NNCI Computation

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Modeling and Simulation

- Modeling and simulation can enhance nanoscale fabrication and characterization:
  - guide experimental research
  - drastically reduce the required number of trial and error iterations
  - enable more in depth interpretation of the characterization results
  - help quantify the true potential value of the fabricated devices

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Current Status

- Abundance of resources and expertise at various sites even though few sites proposed any activities.
- Diverse funding sources for development and maintenance of these resources (inadequate in many cases).
- Ad hoc access and documentation.
- Many gaps and deficiencies.
- Duplicate efforts happen.

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Objectives:

- To facilitate access to the modeling and simulation capabilities and expertise within NNCI sites.
- To identify the strategic areas for growth in modeling and simulation
- To promote and facilitate the development of the new capabilities.

An inventory of available modeling and simulation resources and expertise is being complied. The directory is hosted by nanoHub.org.

So far, 10 sites have reported collectively more than 65 commercial simulation tools and 40 internally developed simulation tools available for internal and/or external users (with and without fee).

8 supercomputers or major computing clusters are available in various sites.

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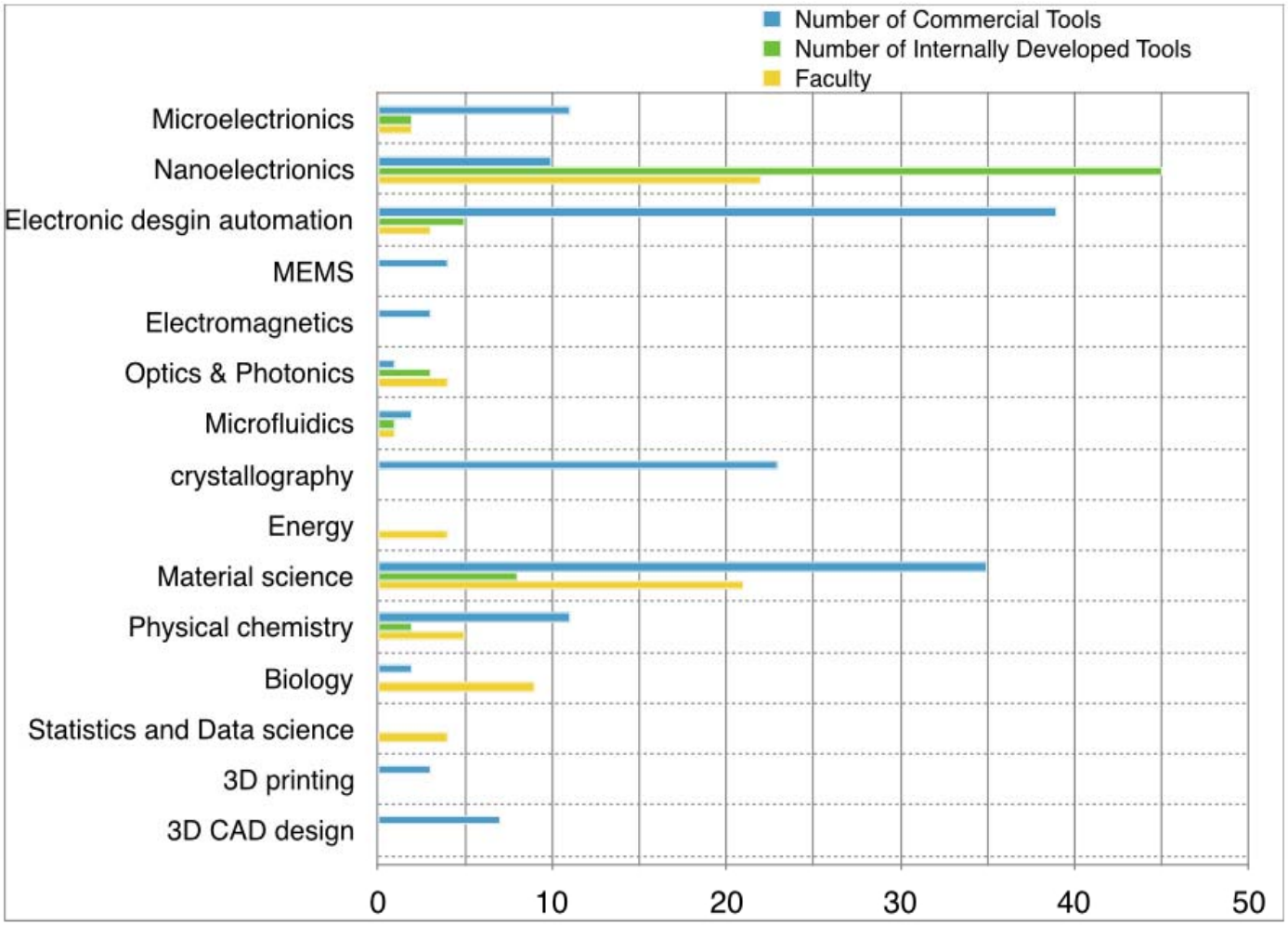
Statistics by Disciplines



