nanoHUB platform not only provide you with an understanding of the reach of your tool into the community but provide a compelling measure of impact.

In the grey box below the tool's description, click the "Usage" tab. Here you'll find a map displaying the geographical location of each of your tool's users since its posting, a graph tracking the growth of your tool's user base over time, a breakdown of users by organization type, and more.

Has your tool been cited by other researchers? Take a look at the "Citations" tab. This page lists citations as they are discovered by nanoHUB and are broken down into authors who are affiliated with nanoHUB, and authors who are non-affiliated.

The data in these documents is updated continuously and provides an easy way to gauge your tool's impact at a glance.

