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nanoHUB: online simulation and data

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Abstract: Access to powerful simulation tools and hardware together with the ability to use machine learning tools to extract information from the large data sets is revolutionizing nanotechnology, nanomaterials and related fields. Unfortunately, utilizing such tools requires significant expertise and has traditionally been restricted to computational experts, furthermore, the data generated has not been accessible or findable except to its creator. To address this gap and make simulation and data products available to end users, more powerful, and easier to create, NSF's Network for Computational Nanotechnology developed and operates nanoHUB. I will discuss how tool developers can make research grade codes and models accessible and useful to a large community via cloud computing and how nanoHUB's cyber-infrastructure makes these products more powerful. Today, over 600 community-contributed simulation & data tools, each indexed by Web of Science and Google Scholar, serve 16,000+ users and 1,000,000 runs every year. Developers and end users benefit from HPC resources, a scientific software development environment, automatic uncertainty quantification, and support for Jupyter notebooks. In addition, every run is automatically stored and indexed, enabling the use data science tools to explore, analyze and extract information from prior, community-generated runs. We find that most tools serve dual education-research purposes and I will exemplify several use scenarios where research-grade tools in the hands of domain experts can are used to train next generation students, for workforce development or to advance science and engineering applications.

Bio: Alejandro Strachan is a Professor of Materials Engineering at Purdue University and the Deputy Director of NSF's Network for Computational Nanotechnology, home of nanoHUB. 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. Prof. Strachan's research focuses on the development of predictive atomistic and multiscale models to describe materials from first principles and their application to problems of technological importance. His group uses these tools to understand how materials work and use this insight to design new materials combining simulation and experimental results with data science tools. Application areas of interest include: high-energy density and active materials, metallic alloys for high-

temperature applications, materials and devices for nanoelectronics and energy, as well as polymers and their composites. Prof. Strachan has published over 150 peer-reviewed scientific papers and his contributions to research have been recognized by the *Early Career Faculty Fellow Award* from TMS in 2009 and his induction as a *Purdue University's Faculty Scholar* (2012-2017). His contributions to education have been recognized with the *Schuhmann Best Undergraduate Teacher Award* from the School of Materials Engineering, Purdue University, in 2007 and 2017.