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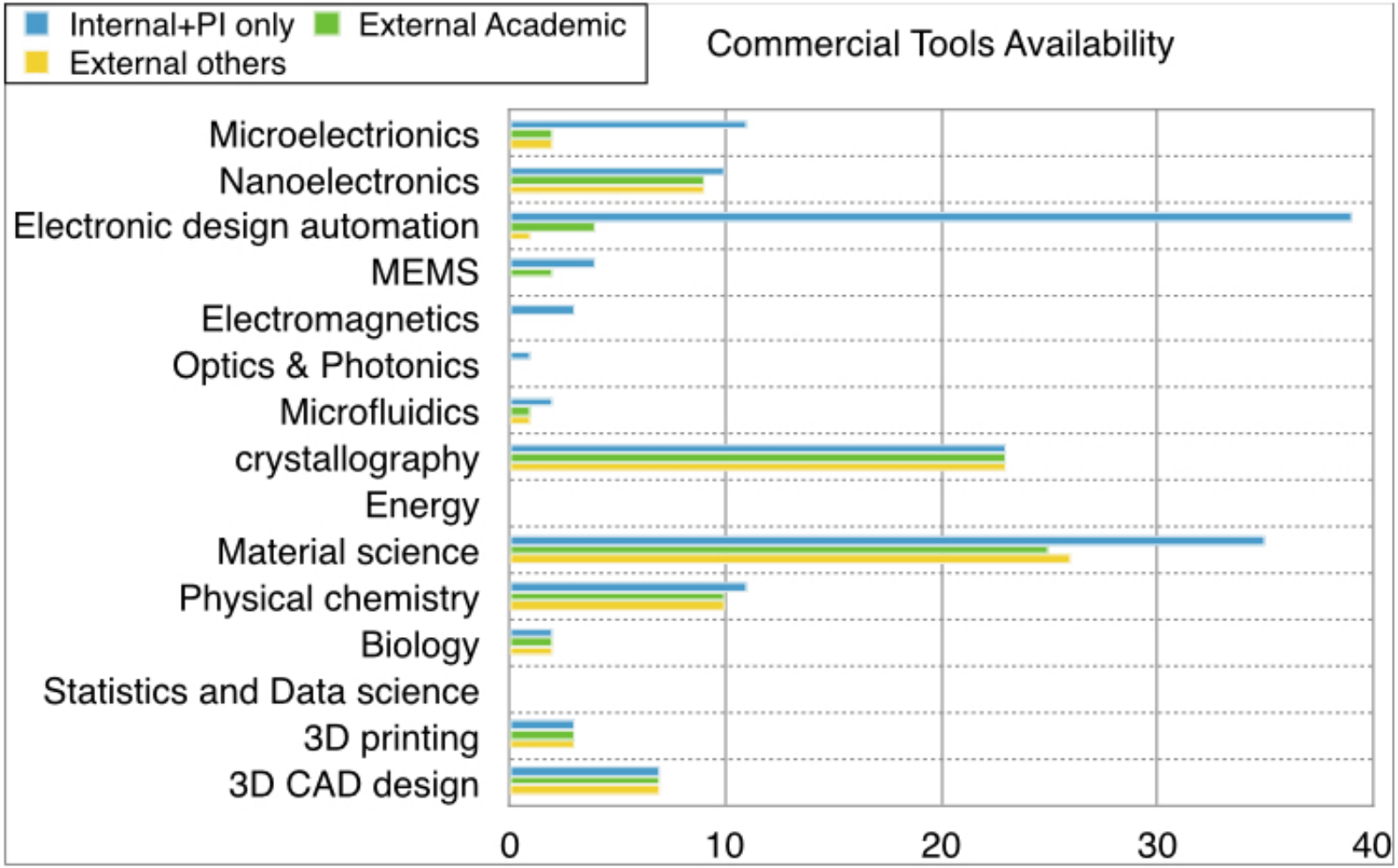
Permission to Access: Commercial Tools



