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Computational nanoelectronics research and education at nanoHUB.org

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Abstract The simulation tools and resources available at nanoHUB.org offer significant opportunities for both research and education in computational nanoelectronics. Users can run simulations on existing powerful computational tools rather than developing yet another niche simulator. The worldwide visibility of nanoHUB provides tool authors with an unparalleled venue for publishing their tools. We have deployed a new quantum transport simulator, OMEN, a state-of-the-art research tool, as the engine driving two tools on nanoHUB.

The educational resources of nanoHUB are one of the most important aspects of the project, according to user surveys. New collections of tools into unified curricula have found a receptive audience in many university classrooms.

The underlying cyberinfrastructure of nanoHUB has been packaged as a generic software platform called HUBzero. The Rappture toolkit, which generates simulation GUIs, is part of HUBzero.

Keywords Computational · Electronics · Nanoelectronics · Modeling · nanoHUB · nanoHUB.org · OMEN · Rappture · GUI

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1 Introduction

1.1 Mission and vision

The Network for Computational Nanotechnology (NCN) was created in 2002, as part of the National Nanotechnology Initiative, to provide computational tools and educational resources related to nanotechnology. The primary vehicle for this mission is the web site nanoHUB.org (nanoHUB). nanoHUB provides 140 simulation tools and over 1400 educational resources which are employed by over 91,000 users all over the world [1]. We define a "user" as someone who downloads content, runs simulations, or spends at least 15 minutes on the site viewing materials. Over 7,200 of our users ran more than 400,000 simulations in the past year.

nanoHUB offers at least two tremendous opportunities for creators and users of simulation tools. The first is for those who want to use simulation tools but not to create them. For example, an experimentalist might want to vary the parameters of a semiconductor device of interest in his laboratory. A good computational model can do this much more quickly than a new device could be manufactured, and modeling can guide the experimental effort. Such a user is not likely to spend the time to code and debug a simulation tool and continue updating and maintaining it. nanoHUB presents a collection of high quality computational tools in one venue, and many of these tools make use of open access grid computing resources (TeraGrid, Open Science Grid), which are not likely available to most users. The second opportunity is for tool creators. Most simulation tools are created and used in a local environment by a few people. Much time and effort is spent re-creating a tool which already exists in another research group. The worldwide audience of the nanoHUB offers unparalleled visibility for a simulation tool. For example, one of us (BPH) has contributed tools to nanoHUB which have been used for almost 27,000 simulations by 1670 people [2].

nanoHUB also offers access to a wide range of educational materials. Resources from nanoHUB were used in 78 classes, at both the graduate and undergraduate levels, at 42 universities worldwide over the past year. These materials, which include lecture videos, tutorials, tool manuals, and learning modules, can be used in conjunction with traditional class lectures or for self-study.

1.2 Overview

In this paper we discuss the research usage of nanoHUB (Sect. 2), as well as educational (classroom) usage (Sect. 3). We also provide some measure of nanoHUB's impact in the nanotechnology community (Sect. 4), and we discuss the cyberinfrastructure which powers nanoHUB (Sect. 5). Section 5.1 gives an introduction to the Rappture toolkit, which generates the tool GUIs that facilitate simulations and are in a large part responsible for the user numbers mentioned in Sect. 1.1.

2 Research usage

2.1 Scholarly citations

Perhaps the most visible measure of the impact of nanoHUB on the nanotechnology community is the number of publications which cite a tool or resource on nanoHUB. We have identified 430 citations to nanoHUB in the scientific literature and 52% of these citations are made by investigators not in any way affiliated with NCN, as visualized by being outside of the dashed line in Fig. 1. Researchers affiliated with, but not funded by, NCN are responsible for many of the remaining citations. The NCN is clearly strongly networked through research papers, and networks are also developing outside the NCN. Some of the outside networks are completely decoupled from the NCN.

