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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 140,000 materials and millions of properties. The resource supports a growing community of data-rich materials research, currently supporting over 220,000 registered users and millions of 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 new materials development, synthesis and characterization and associated machine learning algorithmic tools and data-driven approaches.

Kristin Persson is the Director of the Molecular Foundry, a user facility at Lawrence Berkeley National Lab (LBNL), a Professor at the University of California, Berkeley and a Faculty Senior Scientist at LBNL. She 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 >200,000 users worldwide with thousands of unique users accessing the site every day. She is a leader in the MGI community, and applies modeling and data-driven to the innovation of materials for energy storage and production. She serves as an Associate Editor for Chemistry of Materials, on the advisory board of NanoHub and FAIRmat and she is the appointed MGI ambassador for The Metal, Minerals, and Materials Society (TMS). She has received the DOE Secretary of Energy's Achievement Award, the TMS Faculty Early Career Award, the Falling Walls Science and Innovation Management Award, the LBNL Director's award for Exceptional Scientific Achievement and she is a Kavli Fellow and an APS Fellow. She holds several patents in the clean energy space, and is among the world's 1% most cited researchers. She has co-authored more than 200 peer-reviewed publications (h-index 77).