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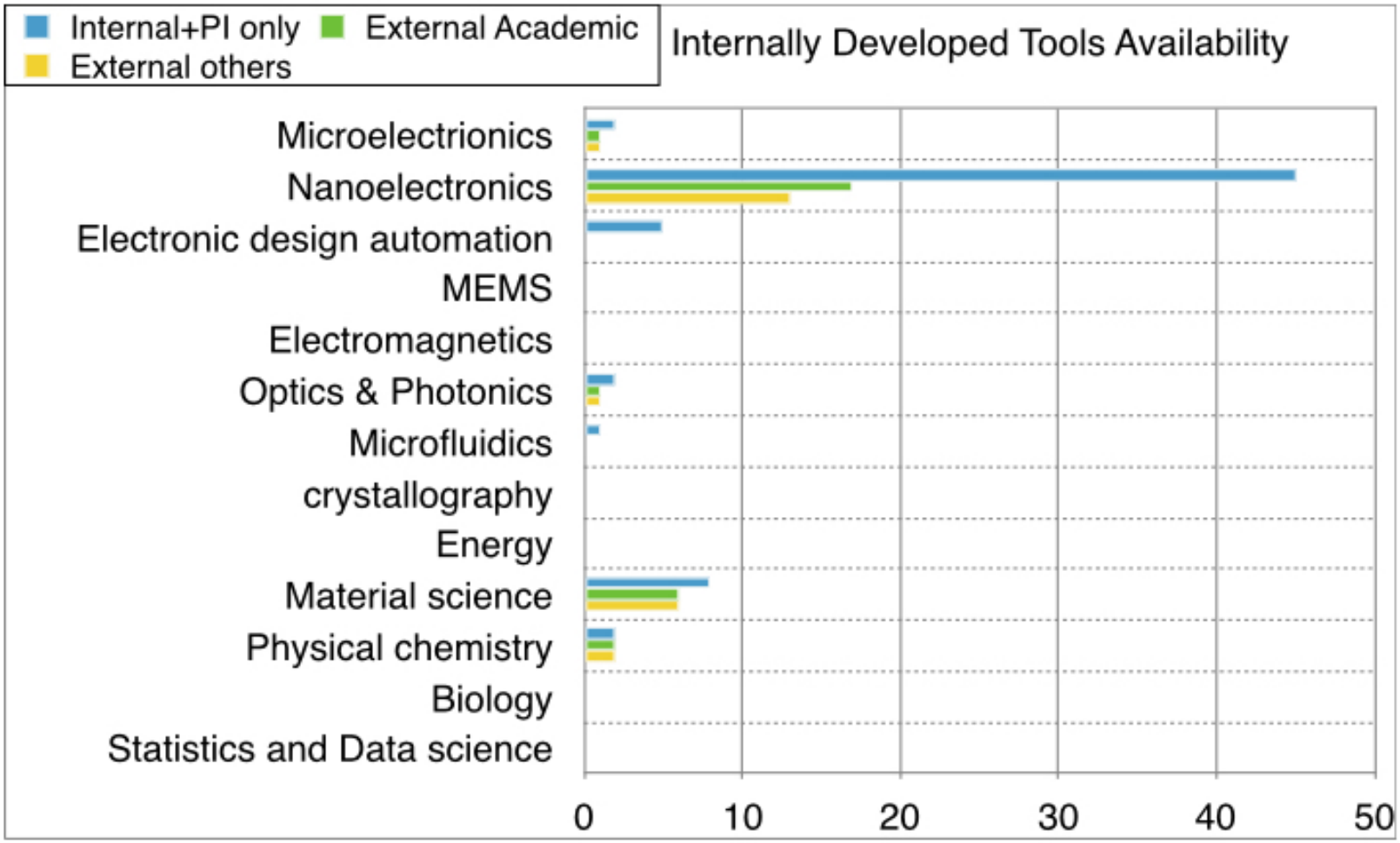
Permission to Access: Internally Developed Tools



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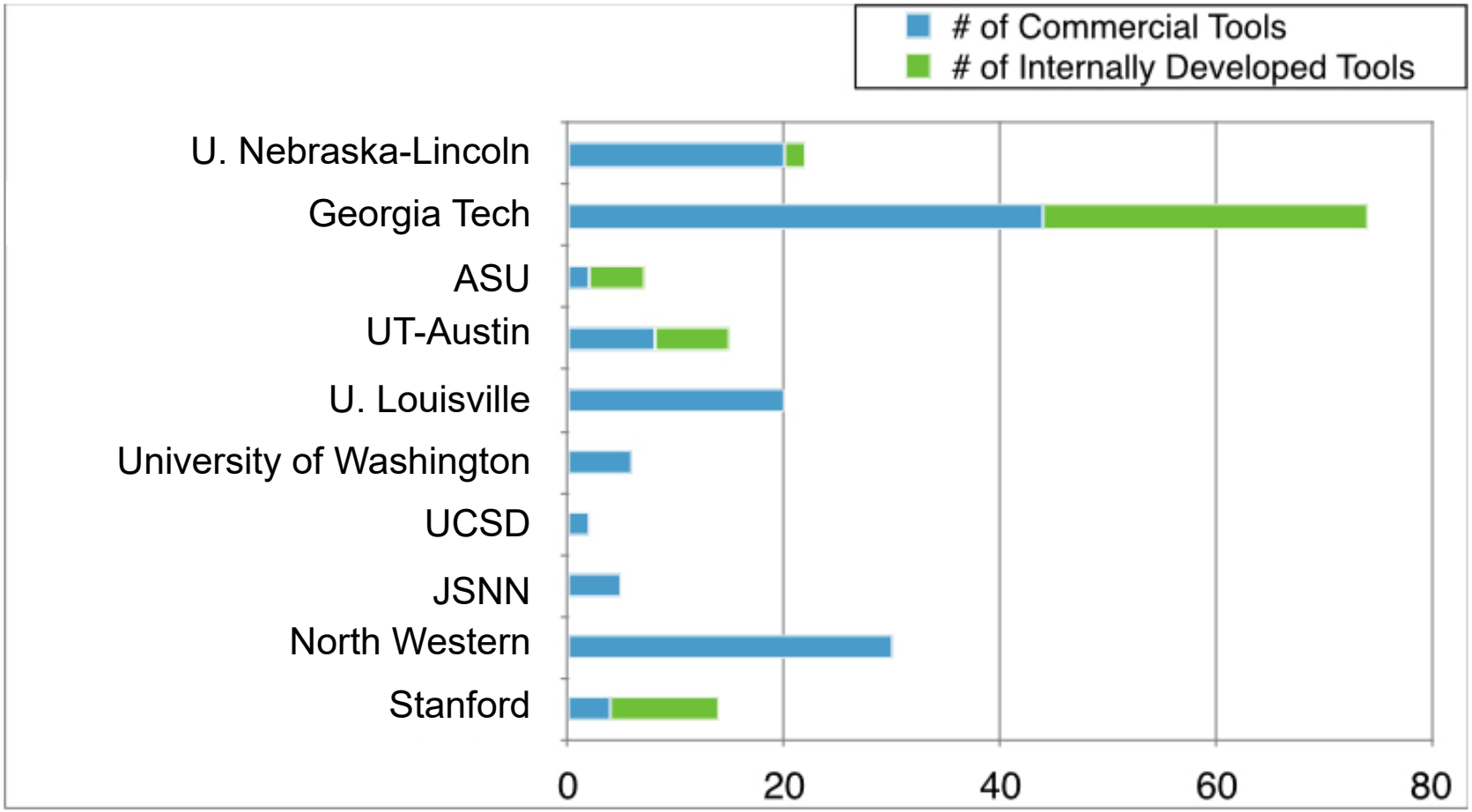
Contributing Universities