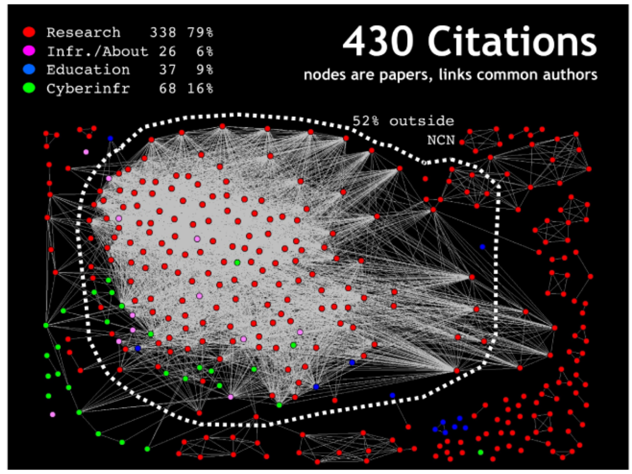

Fig. 1 Connections between nanoHUB citations, inside and outside of NCN

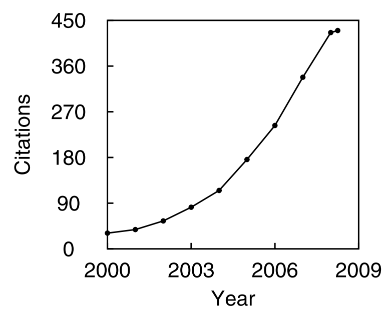

Fig. 2 Cumulative nanoHUB citations

Fully 89% of these citations are found in peer reviewed journals, conference proceedings, book chapters, or dissertations (Ph.D. or Master thesis). The remainder are found in magazine articles or conference presentations. As nanoHUB has grown in visibility and in its impact on the community, the number of citations has grown from 31 in 2000 to 430 at the end of March 2009 (Fig. 2).

Seven of the ten most cited tools on nanoHUB simulate nanoelectronics. These include Schred [3, 4], Band Structure Lab [5–7], (Fig. 3), Quantum Dot Lab [5, 8], and Nanowire [9, 10].

2.2 OMEN

We have recently developed a new 3D atomistic full-band quantum transport simulator, OMEN, which uses a nearest neighbor tight-binding [11] basis. OMEN has been used to study post-CMOS devices such as ultra-thin-body (UTB), nanowire, and tunneling FETs [12–15], as well as the transport properties and the gate length scaling behavior of ideal and rough Si triple-gate nanowires with different crystal orientations [16–18], comparing the output characteristics of n- and p-doped Si double-gate UTB FETs with different transport and confinement directions [19], and reproducing the

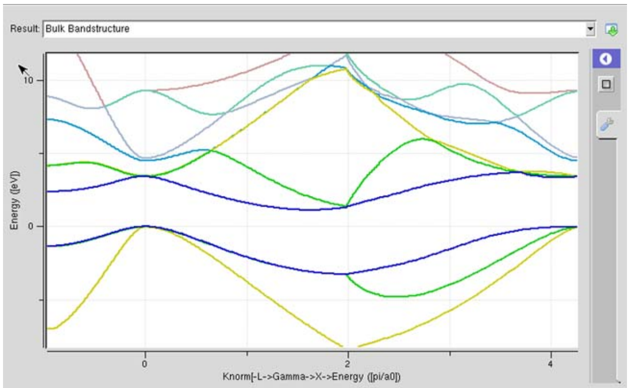

Fig. 3 Band Structure Lab output for bulk Si

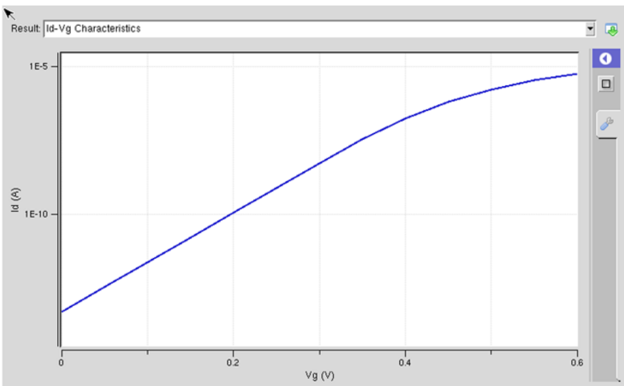

Fig. 4 OMEN Nanowire Id-Vg output for a cylindrical Si ⟨100⟩ nanowire at 300 K

experimental data of an existing InAs high-electron mobility transistor (HEMT) [20].

OMEN employs four levels of parallelism, distributing voltage points, k-points, energy points, and spatial regions across many CPUs. This approach has allowed OMEN to scale almost perfectly to 65536 CPUs (cores) [21], making use of high-performance computing (HPC) resources such as Kraken at NICS and Ranger at TACC.

