THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT WINTER COLLOQUIUM SERIES PRESENTS:

Kristin Persson

Associate Professor, UC Berkeley

Senior Faculty Staff Scientist, LBNL

The Era of Data-driven Materials Innovation and Design

Fueled by our abilities to compute materials properties and characteristics orders of magnitude faster than they can be measured and recent advancements in harnessing literature data, we are entering the era of the fourth paradigm of science: data-driven materials design. The Materials Project (www.materialsproject.org) uses supercomputing together with state-of-the-art quantum mechanical theory to compute the properties of all known inorganic materials and beyond, design novel materials and offer the data for free to the community together with online analysis and design algorithms. The current release contains data derived from quantum mechanical calculations for over 100,000 materials and millions of properties. The resource supports a growing community of data-rich materials research, currently supporting over 100,000 registered users and over 1 million data records served each day through the API. The software infrastructure enables thousands of calculations per week – enabling screening and predictions - for both novel solid as well as molecular species with target properties. However, truly accelerating materials innovation also requires rapid synthesis, testing and feedback. The ability to devise data-driven methodologies to guide synthesis efforts is needed as well as rapid interrogation and recording of results – including 'non-successful' ones. In this talk, I will highlight some of our ongoing work, including efficient harnessing of community data together with our own computational data enabling iteration between ideas, new materials development, synthesis and characterization as enabled by new algorithmic tools and data-driven approaches.

Persson obtained her Ph.D. in Theoretical Physics at the Royal Institute of Technology in Stockholm, Sweden in 2001. She is an Associate Professor in Materials Science and Engineering at UC Berkeley with a joint appointment as Senior Faculty Staff Scientist at LBNL. Persson is the Director and co-founder of the Materials Project (www.materialsproject.org); one of the most visible of the Materials Genome Initiative (MGI) funded programs attracting over a hundred thousand users worldwide. She is a leader in the MGI community, and is known for her advancement of data-driven materials design and advancement of materials informatics.

She is an Associate Editor for Chemistry of Materials and has received the 2018 DOE Secretary of Energy's Achievement Award, the 2017 TMS Faculty Early Career Award, the LBNL Director's award for Exceptional Scientific Achievement (2013) and she is a 2018 Kavli Fellow. She holds several patents in the clean energy space and has co-authored more than 150 peer-reviewed publications.

Tuesday, January 28 • 4 pm | Tech L211

Northwestern | McCORMICK SCHOOL OF ENGINEERING
Materials Science and Engineering