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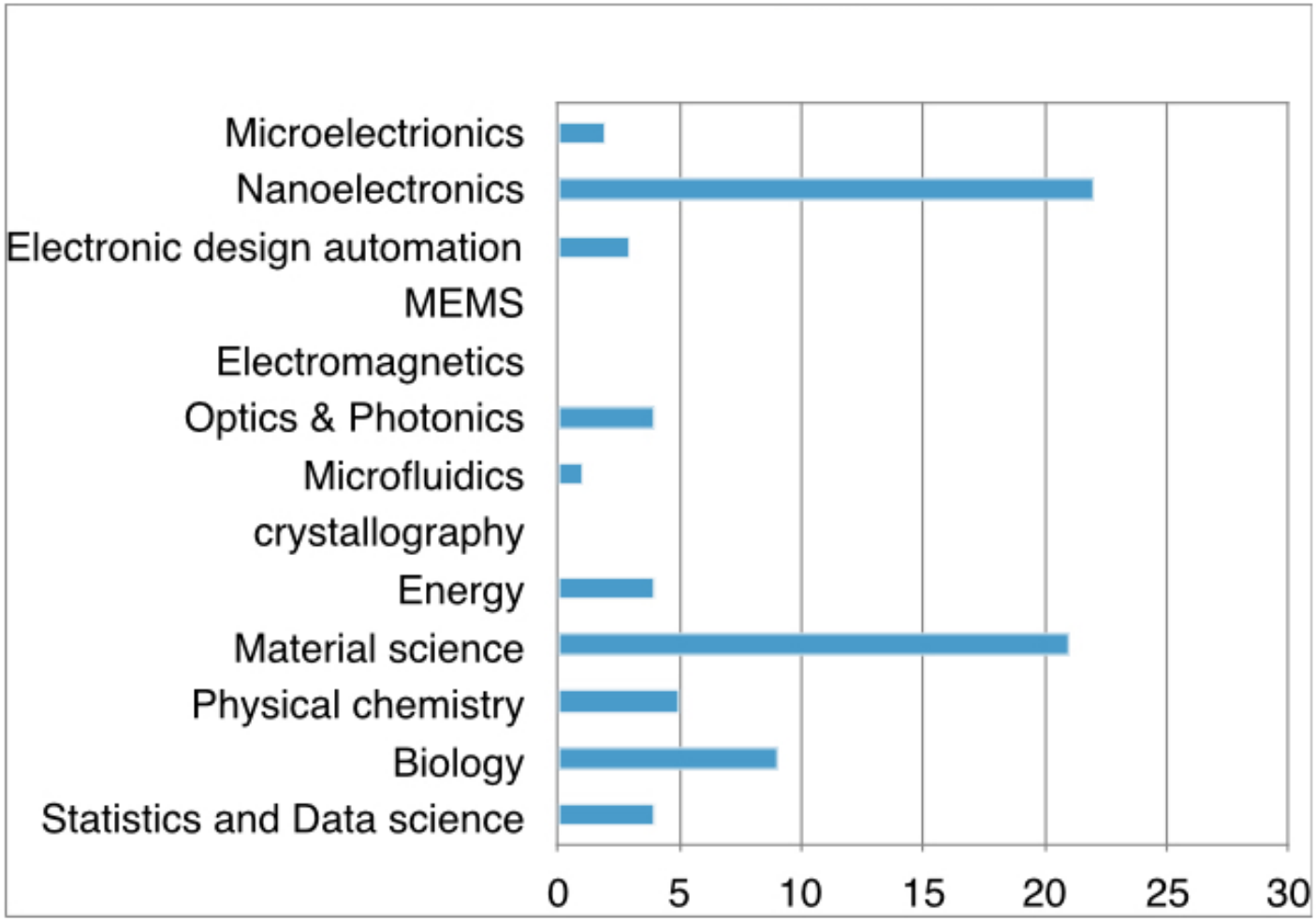
Modeling and Simulation Experts