This powerful research tool now drives two nanoHUB applications: Band Structure Lab [5–7] (Fig. 3), and OMEN Nanowire [12, 22] (Figs. 4 and 5), used by over 2,300 and 100 users, delivering over 18,000 and 720 simulations, requiring on average 8 minutes and 4.3 hours of compute time, respectively. The OMEN nanowire tool can be used to calculate full I–V curves for realistic devices, as shown in Fig. 4, as well as the density of states, seen in Fig. 5.

2.3 Impact: patent application

nanoHUB was used recently in the design process of a new semiconductor device [23], a gated resonant tunnel device based on a standard CMOS production process. The device is realized by changing implant doses and species and is a

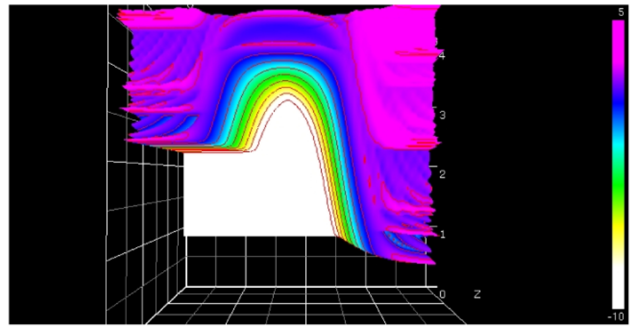

Fig. 5 OMEN Nanowire density of states for the same wire as Fig. 4

single mask-adder to the process flow. The basic idea was to leverage the electrostatic control necessary for resonant tunneling. The resulting device is a four-terminal resonant tunnel device capable of negative differential source-to-drain resistance as a function of either the gate, the drain, or substrate bias. It has potential applications in memory, digital and analog circuitry. One of the inventors, Dr. R. Chris Bowen of Texas Instruments, provided the following statement:

> NanoHUB provided me with a means to quickly test the original concept to see if it was worth pursuing in more detail on local machines and simulation tools. To do this, I pushed the nanoHUB tool into a regime it was never intended to operate and was able to get a concise answer to the question of viability. This was extremely helpful in getting the patent through the initial approval process within Texas Instruments.

3 Educational usage

In the Spring of 2009, 29 universities and colleges in the USA, Canada, Central America, China, Germany, Belgium, Netherlands, Czech Republic, Singapore, India, and Turkey used nanoHUB simulation resources as part of 35 courses. In the Fall of 2008, 34 courses at 21 institutions used nanoHUB. Many of these courses used collections of educational resources organized into coherent curricula. Some of these curricula which are focused on nanoelectronics are shown in Fig. 6 and are discussed in the following sections.

3.1 ABACUS: Assembly of Basic Applications for the Coordinated Understanding of Semiconductors

The popular curriculum entitled "Introduction to Semiconductor Devices" is powered by the tool ABACUS [24]. The ABACUS-powered curriculum is designed to enhance the learning experience of students in existing semiconductor device classes in Electrical Engineering programs. ABACUS is a collection of different nanoHUB tools that model

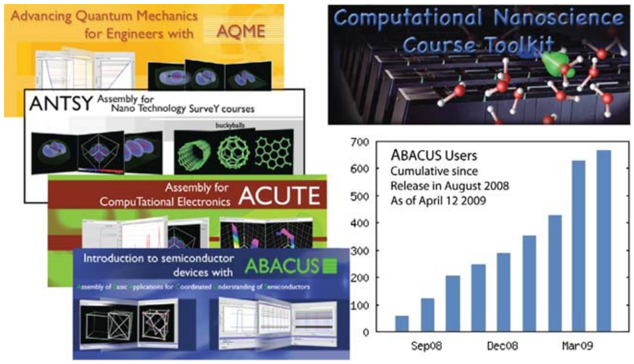

Fig. 6 Tool powered nanoelectronics curricula on nanoHUB

crystals, band structure, pn junctions, MOS capacitors, and transistors. The ABACUS-powered curriculum is a curated page that provides easy access to a variety of different homework and project assignments which are relevant for the teaching of semiconductor devices. Educators can request access to homework solutions. All community members are encouraged to contribute content to nanoHUB. ABACUS was introduced in August 2008 and has served over 660 users through the end of March 2009.

