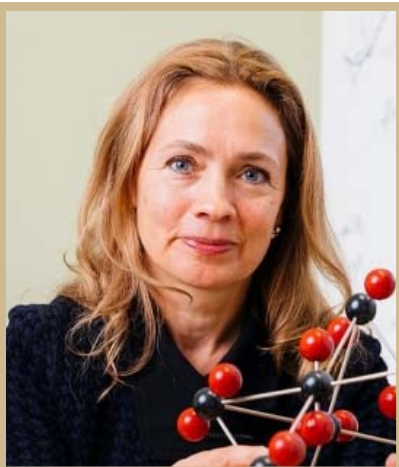


SCHOOL OF
MATERIALS ENGINEERING

DISTINGUISHED LECTURE



KRISTIN PERSSON

*Daniel M. Tellep Distinguished
Professor in Materials Science &
Engineering*

University of California at Berkeley

**“Fueling the Era of Data-Driven
Materials Innovation and Design”**

ABSTRACT

Fueled by our abilities to compute properties and characteristics orders of magnitude faster than they can be measured and recent advancements in harnessing literature data, the materials science field is entering the era of the fourth paradigm of science: data-driven materials design. The Materials Project (www.materialsproject.org) uses supercomputing and a sophisticated software infrastructure 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 combined with online analysis and design algorithms. The current release contains data derived from quantum mechanical calculations for over 150,000 materials and millions of properties. The resource supports a growing community of data-rich materials research, currently supporting over 500,000 registered users and millions of data records served each day through the API. Our resource is inspiring data-driven work across the community and in response, we are seeing a rapid increase in the development of machine learning algorithms for the prediction of materials properties, characteristics and synthesizability. However, we note that truly accelerating materials innovation also requires rapid synthesis, testing and feedback, seamlessly coupled to existing data-driven predictions and computations. 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. This talk will outline the rise of data-driven materials design and predictive synthesis and showcase successes, as well as comment on current pitfalls and future directions.

BIOGRAPHY

Kristin Persson is the Daniel M. Tellep Distinguished Professor at the University of California, Berkeley and a Senior Faculty Scientist at Lawrence Berkeley National Laboratory. Between 2020-2024 she served as the director of the Molecular Foundry, one of the five U.S. Nanoscale Research Centers. In 2011 she founded the Materials Project (materialsproject.org), which has emerged as one of the most visible programs that originated from the Materials Genome Initiative (MGI). She has served as the director of the Materials Project since its inception, and today the Materials Project serves millions of materials data records every day to more than half a million registered users worldwide. In 2021 the Materials Project was recognized by the Department of Energy as an official Public Reusable Research (PuRe) Data resource for materials data and design.

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