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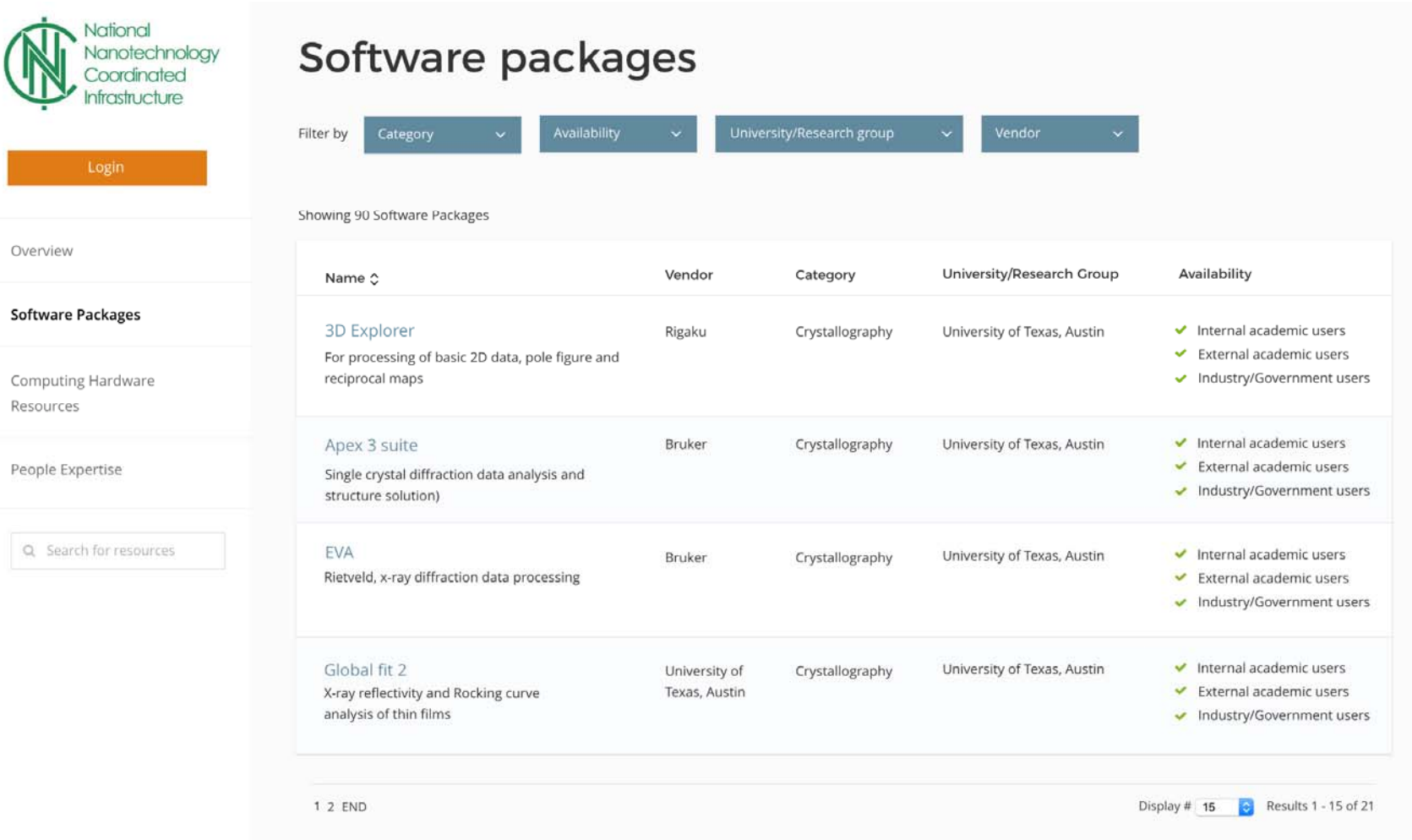
NNCI Computing Page on nanoHUB



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NNCI Computing Page on nanoHUB

nanohub.org/groups/nnci_computation

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Show 50 entries — First Previous 1 2 Next Last — Search:

Title	PI	NNCI Site Name	Brief Description
CatApp	Norskov	Stanford	software for atomic-scale simulations to understand heterogeneous catalytic reactions
CNTmob	Pop	Stanford	calculates the mobility of semiconductor CNTs at various charge densities and temperatures
GFET Tool	Pop	Stanford	calculates I-V curves for graphene transistors
MSMBuilder	Pande	Stanford	software for understanding a molecule's conformational dynamics
nanoJoule	Pop	Stanford	calculates I-V curves for metallic single-wall carbon nanotubes
NEGF-BiSFET	Frank Register	UT Austin	Quantum NEGF transport simuator for BisFETs and ITFETs
piezoD	Pruitt	Stanford	Tool for modeling the performance and optimizing the design of piezoresistive and piezoelectric sensors and
Stanford 2D Semiconductor (S2DS) Transistor Model	Pop	Stanford	a physics-based compact model for transistors based on two-dimensional semiconductors such as MoS2
Stanford Stratified Structure Solver (S4)	Fan	Stanford	open-source software to simulate and anlayze photonic structures
Stanford Virtual-Source Carbon Nanotube Field-Effect Transistors Model	Wong	Stanford	a semi-empirical compact model that captures the scaling properties of CNFETs
SU RRAM Model	Wong	Stanford	a SPICE-compatible model that describes switching for bipolar metal-oxide RRAM
TMDMOSFET	Frank Register	-	Ballistic Transport simulator for 2D layered TMD materials using maximally localized Wannier function techni
TOMCAT	Sanjay Banerjee	UT Austin	General-purpose Monte Carlo simulator of particle transport in arbitrary 2-D structures. The main applicatio
UT-Marlowe	Sanjay Banerjee	UT Austin	Neutron Transport Simulator which models scattering , electronic stopping, and damage accumulation
UT-QUANT	Sanjay Banerjee	UT Austin	CV Simulator for Silicon MOS Structures
UT-SCMC	Frank Register	UT Austin	Ensemble semi-classical Monte Carlo methods employing quantum corrections to address quantum confine
Macrospin LLG Code	Sanjay Banerjee	UT Austin	C++ code for simulating stochastic magnetization dynamics, includes STT
Nanonet	Satish Kumar	Georgia Institute of Technology	A simulation tool for Thin films transistors based on network of nanotubes or nanowires
1D Monte Carlo code	Dragica Vasileska	ASU	calculates drift velocity, average carrier energy and the mobility of electrons in Q1D systems
2D Monte Carlo code	Dragica Vasileska	ASU	calculates drift velocity, average carrier energy and the mobility of electrons in Q2D systems
2D Particle-Based Device Simulator	Dragica Vasileska	ASU	IV Characteristics of n-channel MOSFETs and SOI devices
3D Particle-based Device Simulator	Dragica Vasileska	ASU	IV Characteristics of 3D devices, discrete impurity effects (RDF and RTN)
Bulk Monte Carlo Code	Dragica Vasileska	ASU	calculates drift velocity, average carrier energy and the mobility in bulk materials
Dzyaloshinskii-Moriya ferromagnets	Alexev Kovalev	Nebraska Nanoscale Facilities	spin wave theory in Wolfram and MATLAB
mumax3	Alexev Kovalev	Nebraska Nanoscale Facilities	micromagnetic modelling
Compact thermal model of Microgap flow cooling stacked chips for co-design	Yogendra Joshi	Georgia Institute of Technology	A compact multi-layer pin-fin liquid cooling model with high speed simulation has been established for stead
Power Delivery Network Analysis tool	Muhannad S. Bakir	Georgia Institute of Technology	This is a thermal electrical co-simulation framework especially for 2.5D and 3D Ics. Power Delivery Network C
Thermal Simulation tool for 2.5D and 3D Ics	Muhannad S. Bakir	Georgia Institute of Technology	This is thermal modeling tool which can perform both steady-state and transient thermal analysis Thermal m

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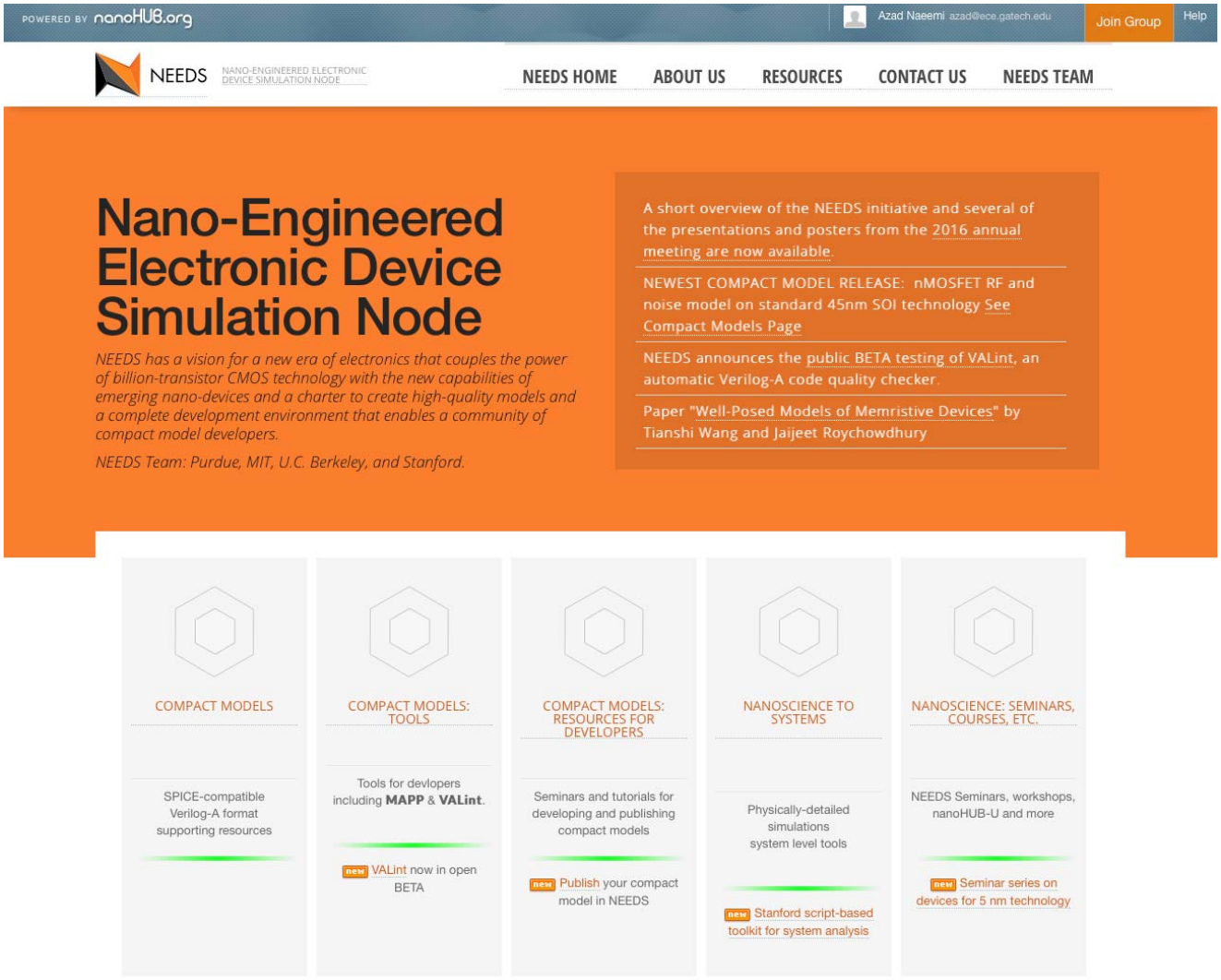
NSF Network for Computational Nanotechnology