3.2 AQME: Advancing Quantum Mechanics for Engineers

The curriculum entitled Advancing Quantum Mechanics for Engineers is powered by the AQME [25] tool, which is an assembly of tools we believe are useful in the teaching of introductory quantum mechanical principles in an Electrical Engineering or Physics curriculum. Commercial semiconductor devices have become as small as a few tens of nanometers, and understanding basic quantum mechanical principles of quantization, energy bands, and tunneling are of critical importance. Topics considered in AQME are superlattices, quantum dots, tunneling diodes, and Ultra-Scaled MOS devices. The AQME-powered curriculum is a curated page that provides access to a variety of different homework and project assignments that are relevant for quantum mechanical principles.

3.3 ANTSY: Assembly for Nanotechnology Survey Courses

The curriculum entitled Assembly for Nanotechnology Survey Courses is powered by the ANTSY tool [26], which is an assembly of tools we believe are useful in the teaching and understanding of simple and oft-discussed nanotechnology devices such as bucky balls, carbon nanotubes, graphene, quantum dots, and resonant tunneling diodes. The ANTSY-powered curriculum is a curated page that provides access to a variety of different homework and project assignments that are relevant for quantum mechanical principles. This tool set was compiled by one of us (GK) after several faculty members across the United States requested information regarding nanotechnology simulation overviews.

3.4 ACUTE: Assembly for Computational Electronics

The ACUTE [27] tool-based curricula is intended to introduce interested scientists from industry and academia to advanced simulation methods needed for proper modeling of state-of-the-art semiconductor devices. The ACUTE-powered curriculum is a curated page that provides access to a variety of different homework and project assignments which illustrate key principles of current nanoelectronics.

3.5 Impact: classroom usage

Dr. Shaikh Ahmed, Assistant Professor in the Electrical and Computer Engineering Department at Southern Illinois University, Carbondale, has used simulation tools on nanoHUB as an integral part of several graduate level nanoelectronics courses. Dr. Ahmed provided the following statement:

> In this connection, I would like to mention that I have taught a junior-level undergraduate course on Microelectronics in fall 2008 and spring 2009 semesters, with 11 and 19 students respectively. The main objective of this course is to introduce the students to the fundamental concepts of electronic devices (diodes, BJTs, and MOSFETs) and their circuit applications. In this course, as case study and in order to find necessary supports in the proper perspective for the above-mentioned curriculum, I have introduced topics on nanoelectronics within the scopes of my lectures, homework assignments (some of which used nanoHUB simulators like BJT Lab and FETtoy), and issue-based group/independent studies. A survey was also conducted, which revealed that 77% students strongly welcomed this form of nanotechnology integration and 73% would strongly support similar activities in other courses too.

4 Assessment of nanoHUB

4.1 User surveys

Measuring the impact of nanoHUB on the nanotechnology community is a challenging task. The citations discussed in Sect. 2.1 form one measure of impact. Another may be found in the responses to periodic surveys of registered users. Users of nanoHUB fall into several categories; three groups of particular interest for assessing the overall utility and direction of nanoHUB are one-time users, non-simulation users, and heavy simulation users.

One-time users The one-time users log in perhaps a few times in a one week period but never return again. They are usually students who are required to use a specific nanoHUB tool for a class. These users identified in their survey responses a strong desire to learn more about nanotechnology but not through simulations.

Non-simulation users Regular users who do not typically run simulations are called non-simulation users. Of these users, 21% are searching for online presentations, while 9% are looking for materials to use as they teach. Their interest is broadening their research and keeping current in nanotechnology.

Heavy simulation users Users who run many simulations are overwhelmingly graduate students and postdocs. Their interest in nanoHUB lies in the quality and free access to powerful computational tools and resources. Their motivation is deepening their research, keeping current in nanotechnology, and learning new technical information.

Overall results Users in all categories want to see more educational materials on nanoelectronics, at both introductory and specialized levels. For simulation users, the quality and availability of the computational tools is paramount. This information is very useful in directing the development of nanoHUB.

4.2 NCN supported tools

The nanoHUB tools discussed in Sect. 2.2 are significant research simulators, and, as discussed in Sect. 4.1, the heavy simulation users of nanoHUB place a high premium on access to such tools with little interruption. In order to more fully support these users, the NCN has identified a limited list of supported tools which we believe produce valid results and for which we commit to the following level of service:

1. Monitor support tickets, questions, wish lists to provide a response to issues within one business day
2. Fix simple bugs within one week
3. Move long term improvement requests to a public wish list

Every nanoHUB tool is displayed on the site along with the numbers of its users, community-contributed reviews, and questions, and citations in the literature. As a distinction, supported tools also receive a gold badge followed by "NCN Supported", shown in Fig. 7.

