nanoHUB tutorial and invitation to join

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Established in 2002, NSF's Network for Computational Nanotechnology developed and operates nanoHUB, a major cyberinfrastructure supporting nanotechnology and related communities, now serving over 1.4 million visitors per year. This talk will introduce nanoHUB's capabilities for online simulations, collaboration and learning and how researchers and educators can both utilize its resources and contribute to it. I will discuss how tool developers can make their produces accessible and useful to a large community via cloud computing. Today, over 500 community-contributed simulation tools, each indexed by Web of Science and Google Scholar, serve 16,000+ users and 1,000,000 runs per year. Developers and users benefit from nanoHUB's HPC resources, automatic uncertainty quantification, support for Jupyter notebooks, and other resources driven by the needs of the communities we serve. We find that most tools serve dual education-research purposes and I will exemplify the use of our resources in various settings. nanoHUB enables translational work, putting research-grade tools in the hands of domain experts who can use them to train next generation students, for workforce development or to advance science and engineering applications and this presentation will be an invitation to take a look and take nanoHUB for a spin.

Alejandro Strachan is a Professor of Materials Engineering at Purdue University and the Deputy Director of the Purdue's Center for Predictive Materials and Devices (c-PRIMED) and of NSF's Network for Computational Nanotechnology. Before joining Purdue, he was a Staff Member in the Theoretical Division of Los Alamos National Laboratory and worked as a Postdoctoral Scholar and Scientist at Caltech. He received a Ph.D. in Physics from the University of Buenos Aires, Argentina, in 1999. Among other recognitions, Prof. Strachan was named a Purdue University Faculty Scholar (2012-2017), received the Early Career Faculty Fellow Award from TMS in 2009 and the Schuhmann Best Undergraduate Teacher Award from the School of Materials Engineering, Purdue University in 2007. Prof. Strachan's research focuses on the development of predictive atomistic and molecular simulation methodologies to describe materials from first principles, their application to problems of technological importance and quantification of associated uncertainties. Application areas of interest include: coupled electronic, chemical and thermo-mechanical processes in devices of interest for nanoelectronics and energy as well as polymers and their composites, molecular solids and active materials, including shape memory and high-energy density materials.