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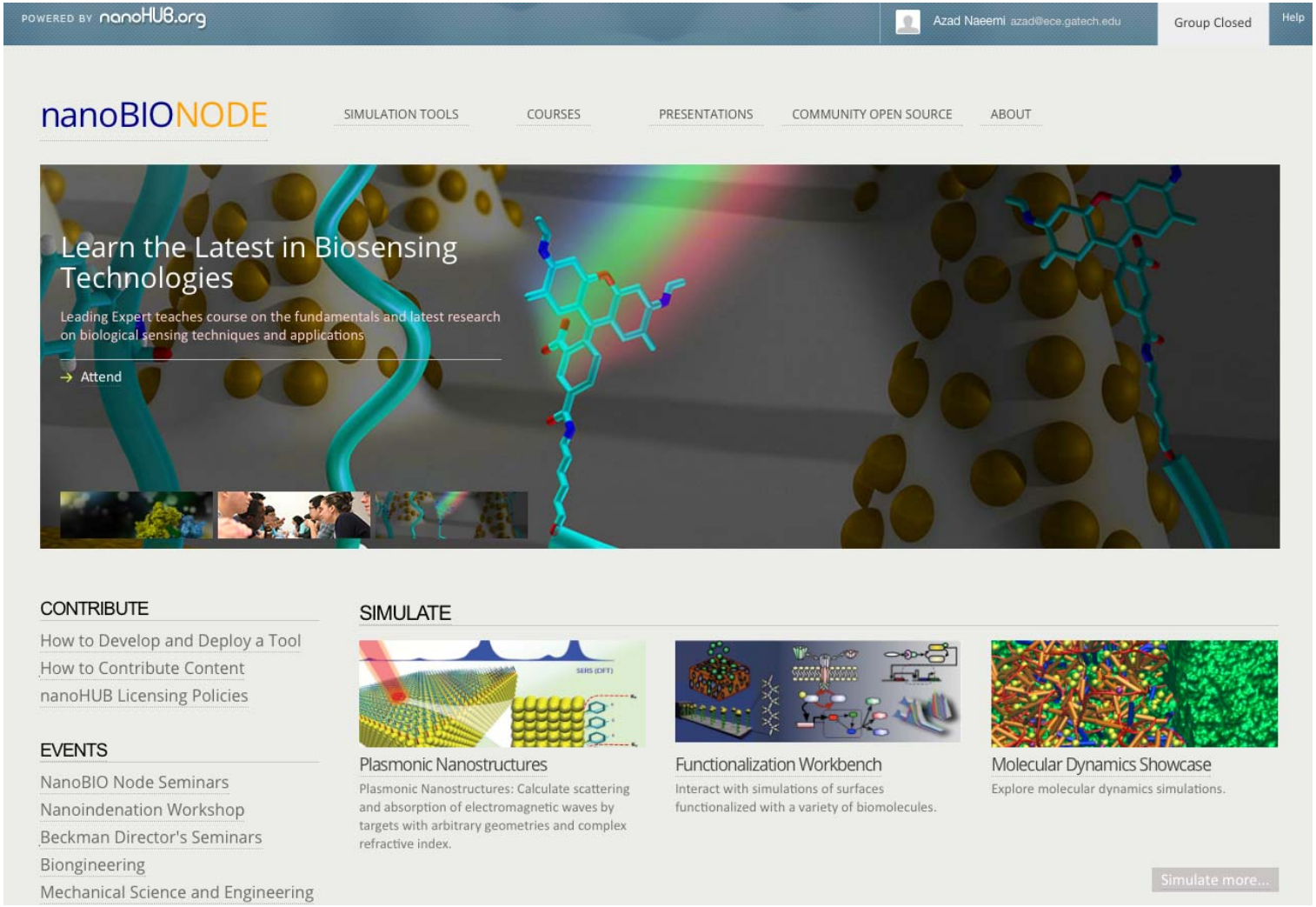
NSF Network for Computational Nanotechnology