4.3 Content characterization

As nanoHUB content increases, we find that users are struggling to find the high quality content. As a result, we have continued to improve the search mechanisms on nanoHUB to enable rapid information retrieval. One key element in this effort is to characterize each content item by a variety of criteria that ultimately influence the ranking of the resource. Each simulation tool is characterized by:

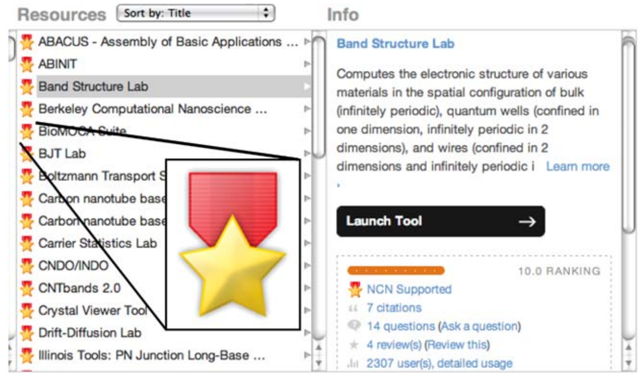

Fig. 7 NCN-Supported tools are specially identified on nanoHUB

1. A Google-like ranking based on user reviews and use.
2. Data including number of users and simulation jobs, average run time, and average number of stars awarded in reviews.
3. Number of citations in the scientific literature; this is a number that indicates the vetting of the tool and its use in research.
4. Number of questions, indicative of the liveliness of the community; a large number of open question suggests a badly supported tool. A large number of closed questions indicates a live code with tool owners interested and dedicated to its support. The introduction of a virtual economy has proved to have a positive influence on the question and answer forum.
5. A newly introduced wish list enables users to express tool improvement wishes and the tool development team to handle tool improvement processes.
6. User reviews: anyone can give a 0- to 5-star review and submit written comments.
7. Users can also now declare nanoHUB content items as their favorites, which they can later easily find again on their favorite list. Furthermore they can share their favorite nanoHUB items on six different social network sites like facebook, twitter, or google.

An example of this characterization is seen in Fig. 8.

4.4 Contributor impact

In Sect. 1.1 we mentioned the impact one of us (BPH) has had through tools deployed on nanoHUB. This analysis of contribution impact may be extended, as we now show for the case of one of our co-authors, Professor Dragica Vasileska. Prof. Vasileska deployed Schred [3, 4] on Purdue's PUNCH system, which predated nanoHUB in 2000.

