THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT SERIES PRESENTS

THE 2019 JOHN E. DORN MEMORIAL LECTURE

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Functional Materials from First Principles

New materials can solve many (though not all) of the world's problems though faster, smaller-scale and cheaper processing and storage of information and energy. Improving and optimizing the materials we already use for these purposes can only take us so far -- what about something really new? How would we know where to look? Information about the structures and properties of experimentally known materials, as organized into a crystallographic database, provides the initial data for a rough map of the space of possible materials. Using the theory of quantum mechanics to perform first-principles computer simulations of the properties of known and as-yet hypothetical materials from first principles, using only their chemical composition as input, we can augment the database with the results of computer experiments to develop the map. Drawing on the unique capability of first-principles calculations to identify low-energy metastable states in addition to the equilibrium phase, we can predict phase transitions and functional properties "de novo": that is, without prior experimental clues. Several examples of such predictions for functional behavior in binary oxides, perovskites and ternary intermetallics will be presented. The challenges and promise of theoretical materials design and theoretical-experimental integration will be discussed.

Karin Rabe is a computational materials physicist with a particular interest in the use of first-principles quantum-mechanical calculations for the study of phase transitions and the theoretical design of new materials. Born in New York City, she attended the Bronx High School of Science and majored in physics at Princeton University. She received a Ph.D. in physics from Massachusetts Institute of Technology (1987) with thesis supervisor John Joannopoulos. Following two postdoctoral years in the theory department at AT&T Bell Laboratories, she joined the Department of Applied Physics and the Department of Physics at Yale University, with tenure in 1995, and moved to the Department of Physics and Astronomy at Rutgers in 2000, where she was promoted to Board of Governors professor of physics in 2013. She served as president of the Aspen Center for Physics from 2013 to 2016. Her recent professional recognition includes fellowship in the American Physical Society (2003), the David Adler Lectureship Award in the Field of Materials Physics from the American Physical Society (2008), fellowship in the American Association for the Advancement of Science (2011) and membership in the American Academy of Arts and Sciences (2013) and the National Academy of Sciences (2013).

Tuesday, May 21 • 4 pm Pancoe Auditorium
Reception to follow | Pancoe Cafe

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Materials Science and Engineering