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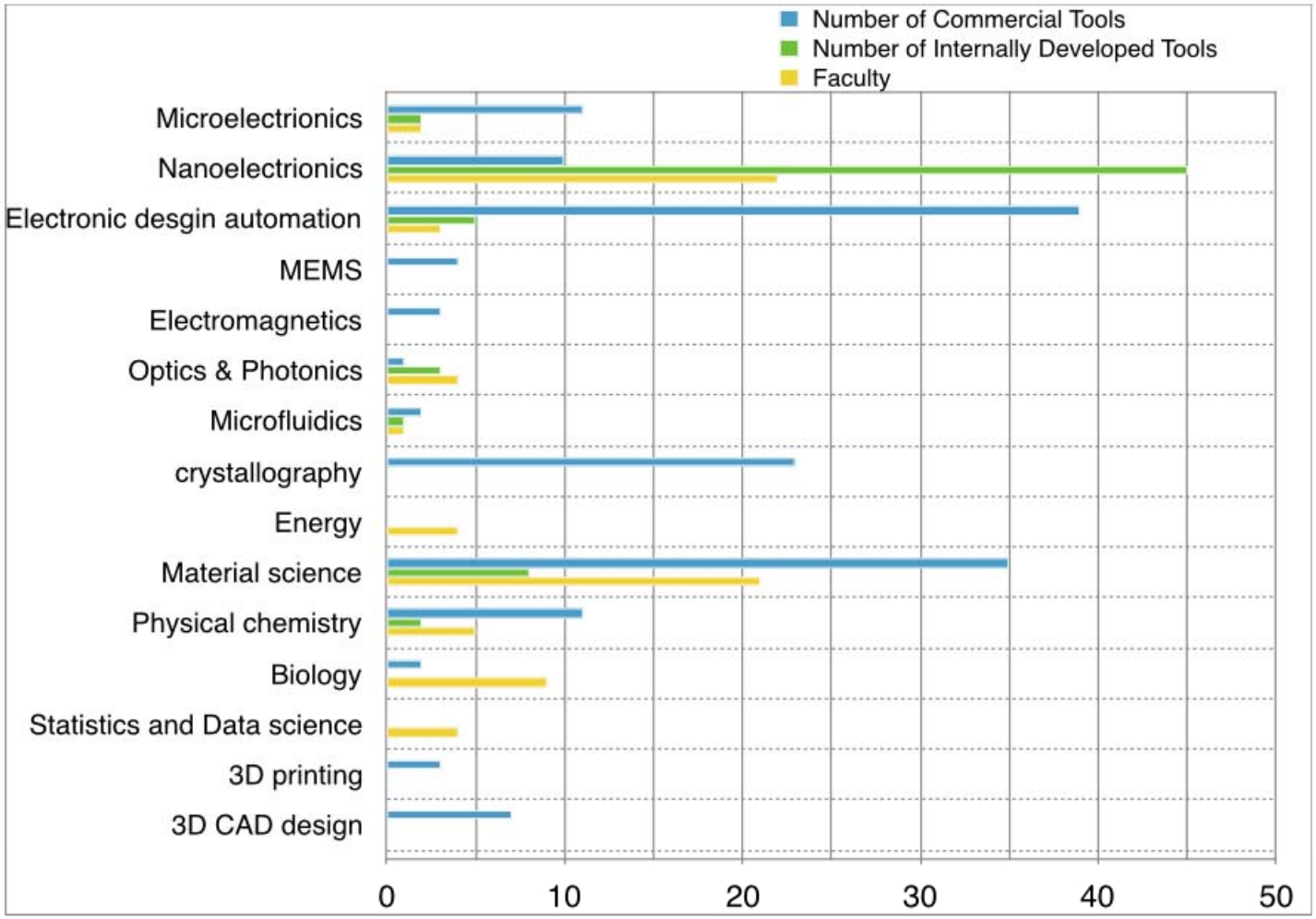
What are Major Gaps?



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Process Simulation Tools

- None of the sites have reported such tools.
- Can greatly help users and staff and cut cost.
- Fabrication complexity is growing and user experience is decreasing.
- Should NNCI invest in such tools?
- Buy commercial tools or develop its own sets of tools?

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Example: Electron Beam Lithography

- Job preparation is a key aspect:
  - CAD patterns must be converted to tool format and dose must be applied to correct for proximity effects.
  - Many other factors (resist, substrate, developer, accel. voltage, etc.) determine "proper" dose.
- Even with advanced knowledge and experience, it is common to do a dose test/skew. some iteration (hopefully < 3 is required)
- Software provided by EBL vendors are very limited.
- Tools to simulate electron scattering are available but are expensive.
- These tools could be improved by have a more process/fabrication oriented outlook.

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Inputs from Devin Brown (GIT)

Opportunities?

- Allow the user to iterate in the software rather than in the fab??
- Provide close to a "final answer" / "right condition"?
- Develop EBL conversion/proximity effect correction tool and share across NNCI network (reduce costs >$100k/license)?
- Envision other process modules (etch, photolithography, etc.) to simulate?

It will not be easy to develop such tools (Funding/resources).

However, if we could create a tool to help users get "right" results faster and cheaper, the upside could be tremendous.

Breakout Session Questions

- How can NNCI Computation can be most useful for the NNCI community?
- What should be the short term and long term goals?
- How can we facilitate tool development and access to the tools?
- Should NNCI identify some very important process simulation tools and invest in their development?
- What are the funding opportunities?

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