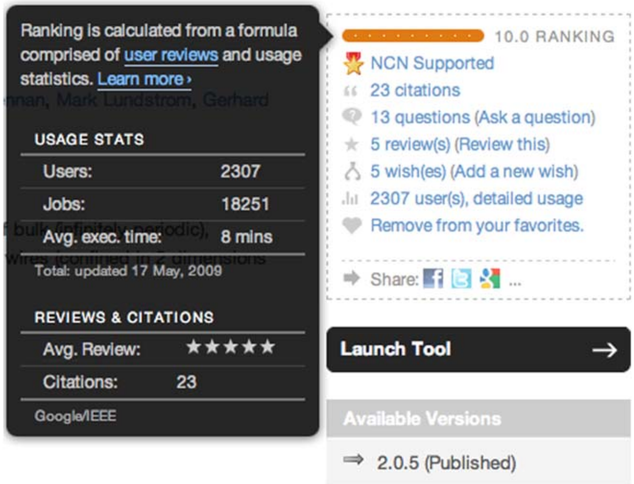

Fig. 8 Characterization of Band Structure Lab

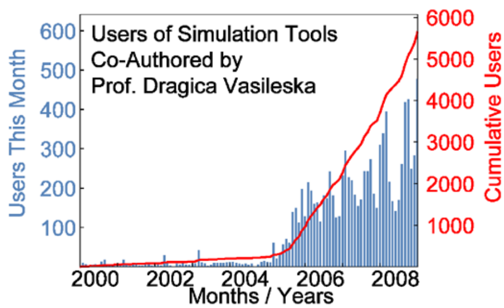

Fig. 9 Monthly and cumulative users of Prof. Vasileska's tools on nanoHUB

Since then, the tool has undergone various improvements and has been deployed also in a fully interactive version. Prof. Vasileska immediately began to use the tool for teaching semiconductor device classes. Neither she nor her students had to install the code. Both theorists and experimentalists found the code powerful enough for research purposes. We have been able to identify 93 citations to this tool on nanoHUB, 81 of which are from users unaffiliated with NCN or nanoHUB. We believe that this is an impressive number of citations for a tool that is community-contributed. The NCN team keeps track of these tool citations, and the number of citations is a key element to validate the science of a particular code. Prof. Vasileska is a co-author on 17 tools on nanoHUB. The usage tracking on nanoHUB can now deliver other data about the impact of a contributor. Figure 9 shows a summary graph of the monthly users of Prof. Vasileska's tools and a cumulative number of unique nanoHUB users who used her tools. Around 200–300 users use her tools on a monthly basis, and in total over 5,500 users have run simulations with her tools. She will soon be able to pull such impact graphs from the nanoHUB directly and can use them as evidence of on-going education and outreach efforts with her work.

The NCN has invested considerable effort to make nanoHUB self-sustaining. The ability described here to quantify and demonstrate the impact of one's contributions to nanoHUB is a compelling incentive to contribute, especially for those who wish to demonstrate significance to prospective employers or funding agencies. As nanoHUB visibility grows, we foresee a reliable stream of new simulation tools deployed on nanoHUB.

5 Technology and infrastructure

Part of the overall mission of nanoHUB is the development of the cyberinfrastructure necessary to serve the community. Sixty-eight papers, meeting the same peer-review criteria as those in Sect. 2.1, have referred to the cyberinfrastructure of nanoHUB; forty-one of these papers come from outside the NCN, which strongly indicates to us that the nanoHUB is considered a leader in cyberinfrastructure development.

5.1 Rappture

In order to significantly reduce the programmer hours required to create intuitive GUIs to a wide variety of powerful simulation codes, NCN created an open source *R*apid *App*lication Infrastruc*ture* toolkit called Rappture [28]. Rappture-based tools are ordinary applications which can run on Windows, Mac OS X, and Linux platforms, irrespective of any Web deployment. Coupled with our unique middleware [29], however, nanoHUB.org delivers them to any web browser which supports Java; no extra work is required to deploy a powerful computational tool online. Not only is the resulting tool easy to use, but it's also easy to develop, typically by graduate students deeply involved with the underlying theory code or undergraduate students working in a team with expert graduate students. Rappture programmers describe the input parameters and output results for a simulation code as a hierarchy of data objects in an XML file. Rappture reads that file and generates a GUI automatically. Each input and output has a description that pops up when users mouse over its associated control. The GUI can include embedded notes in HTML format, with links to tutorials and documentation. Rappture recognizes various output types and automatically invokes the appropriate visualization engine. In the past three years, more than 200 developers have used Rappture on more than 190 projects. Typical projects require a few days of programmer time to create the Rappture interface that facilitated the deployment of a raw simulation code on nanoHUB. Rappture also provides a consistent and accessible presentation, which is extremely important in an educational setting. Instructors interested in constructing a coherent sequence of learning experiences for students, such as the tool based curricula discussed in

Sect. 3, need a common interface for all the tools. For example, the design project for a course might require the synthesis of results from several simulation tools. With a consistent interface, learners will apply their intellectual energy to investigating their questions rather than to learning new interfaces.

5.2 HUBzero

The underlying cyberinfrastructure of nanoHUB has been abstracted into a generic package called HUBzero[30]. We believe the HUB concept is applicable to many engineering and science disciplines, and the NCN is actively deploying new HUBs for discovery and learning. HUBzero is designed as a general-purpose software platform that can support virtual communities focused on nearly any academic discipline. The HUB concept will greatly expand the user base for modeling and simulation and open new possibilities for many people who would otherwise avoid computing.

6 Summary

nanoHUB was created to provide computational tools and educational resources for a global nanotechnology community. The opportunities provided by nanoHUB include simulation tools for users who would not create their own, worldwide visibility and audience for tool authors, and a wide variety of educational materials. Hundreds of peer reviewed articles cite nanoHUB and many of these focus on nanoelectronics. Our new high-performance quantum transport research simulator, OMEN, powers two tools on nanoHUB.

Collections of tools in coherent curricula are used in dozens of university classes in several countries. We find that our users are extremely interested in educational resources in nanoelectronics and high quality simulation tools. The underlying infrastructure of nanoHUB has been extracted into HUBzero, a generic HUB platform which is currently expanding into many diverse disciplines beyond nanoelectronics.

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